Modeling of Gas flows in Steelmaking Decarburization Processes

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A journey of a thousand miles begins with a single step.

-Confucius
Abstract

The purpose of the current study is to increase the understanding of different steelmaking processes at the decarburization stages by use of mathematical modeling. More specifically, two De-Laval nozzles from a VOD (Vacuum Oxygen Decarburization) process, which is used for producing stainless steels with ultra-low carbon grades, was investigated for different vessel pressures. Moreover, the post combustion phenomena in a BOF or LD (Linz-Donawitz) process as well as an AOD (Argon Oxygen Decarburization) process were studied focusing on the decarburization stage.

Two industrial VOD nozzles were numerically studied and compared at different temperatures and ambient pressures. Flow patterns of the oxygen jet under different ambient pressures were predicted and the flow information at different positions from the nozzle was analyzed. In addition, the effects of different ambient temperatures on the jet velocity and the dynamic pressure were compared. The predictions revealed that a little under-expansion is somewhat helpful to improve the dynamic pressure. The jet dynamic pressure and its width for the specific nozzle geometry were also studied. It was observed that a variation in the ambient pressure can influence the jet momentum and its width. In addition, a high ambient temperature was found to have a positive effect on the improvement of the jet dynamic pressure. Furthermore, it was found that a change in ambient pressure has a stronger effect on the jet force than a change in the ambient temperature. In addition, it was proved that the profiles of the dynamic pressure at a certain blowing distance fit well to Multi-Gaussian distribution.

Post combustion in a BOF/LD and an AOD process during decarburization was also studied. Two mathematical models were created to show the post combustion phenomenon inside the converters, respectively. For the CFD modeling of the two processes, the realizable k-ε model, the species transport model and the discrete ordinate were adopted to calculate the turbulence, gas reaction and radiation present in the gas phase in the converter. For the BOF/LD modeling, a series of plant tests were conducted to collect data, which were used in the current model. These include the off-gas information, emissivity data, oxygen blowing parameters and the chemical composition
of steel. After the simulation, the predicted flow pattern and detailed information of the gases taking part in the post combustion were compared to plant data. Specifically, the off-gas data from the plant was used for the model verification. The measured CO$_2$ concentration was 15-20 wt% and the predicted value from the modeling was 16.7 wt%.

For the AOD converter of interest in the current work, a fan is installed in the end of the AOD flue to help extract the off-gas from the converter. The influence of different fan gauge pressures as well as temperatures of the gas mixture, containing the generated CO and argon, on the post combustion in the whole AOD system was studied. It was indicated from the modeling results that the post combustion was only present in the flue for the present modeling conditions. Moreover, a critical fan gauge pressure (approx. -550 Pa) was found which could yield a maximum post combustion in the flue gas.

For both two models (BOF/LD and AOD), simulations indicated that a change of the converter temperature from 1500 to 1700 °C did not influence the post combustion reaction to a large degree. In addition, these two models can be regarded as the first step for a future more in-depth modeling work of the post combustion.

**Key words:** VOD, nozzle, jet, vacuum, BOF, LD, AOD, post combustion, flue, CFD
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*Steel Res. Int.*, 82 (2011), 249

Supplement 2: Mathematical Comparison of Two VOD Nozzle Jets
Zhili Song, Mikael Ersson and Pär Jönsson
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Supplement 3: A Study of Post Combustion in a BOF converter
Zhili Song, Mikael Ersson and Pär Jönsson
Manuscript

Supplement 4: A Study of Post Combustion in an AOD Flue
Zhili Song, Mikael Ersson and Pär Jönsson
Submitted to *Steel Res. Int.*, August 2013

A part of this thesis has been presented at the following conferences:

The contributions by the author to different supplements of this thesis:

**Supplement 1:** Literature survey, numerical calculations, major part of the writing

**Supplement 2:** Literature survey, numerical calculations, major part of the writing

**Supplement 3:** Literature survey, numerical calculations, major part of the writing

**Supplement 4:** Literature survey, numerical calculations, major part of the writing
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1. Introduction

Steelmaking is a huge industry which has continuously been developed for more than 150 years. A deep understanding of steelmaking processes will help to improve the control over processes more precisely and dynamically. A good control of online processes is increasingly important with regard to improving the production efficiency and to saving energy. In the contemporary steelmaking world, there are basically two procedures of steelmaking.

Blast Furnace Steelmaking

Electric Arc Furnace Steelmaking

Figure 1 Overview of two steelmaking processes

Figure 1 shows the two basic steelmaking processes in Sweden. One is the blast furnace steelmaking and the other is the electric arc furnace steelmaking. In the blast furnace steelmaking process, the steel produced from a BOF/LD converter originates from the blast furnace. After a decarburization in the converter, refining is done in a ladle furnace. On the other hand, in the electric arc furnace steelmaking, the steel is charged into the refining processes directly from the EAF, where the scrap, among others, is melted by an electric arc. In the present work, the focus was on a primary steelmaking process – BOF/LD process and two secondary steelmaking processes – VOD and AOD process.

Top blowing of oxygen has been widely employed as a decarburization technic during steelmaking. Here, oxygen reacts with carbon under the formation of a CO gas. Vacuum Oxygen Decarburization, VOD, is one way of producing high alloy steels, such as stainless steel. These grades contain elements with a high affinity to oxygen like
chromium. More specifically, it is a process for further refinement of stainless steel by a reduction of the carbon content. In a VOD process, molten and unrefined steel is stirred and heated through electrical induction. At the same time, oxygen is ejected through an oxygen lance and argon stirring is adopted from the bottom. Undesirable gases can escape from the steel and are evacuated through a vacuum treatment. Additives and alloys can then be added to further improve the steel. Since a very low carbon content is required in VOD, the vacuum environment is very important.

The VOD process could be roughly divided into three stages, i) oxygen blowing, ii) degassing and iii) reduction. The oxygen lance used for blowing is of interest in the present work, including a De Laval nozzle which is mounted at the tip of the oxygen lance. A good understanding of the jet flow in a VOD process is desirable for recognizing the jet behavior for different vessel pressures and temperatures. However, the real environment in a VOD vessel is quite harsh since the vessel is loaded with slag and steel and it endures temperatures of 1600 degree Celsius or more. This opens up the possibility of exploiting mathematical modeling to perform parametric studies to increase the knowledge of the process. Here, CFD (Computational fluid dynamic) modeling has been largely promoted for its effectiveness and economy. Hence, in the current work, two VOD nozzles were modeled by the use of CFD modeling with respect to the nozzle jet behavior.

Several studies have been done on the subject of blowing and jet behavior. Water modeling has been employed to explore different aspects of top blowing processes [1-5]. The research of oxygen lance and VOD process has been reported [6-10]. Also, investigations of jet behaviors have been conducted [11-14]. Ersson et al. [1, 2] employed both water-model experiments and mathematical modeling to study the effects of the top-blown jet on the steel bath in an LD converter. Also, Krishnakumar et al. [3] employed a water model simulation to characterize the mixing phenomena in a VOD ladle. Nordquist et al. [4, 5] focused on the research in the top-blown water model. It was shown that the nozzle diameter, lance height, aspect ratio and the gas flow rate all influence the penetration depth and the swirl phenomena. In a paper by Ding et al. [6], a dynamic model was created to explore the influence of oxygen flow rate, vacuum pressure, and argon flow rate on the VOD process. Oonuki et al. [7] investigated the process and the apparatus for vacuum degassing of molten steel. Fukui et al. [8] studied the oxygen lance equipped in the VOD vessel. Sumi et al. [9] explored the top-blown jet behavior under reduced pressure, using physical and numerical modeling. Also, Hirata et al. [10] showed the stirring effect induced by top and side blown oxygen and bottom blown nitrogen converter. It showed that the appropriate combination of top, side and bottom blowing would produce a high HTE (heat transfer efficiency) and PCR (post combustion ratio). Naito et al. [11] investigated the incorrect jet expansion and multiple jets behavior by cold and hot model experiments. Yuan et al. [12] utilized a small-scale measurement with a double-parameter lance equipped to study the jet velocity and its deviation from the jet centerline. It was shown that by using the double-parameter lance the metallurgical performance could be improved. Also, Tago et al. [13] used cold model experiments and numerical modeling methods to study single nozzles and multi-nozzles. They found that jet dynamic pressures and nozzle inclination angles could influence the jet properties.
Wang et al. [14] developed a three-dimensional mathematical model of multiple jets to comprehend the multi-jet coalescence and its dynamic power.

In the current work, based on the knowledge of mathematical modeling, comparison of real nozzles from a real VOD plant has been carried out as a parametric study. It would, for example, be of great interest to explore the oxygen flow of different oxygen nozzles used for varying ambient pressures.

The research on the post combustion in converters has been conducted for many years. The purpose of increasing the scrap content without a large heat loss drives the research forward. Here, one way of yielding heat apart from the decarburization in converters is to obtain post combustion between O\(_2\) and CO. It is already known from equations (1) and (2) that the heat released from the reaction between the carbon in the liquid and O\(_2\) is less than that between CO and O\(_2\) [15]

\[
\begin{align*}
\text{CO} + \frac{1}{2}\text{O}_2 &= \text{CO}_2 & \Delta G &= -279073 + 84.56 \cdot T \ (J \text{ mol}^{-1}) \\
\text{C} + \frac{1}{2}\text{O}_2 &= \text{CO} & \Delta G &= -139536 - 42.55 \cdot T \ (J \text{ mol}^{-1})
\end{align*}
\]

(1) (2)

Therefore, it is worthwhile to focus research on different ways of improving the post combustion ratio. Moreover, it is also of interest to study the heat transfer efficiency, which measures the heat generated by the post combustion to the steel bath.

A BOF/LD process is a primary steelmaking process for producing basic steels while AOD processes have been widely used for the manufacture of stainless steel. Here, nozzles are employed for injection of a gas mixture containing, among others, oxygen, which performs the main task of decarburization. Also, additions of ferro chromium are made in the AOD process, to obtain the desired chromium level in the steel and to lower the cost.

Despite the fact that it has been a growing interest to investigate the steelmaking process, not much research has been focused on the modeling of the post combustion phenomena in AOD converters. Table 1 shows the post combustion modeling work that has been done by different researchers with respect to different steel making furnaces [16-25]. It can be seen that methods of treating the post combustion reactions are different. Most of the papers were published by using the standard k-\(\varepsilon\) model to simulate turbulence. Furthermore, a common view has been formed that radiation plays a very important role in high temperature post combustion in steel making processes.
### Table 1 CFD work on post combustion in steel making converters

<table>
<thead>
<tr>
<th>Year</th>
<th>Authors</th>
<th>Converter type</th>
<th>Dimension</th>
<th>Reaction rate determination</th>
<th>Turbulence</th>
<th>Radiation model</th>
<th>Multiphase</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td>Finite reaction</td>
<td>Fast reaction</td>
<td>Combined rate</td>
<td>k-ε</td>
</tr>
<tr>
<td>1988</td>
<td>H. Gou et al. [16]</td>
<td>Lab furnace</td>
<td>2D</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
</tr>
<tr>
<td>1988</td>
<td>W. Pei et al. [17]</td>
<td>6t SOP</td>
<td>2D</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
</tr>
<tr>
<td>1992</td>
<td>J. Zhang et al. [18]</td>
<td>180t BOF</td>
<td>3D</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td></td>
</tr>
<tr>
<td>1993</td>
<td>H. Gou et al. [19]</td>
<td>30t KOBM</td>
<td>2D</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td></td>
</tr>
<tr>
<td>1993</td>
<td>M. Shin et al. [20]</td>
<td>100t converter</td>
<td>2D</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td></td>
</tr>
<tr>
<td>1998</td>
<td>S. Story et al. [21]</td>
<td>EAF</td>
<td>2D</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td></td>
</tr>
<tr>
<td>2003</td>
<td>X. Tang et al. [22]</td>
<td>EAF</td>
<td>3D</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td></td>
</tr>
<tr>
<td>2003</td>
<td>Y. Li et al. [23]</td>
<td>165t EAF</td>
<td>3D</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td></td>
</tr>
<tr>
<td>2005</td>
<td>Y. Tang et al. [24]</td>
<td>90t AOD</td>
<td>3D</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td></td>
</tr>
<tr>
<td>2013</td>
<td>Supplement 3</td>
<td>130t LD converter</td>
<td>2D</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
</tr>
<tr>
<td>2013</td>
<td>Supplement 4</td>
<td>75t AOD</td>
<td>3D</td>
<td>x</td>
<td>x</td>
<td>x</td>
<td>x</td>
</tr>
</tbody>
</table>
In the present work, a more complex converter model was developed compared to those presented in the literature. It considers turbulence, reactions and radiation. The realizable k-ε model was employed to compute the turbulence; the discrete ordinate model was utilized for the radiation modeling. In addition, the slowest step from either turbulence mixing or the Arrhenius kinetics was considered to determine the reaction rate for post combustion. For the BOF/LD modeling, the modeling results were compared to the industrial data from a LD converter. For the AOD process, different fan gauge pressures at the end of the off-gas flue as well as the temperature effects on the post combustion were explored by use of a mathematical model.

![Diagram of Steelmaking Decarburization Processes](image)

**Figure 2 Connections between different supplements**

**Figure 2** shows how the four supplements are connected to each other. The first two supplements include the comparison of two De Laval nozzles of different lengths which are being used in a production VOD vessel. One VOD nozzle was first developed to fundamentally understand the flow field in the process of blowing. This was focused in **Supplement 1**. Different ambient temperatures were applied to explore the dynamic change of the flow. The oxygen jet width was also studied. In particular, a high oxygen flow rate was applied and a fairly low ambient pressure was tested. Finally, a variable ambient temperature was employed. In **Supplement 2**, another VOD nozzle designed for real VOD was introduced and simulated to compare with the Nozzle in **Supplement 1**. It was aimed at uncovering the different blowing behaviors affected by ambient pressures and temperatures by means of numerical modeling. Furthermore, it is intended to try to find the better nozzle for a specific ambient pressure. The flow patterns and dynamic
pressures of two nozzles were compared for different ambient pressures. Moreover, the
temperature effects on the jets for the two nozzles were studied. Also, suggestions as how
to choose the better nozzle for a certain ambient pressure were proposed. Besides, a
Multi-Gaussian function was employed to fit profiles of the jet dynamic pressure.

The investigation of post combustion phenomena in converter processes was summarized
in Supplement 3 and 4. Specifically, in Supplement 3, the post combustion phenomenon
in a BOF/LD process was studied whereas in Supplement 4, the post combustion in a
AOD flue was explored. All the work was carried out by means of CFD calculations.
2. Nozzle and Jet Theory

The nozzle theory has been used as the principle of designing a convergent-divergent nozzle. In Supplement 2 and 3, all the modeling work of two VOD nozzles is based on the nozzle theory. The understanding of the theory helps to calculate the relations between properties in the nozzle flow, and in turn, to design or control flow conditions for a nozzle. Also, the knowledge needed for comprehending the jet behavior is summarized in this chapter.

2.1 De Laval nozzle

The schematic appearance of a De Laval nozzle is shown in Figure 3. The nozzle converges from its inlet to throat, and diverges from its throat to the outlet. The function of this typical characteristic is to guide and accelerate the fluid of interest. Furthermore, it can maximize the flow velocity to a supersonic velocity at the nozzle outlet.

![Figure 3 Flow in a De Laval nozzle](image)

The De Laval nozzle theory includes assumptions. The fluid of interest is assumed to be a compressible ideal gas in the form of a steady one-dimensional flow. The gas is assumed ideal to create a correlation among different properties of it, such as density, temperature and pressure. The assumption that the fluid is compressible indicates that the fluid density is a function of the local fluid pressure. Friction and heat loss are two other factors that could complicate the study. Therefore, the flow in the nozzle is regarded as an isentropic flow, which means that the flow is frictionless and adiabatic.

The basic relations in the nozzle theory that were used in the present work for calculations are as follows:

\[ \frac{T_0}{T} = 1 + \frac{\gamma - 1}{2} M_a^2 \]  \hspace{1cm} (3)

\[ \frac{p_0}{p} = \left(1 + \frac{\gamma - 1}{2} M_a^2 \right)^{\frac{\gamma}{\gamma - 1}} \]  \hspace{1cm} (4)

\[ \frac{\rho_0}{\rho} = \left(1 + \frac{\gamma - 1}{2} M_a^2 \right)^{\frac{1}{\gamma - 1}} \]  \hspace{1cm} (5)

where \( T_0, p_0, \rho_0 \) are the inlet temperature, inlet pressure and inlet density, respectively. The parameter \( M_a \) is the Mach Number and \( \gamma \) is the isentropic exponent, which is 1.4 in
this work. At the nozzle throat where $M_a = 1$, we have $\frac{T^*}{T_0} = 0.833, \frac{p^*}{p_0} = 0.528$ and $\frac{\rho^*}{\rho_0} = 0.634$. The parameters $T^*$, $p^*$ and $\rho^*$ are the temperature, the pressure and the density at the throat. To obtain the design point of a De Laval nozzle, the $\dot{m}$ (mass flow rate), $p_0$ (inlet pressure) and ambient pressure should be specified. The equation involved in the calculation would be:

$$A^* = \frac{\dot{m}}{\sqrt{\frac{2 p_0 \rho_0 \gamma}{\gamma - 1} \left[ \left( \frac{p^*}{p_0} \right)^\gamma - \left( \frac{p^*}{p_0} \right)^\gamma + 1 \right]}}$$

(6)

where $A^*$ is the cross-sectional area of the nozzle at the throat.

For illustrating the flow patterns in the work, terms of under-expansion and over-expansion were employed in the thesis (Figure 4). When the ambient pressure is smaller than the exit pressure, an under-expansion can occur. Moreover, shock waves and expansion waves will be released if an incorrect expansion takes place. However, neither of the two phenomena is expected by people designing the nozzle. The optimum expansion of the nozzle would only be achieved if the ambient pressure is equal to the exit pressure. In the present work, all nozzle-theory calculations were based on the assumption of an ambient pressure equal to an exit pressure.

Over-expansion and under-expansion would happen when the ambient pressure is larger or smaller than the exit pressure. Furthermore, when the ambient pressure is equal to the exit pressure, optimum expansion can be obtained. More specifically, if the exit pressure is larger than the ambient pressure, expansion waves would form. Shock waves are released with diamond patterns appearing when the exit pressure is smaller than the ambient pressure [26]. In many cases when it comes to the nozzle design, it is correct to base all nozzle calculations on the assumption that no separation occurs [27]. Also, in this work all calculations were done under this pre-requisite.
2.2 Gas jet
Nozzle jets can be investigated from different perspectives. The behavior of a gas jet can affect the gas impinging effects on a steel bath, which correspondingly has a strong impact on the decarburization efficiency. In this work, the jet attenuation from both the blowing direction and the radical direction were analyzed. The jet momentum along the blowing axis can be expressed as: [28]

\[ M = \frac{1}{4} \pi d_{\text{outlet}}^2 \rho u_{\text{outlet}}^2 \]  \hspace{1cm} (7)

where \( M \) is jet momentum flow and \( d_{\text{outlet}} \) and \( u_{\text{outlet}} \) are the nozzle outlet diameter and the flow velocity at the nozzle outlet. In addition, the jet momentum can be related to other jet properties as follows: [29]

\[ \gamma_v \propto \frac{M x_u}{\nu v^2} \]  \hspace{1cm} (6)

where the jet width \( \gamma_v \) depends on the momentum flow \( M \), on the density \( \rho \), on the kinematic viscosity \( \nu \) of the fluid and on the downstream distance \( x_u \) from the nozzle.
It could further be found that:

\[ M = \text{constant} \times \rho y_v^2 u_c^2 \]  

(8)

where \( u_c \) is velocity along the centerline and it is seen that the jet width is proportional to the downstream distance \( x_u \). In addition, it could also be found that the momentum flux \( \rho u_c^2 \) is dependent on the jet width \( y_v \) and the jet momentum flow \( M \) is independent of the downstream distance \( x_u \).

For investigating the jet momentum and its width, another property, the dynamic pressure, \( P_{dy} \), needs to be introduced as:

\[ P_{dy} = \frac{1}{2} \rho u^2 \]  

(9)

In this work, the jet momentum change will be illustrated using the dynamic pressure \( P_{dy} \).

The dimensionless velocity \( \frac{u}{u_c} \) was defined to show the jet width change at a certain axial position \( x_u \). In the present work a jet width definition was exploited: [29]

\[ \frac{u(y_v)}{u_c} = \frac{1}{2} \]  

(10)
3. Experimental Work
For all the supplements, experimental data from industries were obtained either for the boundary condition settings in the created models or for the result verifications.

In Supplement 1 and 2, boundary conditions for the nozzle models are obtained from a real VOD process. The detailed settings of boundary conditions are explained in the thesis part of Numerical Modeling Setting.

A SSAB BOF/LD-converter blueprint was employed for creating the geometry in Supplement 3. Figure 5 shows the schematic figure of the BOF/LD. The model dimension that is employed for simulation is based on the design in the figure. A large amount of experimental data was obtained from the converter process control system. First, the carbon content of the hot metal and the steel after oxygen blowing was analyzed to estimate the decarburization rate and the CO generation temperature. Subsequently, the information for the oxygen blowing was collected. Specifically, the mass flow rate, temperature, lance height and the average blowing time were determined based on the industrial production conditions.

![Figure 5 A schematic figure of the BOF converter at SSAB](image)

Figure 5 A schematic figure of the BOF converter at SSAB
Off-gas information in terms of the time point data was similarly obtained from the SSAB database. Off-gas analysis data from industrial productions is of high importance, since it can rapidly reflect the process condition. Based on the analysis, many necessary actions towards the steel making can be taken online to immediately adjust the whole process. In addition, the off-gas information was analyzed for the purpose of verifying the modeling results.

Radiation plays a very important role, especially for the combustion at high temperatures. In order to select a suitable radiation model for the modeling, it is necessary to identify the emissivity of the materials in the converter. In this project, a test to measure the emissivity was conducted for the converter of concern at SSAB. The measurements were done using a FLIR ThermoVision instrument and the software for the analysis was ThermaCAM Researcher 2.10 PRO. This device captures the picture and form images through infrared radiation. It is practical to use when high temperature data are needed. The emissivity of the inner lining is of interest in this test. In the present work, a calibrated Thermo Vision was employed for the measurements. However, the environment for the measurement when the oxygen is being blown is extremely harsh. Therefore, the emissivity measurements towards the inner lining of the converter were conducted after the converter tapping.

It should also be noted that converter linings are unique for different steel plants. For the SSAB converter, the lining information was also summarized and used for the mathematical modeling later on.

In Supplement 4, a mathematical model of the 75 ton AOD converter including the off-gas flue at Sandvik Materials Technology (SMT) was developed. Figure 6 shows a schematic view of the AOD and its flue’s structure. Two simplifications were made in the geometry of the mathematical model. Specifically, the inlet of the off-gas flue lies on the same horizontal plane as the outlet of the AOD converter, while the AOD converter at SMT has a tilted surface. The entire flue was not modeled due to time constrains. However, the part that was modeled is also the part where most of the post combustion is likely to take place.
A gas mixture containing argon and oxygen was blown into the converter from the side. An argon and oxygen gas were injected with a speed of 30 Nm$^3$/min and 75 Nm$^3$/min, respectively.
4. Numerical Modeling Setup

Numerical Modeling was performed in all four supplements. First, two nozzle models based on a VOD converter were created and investigated in Supplement 1 and 2. Thereafter, two converter models based on a real BOF/LD converter and an AOD converter were established and studied in Supplement 3 and 4, respectively. All mathematical modeling work was carried out by using the commercial computational fluid dynamics (CFD) code ANSYS FLUENT.

4.1 Geometry design

4.1.1 VOD nozzles

Two nozzles (Figure 7) were mathematically modeled with CFD approach and compared with each other under different conditions. A parametric study was conducted to investigate the blowing jet conditions.

4.1.2 BOF/LD converter

Figure 8 shows the geometry that is utilized for the modeling. Considering the limited computational resources, an axial symmetrical geometry was created in order to diminish the meshing density for the real 3D converter. Only the chamber of the converter is created for meshing, but the refractories used for the lining are not considered. Instead, the lining properties in the model were set to the same as the production lining data introduced in this work. The diameter of the oxygen lance outlet is assumed to be one
single nozzle with a radius of 0.1m. Based on the industry data, a lance height of 1.7m was employed. In addition, since in the real production, the chamber volume for the post combustion is partly taken up by the formation of the slag, an assumed slag zone was excluded when calculating the post combustion.

![Figure 8 Modeling geometry including relevant dimensions](image)

**4.1.3 AOD converter**

A simplified mathematical model was developed to simulate the real AOD converter and its flue at SMT’s plant in Sandviken. Only the front part of the gas flue close to the AOD was studied in the model. Furthermore, since the post combustion was the main focus, the chamber of the converter above the steel surface was modeled by only considering the gas phase.

*Figure 9* shows the front view of the mathematical model including its dimensions. It can be seen that the lower part of the model represents the upper part of the actual AOD converter, where only gases are present. Thus, the lower part of the AOD that is filled with steel and slag is not considered here, as mentioned above. Above the AOD converter mouth, the gas flows through a cone frustum, which has a larger inlet area than the AOD mouth. After this part, an off-gas flue with a uniform diameter leads the process gases away from the furnace.
4.2 Governing equations

The commercial software ANSYS FLUENT was employed for all the modeling work. Conservation equations of mass, momentum, energy, species transport, turbulence were included for the mathematical modeling. Equation (11) shows the general transport equation for any property \( \Phi \).

\[
\frac{\partial}{\partial t} \left( \rho \Phi \right) + \nabla \cdot \left( \rho \Phi \vec{u} \right) = \nabla \cdot \left( \Gamma \nabla \Phi \right) + S_\Phi
\]  

(11)

where \( \Gamma \) is the diffusion coefficient and \( S_\Phi \) is the source term. The detailed three dimensional transport of different properties is summarized in Table 2. In the current work, the Reynolds-averaged Navier-Stokes (RANS) equations were used in order to decompose the instantaneous Navier-Stokes equations into the average fluctuation components. The detailed equations for each supplement are shown in their corresponding articles.
### Table 2 Governing equations

<table>
<thead>
<tr>
<th>Conservation term</th>
<th>( \Phi )</th>
<th>( \Gamma )</th>
<th>( S_\Phi )</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Mass</strong></td>
<td>1</td>
<td>0</td>
<td>(-\frac{\partial p}{\partial x} + \frac{\partial}{\partial y} \left( \mu_{\text{eff}} \frac{\partial u_x}{\partial x} + \mu_{\text{eff}} \frac{\partial u_y}{\partial y} \right) + \frac{\partial}{\partial z} \left( \mu_{\text{eff}} \frac{\partial u_x}{\partial z} + \mu_{\text{eff}} \frac{\partial u_y}{\partial z} \right) - \frac{2}{3} \mu_{\text{eff}} \left( \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} \right) )</td>
</tr>
<tr>
<td>X momentum, ( u_x )</td>
<td>( \mu_{\text{eff}} )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Y momentum, ( u_y )</td>
<td>( \mu_{\text{eff}} )</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Z momentum, ( u_y )</td>
<td>( \mu_{\text{eff}} )</td>
<td></td>
<td></td>
</tr>
<tr>
<td><strong>Energy</strong></td>
<td>( \rho c_p T - p )</td>
<td>( k_{\text{eff}} )</td>
<td></td>
</tr>
<tr>
<td><strong>Species</strong></td>
<td>( w_i )</td>
<td>( \rho D_{i,m} + \frac{\mu_i}{S_{C_i}} )</td>
<td>( R_i )</td>
</tr>
<tr>
<td><strong>Realizable, ( k )</strong></td>
<td>( \mu + \frac{\mu_i}{\sigma_k} )</td>
<td></td>
<td>( G_k - \rho \varepsilon - 2 \rho \varepsilon \frac{k_{\text{eff}}}{c_i^2} )</td>
</tr>
<tr>
<td><strong>Realizable, ( \varepsilon )</strong></td>
<td>( \mu + \frac{\mu_i}{\sigma_\varepsilon} )</td>
<td></td>
<td>( \rho C_{i,\varepsilon} \frac{G_k}{\mu_i} - \rho C_{i,\varepsilon} \frac{\varepsilon^2}{k + \sqrt{\varepsilon}} )</td>
</tr>
</tbody>
</table>

**Notes**

\[
\mu_i = \rho C_{\mu} \frac{k^2}{\varepsilon} \quad C_z = 1.9 \quad k_{\text{eff}} = k_x + \frac{c_{\mu} \mu_i}{P_{t_i}} \quad G_k = 2 \mu_i \left[ \left( \frac{\partial u_x}{\partial x} \right)^2 + \left( \frac{\partial u_y}{\partial y} \right)^2 + \left( \frac{\partial u_z}{\partial z} \right)^2 + \frac{1}{2} \left( \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} \right)^2 + \frac{1}{2} \left( \frac{\partial u_x}{\partial z} + \frac{\partial u_y}{\partial z} \right)^2 + \frac{1}{2} \left( \frac{\partial u_z}{\partial x} + \frac{\partial u_z}{\partial y} \right)^2 \right]
\]

\[
\eta = \frac{k}{\varepsilon} \sqrt{\frac{G_k}{\mu_i}} \quad \sigma_k = 1.0 \quad \mu_{\text{eff}} = \mu + \mu_i \quad \Phi_v = 2 \left[ \left( \frac{\partial u_x}{\partial x} \right)^2 + \left( \frac{\partial u_y}{\partial y} \right)^2 + \left( \frac{\partial u_z}{\partial z} \right)^2 \right] + \left( \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} \right)^2 + \left( \frac{\partial u_x + \partial u_y}{\partial y} \right)^2 + \left( \frac{\partial u_x + \partial u_y}{\partial z} \right)^2 + \frac{2}{3} \left( \frac{\partial u_x}{\partial x} + \frac{\partial u_y}{\partial y} + \frac{\partial u_z}{\partial z} \right)^2
\]

\[
v = \frac{\mu}{\rho} \quad \sigma_\varepsilon = 1.2 \quad C_i = \max \left[ 0.43, \frac{\eta}{\eta + 5} \right]
\]
4.3 Boundary condition

4.3.1 Boundaries

4.3.1.1 VOD nozzles

The mesh was created with quadrilateral cells of uneven sizes in Supplement 1 and 2. The boundary conditions of the two nozzle geometries are shown in Figure 10. The specifications are listed in Table 3:

<table>
<thead>
<tr>
<th>Boundary types</th>
<th>Specifications</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mass flow Inlet</td>
<td>Fixed mass flow rate</td>
</tr>
<tr>
<td></td>
<td>Fixed temperature</td>
</tr>
<tr>
<td>Pressure Outlet</td>
<td>Different pressures adopted with variable temperature</td>
</tr>
<tr>
<td>Wall</td>
<td>No-slip Wall</td>
</tr>
<tr>
<td>Axis</td>
<td>Axisymmetry</td>
</tr>
</tbody>
</table>

![Figure 10 Boundary conditions of Nozzle A and Nozzle B](image1)

Figure 10 Boundary conditions of Nozzle A and Nozzle B
4.3.1.2 BOF/LD converter
For the BOF/LD model, boundary conditions were assigned at different positions (Figure 11) in Supplement 3. The axisymmetric boundary condition was employed for the computational domain axial symmetry was used to simplify the model. The oxygen inlet and the outlet were also shown. Furthermore, the CO inlet was employed at the top curve of the slag zone. The complete estimation process for different boundary conditions is shown in Chapter 5 – Results and Discussion. The detailed setting of boundary conditions is described below:

**Figure 11 Boundary conditions**

**Oxygen Inlet.** Based on the calculation from the data obtained from SSAB, an oxygen flow rate of 385 Nm³/min at a temperature of 0 °C is injected into the converter. Therefore, a mass flow boundary condition was selected at the inlet.

**CO inlet.** Since it is not possible in the present work to know the exact position where CO is generated, a CO mass flow inlet along the slag top curve was chosen as a boundary condition. As explained before, some of the CO will be used for the post combustion and some will be transported upwards to the converter mouth. The iron liquid temperature increases from 1370 °C to 1630 °C due to the oxygen blowing and the simulation is run for a steady state. Thus, the temperature of the generated CO was estimated to be 1500 °C.

**Axisymmetry.** Based on the computational conditions, the converter is considered as an axial symmetric reactor.

**Outlet.** Since the outlet of the converter faces the surrounding directly with a pressure of 1 atm, a pressure boundary condition was adopted at the outlet. The gas was assumed to be air containing nitrogen (77 wt%) and oxygen (23 wt%).
Walls. For the converter linings, mixed thermal conditions were adopted. According to the emissivity measurement carried out at SSAB, the emissivity of the MgO-C lining is set to be 0.7. Also, the heat transfer coefficient is of importance for modeling the heat transfer through the wall. The value of heat transfer coefficient can be calculated for the different wall geometries. For the forced convection and the natural convection, it is usually estimated by Equation (12) and (13), respectively:

$$h_f = a \cdot Gr^b \cdot Pr^c$$  \hspace{1cm} (12)
$$h_n = k \cdot Re^m \cdot Pr^n$$  \hspace{1cm} (13)

where \(h_f\) and \(h_n\) are the heat transfer coefficient for the forced and natural convection, respectively. \(Gr\), \(Pr\) and \(Re\) are Grashof, Prandtl and Reynolds Number; \(a, b, c, k, m, n\) are indices that are different for various situations.

For the flow convection around the converter, the flow surrounding the converter was confined by a dog house (a big chamber embracing the converter), which separates the converter from the factory environment. However, due to the off-gas system working on the top and the rigorous blowing condition, the air near to the converter is also to some extent forced to circulate. Hence, the convection near the converter cannot be considered to be pure natural convection. In a previous paper, the heat transfer coefficient around an industrial ladle was taken as 8.5 W/(m\(^2\)-k), since it best fitted the industrial experimental data \[30\]. In the current work, a heat transfer coefficient of 13 W/(m\(^2\)-k) was employed for a wall with a thickness of 0.6m.

4.3.1.3 AOD converter
In Supplement 4, the model boundaries were designed as follows:

Symmetry. Due to the large size of the geometry, only a half of the AOD converter was taken into consideration. More specifically, the geometry is symmetric if it is cut at the shadow plane shown in Figure 12a.

Air inlet. Figure 12b shows the air inlet boundary. A zero gauge pressure inlet (i.e. atmospheric pressure) was adopted here. The air containing 23 wt% oxygen and 77 wt% nitrogen was sucked in with a temperature of 300k, by the negative pressure gradient created by the ascending off-gas and the fan located in the end of the flue.

Converter gas inlet. Figure 12c shows an inlet of CO and argon. The mass flow rate of CO is calculated based on the decarburization rate (from plant data) and the argon flow rate is based on the AOD operation flow rate. Since the nozzle for the gas injection is installed on the side of the AOD converter, CO and argon come up and emerge eccentrically on the steel bath surface. Therefore, it was assumed that these two gases flow into the computational domain through a restricted circular area with a diameter of 1m. A mass flow inlet was hence assigned as the boundary condition with a certain mass proportion of argon (33.2 wt%) and CO (66.8 wt%). In addition, a half deducted mass flow value of 1.345 kg/s at a temperature of 1600 °C was used thanks to the symmetric boundary setting.
**Pressure Outlet.** Figure 12d shows a pressure outlet. A fan is installed with the aim of sucking the off-gas from the AOD converter into the flue. In the present work, different fan pressures were tested by valuing the boundary condition at the pressure outlet. In addition, an operating pressure of 101325pa was adopted as the standard pressure. Hence, the pressure terms used in this work is the pressure difference (gauge) compared to the standard pressure.

**Wall boundary.** No-slip, adiabatic walls with standard turbulence wall functions were used in this work [31].

---

**Figure 12** Different boundaries of the AOD model

a. Symmetry  
b. Air inlet  
c. Converter gas inlet  
d. Pressure outlet
4.3.2 Decarburization zone

In Supplement 3, decarburization occurs when the injected oxygen thrust into the steel bath with a high velocity. The impinging effect of the oxygen jet will give rise to a region where the carbon instantaneously reacts with oxygen to form a CO gas. Around this region, a great deal of heat is released, since the reaction equation (2) is an exothermic reaction. In the present work, a hypothetical decarburization region was created at the bottom of the center of the converter domain. The decarburization zone is created as a cylinder with a radius of 0.2m and a height of 0.4m. Thus the volume of this decarburization zone is obtained by equation (14):

\[ V_{de} = \pi \cdot r^2 \cdot h = \pi \cdot 0.2^2 \cdot 0.4 = 0.0503 \, m^3 \]  \hspace{1cm} (14)

where \( V_{de} \) is the volume of decarburization zone (m\(^3\)), \( r \) is the radius of decarburization zone (m) and \( h \) is the height of decarburization zone (m).

The oxygen injected into this zone is consumed for the purpose of decarburization at a mass reduction rate of 7.19 kg/s. The estimation process will be explained later. Thus, for the modeling, a mass source sink was added into the continuity equation in order to remove the oxygen consumed by a reaction with carbon in the steel.

4.3.3 Materials properties

For the Supplement 3 and 4, three ideal gases (O\(_2\), CO and CO\(_2\)) are active for the post combustion reactions. A mixing law was chosen to determine the heat capacity of the gas mixtures [25]. Similarly, an ideal gas mixing law was selected for calculating the viscosity and the thermal conductivity of the gas mixtures. Specifically, the density, viscosity, thermal conductivity and heat capacity of the gases were treated as follows:

\[ \rho = \frac{p + p_{op}}{RT \sum_i w_i M_i} \]  \hspace{1cm} (15)

where \( \rho \) is the density (kg/m\(^3\)), \( p \) and \( p_{op} \) represent the Gauge pressure and the operating pressure (Pa), respectively. The term of \( w_i \) is the mass fraction of the \( i^{th} \) species and \( M_i \) is its molar mass (kg/mol).

\[ \gamma = \sum_i \frac{x_i \gamma_i}{\sum_j x_j \Phi_{ij}} \]  \hspace{1cm} (16)

\[ \Phi_{ij} = \sqrt{\frac{8\left[1 + \left(\frac{\gamma_i}{\gamma_j}\right)^{1/2} \left(\frac{M_j}{M_i}\right)^{1/4}\right]^{2}}{\gamma_j}} \]  \hspace{1cm} (17)
where $\gamma_i$ is the viscosity (kg/(m·s)) or thermal conductivity (W/(m·K)) of the $i$th species;
$x_i$ is the mole fraction of the $i$th species.

\[ c_p = \sum_i w_i c_{p,i} \]

where $c_{p,i}$ is the heat capacity of the $i$th species (J/(kg·K)).

### 4.3.4 Reaction

For the post combustion reaction in **Supplement 3** and **4**, only one reaction with one step was assumed for the gas reaction. Conservation equations for all species were solved considering the mass convection and diffusion among the different gases. The laminar finite-rate model and eddy-dissipation model have been widely used as species transport models [16,19,32]. Since a high temperature condition exists throughout the modeling, the species react with each other at high chemical reaction rates when they meet. Therefore, apart from the Arrhenius rate, the reaction rates are also controlled by the turbulence mixing, which is a prerequisite for using the dissipation model. Also, the reaction rate was set to be controlled by the lowest rate defined by either the Arrhenius rate or the turbulence mixing.

### 4.3.5 Radiation

In a high temperature process, radiation has been proved to be significant with respect to heat transfer. The Discrete Ordinates model has been proved to be a robust and comprehensive radiation model in ANSYS FLUENT [22,23]. Thus, the Discrete Ordinates model was employed as the radiation model since this model in ANSYS FLUENT is regarded as a comprehensive radiation model with a reasonable accuracy with respect to the computational time [25].

### 4.3.6 Solver

In **Supplement 1** and **2**, the domain size is 0.4×2m with 171609 and 135367 number of cells for Nozzle A and Nozzle B, respectively. The mesh of the domain decreases its density gradually down from the nozzle outlet. ANSYS 13.0 was employed for all the mathematical modeling in the two supplements. Double precision and a steady solution were employed. The steady-state simulations were executed with the pressure-based coupled solver, which resolves a coupled system of momentum and pressure-based continuity equations simultaneously. Furthermore, both first-order and second-order upwind schemes were used to perform the discretization. For all simulations, the residual of the energy was monitored with a criterion of $10^{-6}$. However, for the velocity and the turbulence residual, the criterion was set to $10^{-3}$. A typical simulation took on average one day on a computer with a CPU of Intel(R) Core(TM) 2 Duo CPU E8500@3.16GHz and with Linux Opensuse 11 OS.

For the BOF/LD and AOD model in **Supplement 3** and **4**, ANSYS 14.0 was employed for all the mathematical modeling. The steady-state simulation ran on a computer with a model of Intel® Core™ i7-950 @ 3.07GHz and a 6.0 GB RAM based on a Windows 7
system. A pressure-based coupled solver was employed for the computation. This solver enables a full pressure-velocity coupling. Furthermore, it can give rise to a robust and efficient result for steady-state flows. The PRESTO! scheme was used for discretizing the pressure. For other terms, both the first order and the second order schemes were adopted for the discretization. A convergent solution was deemed to be obtained when all the scaled residuals stayed at a level below $10^{-5}$. The BOF/LD model contained 89221 cells consisting of quadrilateral cells while the AOD model is comprised of polyhedral cells with 492550 nodes.
5. Results and Discussion
The Results from all mathematical simulations are presented in this chapter. This chapter consists of three parts. First, the modeling results from two VOD nozzles were shown and discussed. Thereafter, post combustion in the BOF/LD converter is presented. Finally, the post combustion phenomena in the AOD flue are shown and analyzed.

5.1 VOD nozzle modeling
CFD modeling was employed to obtain the flow information for Nozzle A and Nozzle B. All results and analyses based on the simulations are shown in this part.

5.1.1 Flow pattern
To explore flow patterns for both nozzles, Mach number contours are shown. Four ambient pressures (400mbar, 200bar, 100mbar, 10mbar) that are present in a real VOD vessel, were exerted on the domain outlet boundaries for a temperature of 1873K. This is assumed because the steel temperature in the VOD vessel could be around 1600 °C.

**Figure 13** displays the Mach number contours of both nozzles from the overall view. The distinct difference between **Figure 14a** and **14b** would be the flow pattern around the outlet, where the flow is choked in the case of Nozzle B. **Figure 14b** clearly shows the phenomenon of choking, with a sudden increase of Mach number to around 3 followed by a sharp drop. In addition, it can be noticed that the separations between the nozzle wall and the flow occur at the fringe of the outlet. On the contrary, Nozzle A (see **Figure 14a**) doesn’t show a rapid velocity drop, but a velocity attenuation with oscillations. From the results it can be concluded that the ambient pressure of 400mbar for Nozzle B is so high that it causes an over-expansion behavior. Furthermore, Nozzle A works normally for this pressure. These observations correspond to the nozzle theory calculations for a 400mbar ambient pressure, where the calculated outlet diameter for Nozzle A is closer to its real outlet diameter. Hence, this results in a smoother blowing, than for Nozzle B, where the calculated diameter is quite lower than its real diameter resulting in a choked flow.
Figure 13 shows the Mach number contours for Nozzle A and B for the ambient pressure 200mbar. It can be seen that this time the flow can extend more from Nozzle B (Figure 15b) instead of choking at the outlet as in the previous case (Figure 14b). The velocity peak for both nozzles appears near the nozzle in the domain with a Mach number of 2.58 and 3.3 for Nozzle A and Nozzle B, respectively. Besides, a clear under-expansion can be seen for Nozzle A, while an obvious over-expansion can be observed for Nozzle B. This agrees with the nozzle-theory calculations, where the calculated outlet diameter for Nozzle A is higher than its real diameter. However, for Nozzle B it is lower.
The reason is that oscillations begin to appear for Nozzle B for this ambient pressure value. 

[Figure 15 Mach number contours for an ambient pressure of 200mbar]

Severe under-expansion takes place for Nozzle A when the ambient pressure is decreased to 100mbar (Figure 16a). Moreover, the flow is still over-expanded for Nozzle B for this specific ambient pressure (Figure 16b). However, the expansion situation is better compared to the former case (Figure 15b). The Mach number peak for Nozzle A (3.82) is even larger than that of Nozzle B. Furthermore, the flow from Nozzle A becomes much more unstable than that for Nozzle B. This could indicate that for this certain mass flow rate, the ambient pressure 100mbar is a bit little too low to be used for Nozzle A. However, it is still too high to be used for Nozzle B. Also, the calculation results show two different calculation deviations for both nozzles.

[Figure 16 Mach number contours for an ambient pressure of 100mbar]

Figure 17 illustrates the Mach number contours of both nozzles for an ambient pressure of 10mbar. For Nozzle A, a big Mach disk forms near the nozzle outlet and a velocity vacuum appears. Despite a heavy under-expansion flow, the situation for Nozzle B is better and the flow remains continuous, without a drastic velocity drop behind the Mach disk. It can be concluded from the results that an extremely low ambient pressure might induce a severe turbulence, which results in a severely unstable blowing.

Over-expansion and under-expansion should in principle be considered in a nozzle design. Over-expansion makes a nozzle suck hot surrounding gases into the jet and causes nozzle
wear. However, even though under-expansion would not experience this, the oscillations brought by it might also induce nozzle wear.

![Mach number contours for an ambient pressure of 10mbar](image)

**Figure 17** Mach number contours for an ambient pressure of 10mbar

### 5.1.2 Blowing velocity

The blowing velocity is studied both in the radical and axial direction. The oxygen lance equipped with a De Laval nozzle is mounted at a certain height above the surface of the molten steel, where the oxygen impinges the slag and the melt surface. Furthermore, jet penetration and splashing as well as decarburization happen. By keeping the elevation height constant, the decarburization process can be performed. An elevation height of 1.3m was assumed in the mathematical modeling. In this section, the Mach number change for Nozzle A and Nozzle B along the axis will firstly be showed. Then, the radical attenuation of the blowing velocity of Nozzle A at a blowing distance 1.3m will be investigated. The ambient temperature was assumed as 1873K.

![Mach number profiles along the blowing axis](image)

**Figure 18** Mach number profiles along the blowing axis

**Figure 18** shows the Mach number changes of both nozzles along the blowing axis for the following ambient pressures, 400mbar, 200mbar, 100mbar and 10mbar. For Nozzle A (**Figure 18a**), it shows that the Mach number increases to a peak value. Thereafter, it decreases gradually with slight oscillations for an ambient pressure of 400mbar. The oscillation becomes heavier when the ambient pressure drops to a value of 200mbar. Furthermore, it is seen that the Mach number in the whole jet area in this case is larger than that for a 400mbar pressure value. The same tendency as for the previous two ambient pressures is seen for a 100mbar pressure. However, the flow fluctuates with even
larger oscillations at the start. In addition, a higher Mach number value can be obtained throughout the whole domain axis. In *Figure 17a* it was shown that the blowing failed due to the too low ambient pressure. Hence, in the Mach number profile for an ambient pressure of 10mbar, the Mach number sharply decreases to a subsonic value after a steep increase, which is represented by a Mach disk. Due to the stiff oscillation of the jet for this ambient pressure, the whole domain is not able to reflect all flow fluctuation in this case.

Similar observations are seen from *Figure 18b* except two cases of ambient pressures of 400mbar and 10mbar. A flow separation happens which is attributed to the ambient pressure of 400mbar. For the ambient pressure of 10mbar, the flow fluctuates severely and the fluctuation has not even stopped at the end of the domain.

It is noticed for both nozzles that for a higher ambient pressure, the Mach number shows on average a lower value. On the contrary, a low ambient pressure of 10mbar makes the flow extremely unstable, which results in heavy fluctuations. For this ambient pressure, a failed flow happens which shows a big Mach disk behind the velocity peak for Nozzle A. However, for Nozzle B, severe fluctuations emerge, which gives rise to a high Mach number throughout the whole domain. A supersonic region (Ma>1) can also be compared here to investigate the supersonic flowing distance. In the case of Nozzle A, the supersonic region increases from 0.57m to 1.21m when the ambient pressure decreases from 400mbar to 100mbar. The supersonic region of Nozzle B increases from 0.55m to 1.44m. It can hence be concluded that a lower ambient pressure improves the blowing velocity. On the other hand, it is of interest to note that the supersonic region of Nozzle B for the ambient pressures of 200mbar and 100mbar (0.92m, 1.44m) is larger than that for Nozzle A (0.85m, 1.21m). However, for the ambient pressure of 400mbar (0.55m), it is smaller than for Nozzle A (0.57m). Therefore, it can be concluded that Nozzle B is more suitable to be used at a lower ambient pressure than Nozzle A, since it produces higher velocities.

![Mach number along the radial direction at a blowing distance X=1.3m. Data are given for Nozzle A for four different ambient pressures at 1873K.](image)

*Figure 19* illustrates the velocity change at a distance of 1.3m away from the outlet of Nozzle A along the radius. It can be noticed that the jet radically attenuates from the jet center for ambient pressures of 400mbar, 200mbar and 100mbar. However, for an ambient pressure of 10mbar, the Mach number initially increases and then decrease. This
can be attributed by the low ambient pressure introducing severe jet oscillation. Therefore, stable jet attenuation from a radical direction cannot be formed for too low ambient pressures.

5.1.3 Jet dynamic pressure and jet force

A high jet force can yield a strong impinging effect on the steel surface, which leads to good reaction and stirring conditions. The dynamic pressures and forces of jets from both nozzles were compared. It was assumed that the steel bath was located 1.3m straight down from the nozzle. Therefore, the jet dynamic pressure and force at a blowing distance of 1.3m was investigated. The temperatures were still 1873K at the outlet boundaries. Furthermore, the jet dynamic pressure is displayed with a pressure unit of Pascal (Pa) in order to avoid the confusion to the ambient pressure (mbar).

Figure 20 Dynamic pressures along the radial direction at a blowing distance X=1.3m for four ambient pressures, 1873K

**Figure 20** shows the dynamic pressure for Nozzle A along the radius at a blowing distance of 1.3m. It is seen that when the ambient pressure decreases from 400mbar to 100mbar, the dynamic pressure can be increased from 2.4kpa to 5.1kpa. However, if the ambient pressure is too low, as when the domain pressure 10 mbar is used, the dynamic pressure instead dramatically decreases to less than 2kpa. Compared to the Mach number profile (**Figure 19**), it is interesting to see that the flow has a very high velocity for an ambient pressure of 10mbar. However, it yields a quite low dynamic pressure, which indicates that the density of the flow becomes very low at z=1.3m. **Figure 19** and **20** have indicated that the flow instability caused by a decreasing ambient pressure can be compensated by an increased flow velocity. Nevertheless, it also shows that the flow will crash due to its unsteadiness if the vacuum degree is excessively large. Therefore, it can be concluded that to some extent a decreasing ambient pressure can improve the dynamic pressure of the oxygen flow at the centerline. Furthermore, a too low ambient pressure may contribute nothing to the increase of momentum flux at a certain blowing distance. Moreover, it could also be found that a little under-expansion is somewhat helpful for the improvement of the dynamic pressure at z=1.3m in spite of the flow unsteadiness. However, a too heavy under-expansion makes the flow too unsound to have a larger dynamic pressure at z=1.3m.
To compare both Nozzle A and Nozzle B with regard to the dynamic pressure, Figure 21 was created below. It shows the dynamic pressures for both nozzles for four ambient pressures. In the case of an ambient pressure of 400mbar, the dynamic pressure of Nozzle A at a distance of 1.3m is higher than that of Nozzle B. This can be explained by the calculations and flow patterns. More specifically, the flow from Nozzle B for a 400mbar ambient pressure is choked at the outlet, bringing about a limitation of the blowing velocity. As the ambient pressure is lowered to 200mbar, the dynamic pressures for both nozzles increase and the values of them become similar. Furthermore, for the flow patterns, the flow for Nozzle A shows an under-expansion while the flow for Nozzle B shows an over-expansion. When the ambient pressure is decreased to 100mbar, an opposite situation arises. More specifically, the dynamic pressure of Nozzle B is higher than that of Nozzle A. In this case, a little heavier under-expansion is shown for Nozzle A and a minor over-expansion is seen for Nozzle B. However, both nozzles give rise to a lower dynamic pressure for the ambient pressure of 10mbar, which is due to the failed blowing for Nozzle A and the unfinished oscillation for Nozzle B. Still, Nozzle B shows a higher dynamic pressure than Nozzle A for a blowing distance of 1.3m. To summarize, it can be concluded that Nozzle B would produce a stronger impinging force at lower ambient pressures than Nozzle A would.

Figure 21 Centerline dynamic pressures at a blowing distance of 1.3m

The total jet force at the blowing distance of 1.3m was captured in the mathematical modeling for a 1873K temperature (Table 4). It can be noticed that for both nozzles, the jet force continues to increase from an ambient pressure of 400mbar to 100mbar. This would be attributed to the ambient pressure decrease, resulting in a jet force increase to meet the energy conservation. Moreover, as the same trend found in the dynamic pressure, Nozzle B is more competent for a lower ambient pressure with respect to giving a higher jet force.

<table>
<thead>
<tr>
<th>Temperature: 1873K</th>
<th>Jet Force (N)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ambient Pressure</td>
<td>400mbar</td>
</tr>
<tr>
<td>Nozzle A</td>
<td>135.33</td>
</tr>
<tr>
<td>Nozzle B</td>
<td>122.83</td>
</tr>
</tbody>
</table>
5.1.4 Jet width

The jet width was studied to investigate the jet attenuation trend radically. The jet width for Nozzle A of the oxygen flow at z=1.3m could be calculated as showed in Figure 22. With an increasing vacuum degree, the oxygen jet becomes narrower. In addition, and at an ambient pressure of 100mbar, the half jet width decreases to approximately 80mm. This means that lowering the ambient pressure, to a certain degree, can make the oxygen flow more intensive. However, if a too low ambient pressure is employed, the half jet width in fact increases to about 140mm. The reason could be explained by that a too large vacuum degree makes the flow heavily fluctuating and dispersed. In combination with the plot of a dynamic pressure against the ambient pressure, it can be noticed that at the ambient pressure value of 10mbar, the dynamic pressure is lower than that in other cases notwithstanding a broader jet width.

![Figure 22 Half jet width at a blowing distance X=1.3m, 1873K, Nozzle A](image1)

![Figure 23 Dimensionless velocity change along the radial direction at a blowing distance X=1.3m, 1873K, Nozzle A](image2)

Figure 22 shows the velocity distribution for Nozzle A at an axial distance of 1.3m along different radial positions. For the ambient pressure data of 400mbar, 200mbar and 100mbar, their velocity profiles behave almost in the same way. More specifically, the velocity continuously declines from the centerline outwards. In addition, a 10mbar value gives rise to a totally different velocity trend where the dimensionless velocity at the centerline first increases to a value of approximately 1.3 before it decreases. From the
discussion above it can be summarized that a flow that is not crashed will have a very similar velocity distribution along different radial positions. In addition, it can be noted that a jet can be regularly controlled by changing the ambient pressure in a certain range.

5.1.5 Temperature effects

The simulation results of temperature impact on Nozzle A and Nozzle B will be shown in this section. Three boundary temperatures, 1873K, 1000K, and 293 K were exerted on the outlet of the nozzle domain for both nozzles to investigate the thermal impact on the oxygen jet characteristics. In addition, ambient pressures of 400mbar, 200mbar and 100mbar were simulated.

![Graphs showing velocity change for Nozzle A at different temperatures and ambient pressures.](image)

**Figure 24** Centerline velocities along the blowing axis for Nozzle A

**Figure 24** shows the jet velocity change for Nozzle A along the blowing axis for three ambient pressures. It displays an increasing jet oscillation at the start of the blowing from an ambient pressure value of 400mbar to 100mbar, since the phenomenon of under-expansion is more serious for a lower ambient pressure. Moreover, higher temperatures yield higher blowing velocities after oscillations for all ambient pressures. In addition, no big difference can be found within the oscillation period for different temperatures. In the case of Nozzle B, **Figure 25** shows a similar trend in terms of the velocity change as observed for Nozzle A. The velocities at higher temperatures for these three ambient
pressures are always larger than those at lower temperatures. However, the oscillation extent becomes weaker as the ambient pressure decreases and the blowing tends to be smoother. This is due to that the over-expansion becomes less obvious. The lower velocities at lower temperatures result from the higher density of the surrounding gas at lower temperatures. A higher density of the surrounding gas results in a higher resistance to the flow of the jet.

When it comes to the dynamic pressure change along the axis at different temperatures, distinction would be found in Figure 26 and 27.

**Figure 25** Centerline velocities along the blowing axis for Nozzle B

a. 400mbar  
b. 200mbar  
c. 100mbar
Unlike the case for the velocity change, it can be seen that the difference for the temperature impact to the dynamic pressures is not obvious. However, still, a positive effect on the jet is found with a temperature increase. In the case of Nozzle A (Figure 26), the dynamic pressure for a higher temperature is only slightly larger than that for a lower temperature after the oscillations before a distance around 1m from the nozzle. However, the dynamic pressure values for different temperatures converge at the end of the domain.
The difference in dynamic pressures for Nozzle B (Figure 27) becomes even smaller, showing that the three curves of dynamic pressures are very close to each other. Nevertheless, for the initial part (before 1m) from the nozzle exit of the curves after the oscillation region, it can be still noticed that the dynamic pressures for these three ambient pressures are higher at higher temperatures. This also means that the jet can move with a high force in a low-resistant ambiance, even though undergoing a density decrease. From the results so far shown, it can be concluded that an increased temperature favors an increase of the dynamic pressure in a certain region of the domain. However, the effects are quite small compared to a variation of the ambient pressure. This is in conformity to the physical modeling results from previous results [34]. In addition, the temperature effects for Nozzle A seem to be larger than for Nozzle B.

To summarize, the temperature change shows little contribution to the alteration of the jet force. This can be further noticed in Table 5 and 6, which reveal the jet force for different temperatures for three ambient pressures. Horizontally considering the jet force value in the tables, it shows that temperature change is not favorable with respect to the increase of the total jet force. The comparison indicates that increasing the temperature is not as satisfactory as decreasing the ambient pressure when a high jet force is desired.

<table>
<thead>
<tr>
<th>Nozzle A</th>
<th>Jet Force (N)</th>
<th>Temperature (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Ambient Pressure (mbar)</td>
<td>1873</td>
</tr>
<tr>
<td></td>
<td>400</td>
<td>135.33</td>
</tr>
<tr>
<td></td>
<td>200</td>
<td>159.95</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>171.87</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Nozzle B</th>
<th>Jet Force (N)</th>
<th>Temperature (K)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>Ambient Pressure (mbar)</td>
<td>1873</td>
</tr>
<tr>
<td></td>
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<td>122.83</td>
</tr>
<tr>
<td></td>
<td>200</td>
<td>166.39</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>190.81</td>
</tr>
</tbody>
</table>

5.1.6 Metallurgical discussion

The results from the mathematical modeling of the VOD nozzle jets will be discussed in this part. Modeling results and curve fitting results will be analyzed for a deeper understanding of the jet behavior.

A high jet impinging force is required in an industrial blowing process since it can result in a deep penetration depth and improved reaction efficiency. It has been reported that a
higher oxygen total pressure increases the penetration depth [21, 22]. Nevertheless, in the present work, the jet dynamic pressure can be improved through another two ways. More specifically, it can be increased by decreasing the ambient pressure or increasing the ambient temperature.

![Figure 28](image)

**Figure 28** Centerline dynamic pressures at 1.3m

**Figure 28a** and **28b** reflect both the temperature and ambient pressure effects on Nozzle A and B, respectively. In order to show the dynamic pressure for a blowing distance away from the nozzle, the blowing distance of 1.3m is still selected for the study. Different results can be noticed for Nozzle B. More specifically, higher temperatures cannot all the time give rise to high dynamic pressures. This is especially true for the cases of the temperatures of 293K and 1000K. Here, the dynamic pressures for a 293K temperature are larger than that for a 1000K temperature for the Nozzle A cases (400mbar), Nozzle B cases (200mbar and 100mbar). This can somehow be explained by that the jet energy attenuates at the end of the domain. Thus, it will not be able to support a higher dynamic pressure at a higher temperature. On the other hand, it is clearly seen that on average the jet dynamic pressure is always higher at a lower ambient pressure for both nozzles. In addition, the temperature in a real VOD vessel is not possible to alter within reasonable values. However, the ambient pressure changes from 1bar at the start of the blowing to approximately 10mbar for the last five minutes of the blowing, under production conditions. This means that for a normal VOD operation, the changes in ambient pressure will have a larger impact on the jet dynamic pressure than the temperature changes will.

On the other hand, Nozzle A shows a large dynamic pressure difference for temperatures between 1873K and 293.15K. Specifically, it is 600 and 1234Pa for the ambient pressure of 200mbar and 100mbar, respectively. However, the case of Nozzle B indicates a smaller dynamic pressure difference, which is 199Pa for 200mbar and 379Pa for 100mbar. Hence, this implies that the temperature change has a greater effect on Nozzle A than on Nozzle B for an environment of low ambient pressures.
Figure 29 Dynamic pressure profiles at a distance of 1.3m from the nozzle exit, 1873K

Figure 29a and 29b show the dynamic pressure profiles at the blowing distance of 1.3m from the nozzle exit and for a temperature of 1873K for Nozzle A and Nozzle B respectively. For ambient pressures of 400mbar, 200mbar and 100mbar, it is found that the dynamic pressure curve fits well to the Multi-Gaussian distribution for both nozzles (Table 7). However, the curve representing a 10 mbar ambient pressure does not show a good correlation with a Gaussian distribution for the two nozzles. This is probably due to the rigorous blowing environment.

Table 7 Multi-Gaussian fitting for dynamic pressures

(R² is the coefficient of determination)

<table>
<thead>
<tr>
<th>Multi-Gaussian Fitting</th>
<th>Ambient Pressure (mbar)</th>
<th>Fitting functions</th>
<th>R²</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nozzle A</td>
<td>400</td>
<td>( P_{jet} = 682.6e^{-(\frac{y}{0.0606})^2} + 1749e^{-(\frac{y}{0.1042})^2} )</td>
<td></td>
</tr>
<tr>
<td></td>
<td>200</td>
<td>( P_{jet} = 1277e^{-(\frac{y}{0.05259})^2} + 2400e^{-(\frac{y}{0.09521})^2} )</td>
<td>&gt; 0.9999</td>
</tr>
<tr>
<td></td>
<td>100</td>
<td>( P_{jet} = 2084e^{-(\frac{y}{0.04261})^2} + 3027e^{-(\frac{y}{0.08724})^2} )</td>
<td></td>
</tr>
<tr>
<td>Nozzle B</td>
<td>400</td>
<td>( P_{jet} = 554.3e^{-(\frac{y}{0.06457})^2} + 1409e^{-(\frac{y}{0.1104})^2} )</td>
<td></td>
</tr>
</tbody>
</table>
Table 7 shows that the dynamic pressure value complies well with the Multi-Gaussian distribution. In addition, by integrating the jet momentum flux over the cross-sectional area of the domain at the blowing distance of 1.3m, the jet impinging force can be obtained from equation (16):

\[ F = \int_0^{2\pi} \int_0^{r_{\text{max}}} \rho_{\text{gas}} u^2 r dr d\theta \]  

(16)

where \( F \) is the jet force, \( u \) is jet velocity and \( r_{\text{max}} \) is the blowing cross-sectional radius which is 0.4m in this work. In connection with \( P_{\text{jet}} \), the jet force can be expressed as:

\[ F = 2 \int_0^{2\pi} \int_0^{y_{\text{max}}} P_{\text{jet}}(y) y dy d\theta \]  

(17)

Table 8 Comparison of jet force calculations from fitting and modeling results

| Ambient Pressure (Pa) | Jet force (N) From Multi-Gaussian fitting \( (F_f) \) | Jet force (N) From mathematical modeling \( (F_m) \) | Error (%) \( 100 \cdot \left| \frac{F_f - F_m}{F_m} \right| \) |
|-----------------------|---------------------------------------------|---------------------------------------------|---------------------------------------------|
| 400mbar               | 135.07                                      | 135.33                                      | 0.19                                        |
| Nozzle A              | 158.89                                      | 159.95                                      | 0.66                                        |
| 200mbar               | 168.53                                      | 171.87                                      | 1.94                                        |
| 100mbar               | 122.42                                      | 122.83                                      | 0.33                                        |
| 400mbar               | 165.33                                      | 166.39                                      | 0.63                                        |
| Nozzle B              | 187.15                                      | 190.81                                      | 1.91                                        |
| 200mbar               |                                            |                                            |                                              |
| 100mbar               |                                            |                                            |                                              |

By employing the fitting functions, the jet force can be calculated from equation (17) and compared to that obtained from the mathematical modeling. Table 8 shows calculated jet force values from Multi-Gaussian fitting and mathematical modeling. The comparison of the error calculations shows that the jet force values from the fitting and from the modeling are almost identical. More specifically, this is seen from an error smaller than
5%. This can further verify the rationality of the curve fitting. The discussions above also imply that, among these four ambient pressures, the jet at the ambient pressure of 100mbar can probably penetrate the bath surface the most.

5.2 BOF/LD modeling

5.2.1 Measurement results

5.2.1.1 Process data with respect to heat number

The obtained process data are the carbon content in the hot metal charged into the converter and in the steel when it is tapped. The data were collected during seven days from 17 January 2012 to 24 January 2012. In this work, only the last 41 heats (Heat 22541 to 22581) from the 177 heats were analyzed. This is due to that these data were dynamically registered with respect to the time and at a sampling interval of two seconds. The converter yields an amount of steel with its weight of slightly less than 130 tons. The carbon content drops from 4.68 wt% to 0.06 wt%. It should be mentioned that some data were not registered or wrongly registered in the database due to technical problems. Furthermore, some measurements of the temperature data were affected by the steel which was returned to the converter. These data were thus discarded during the post processing. In order to estimate the decarburization rate, the average values of all the data were adopted. Equation (18) shows the calculation process.

\[ R_{de} = \frac{m_{steel} \cdot [\text{wt}\% C]_{steel} - m_{metal} \cdot [\text{wt}\% C]_{metal}}{t_{blowing} \cdot 60} \]

where \( R_{de} \) indicates the decarburization rate (kg/s); \( m_{steel} \) and \( m_{metal} \) represents the average of steel and metal weight (kg/s); \( [\text{wt}\% C]_{steel} \) and \( [\text{wt}\% C]_{metal} \) represents the average carbon weight fraction in the hot metal and steel (wt%) and \( t_{blowing} \) represents the average blowing time (min).

The average temperature data of the 41 heats were also obtained. It can be calculated that the average sampling temperatures during the blowing is 1370 °C and the average of the steel temperatures obtained by the sampling is 1630 °C.

5.2.1.2 Process data with respect to time point

In addition to the data in terms of the heat number, the process data for every two seconds were also taken into consideration. These data were logged from January 22, 2012 to January 24, 2012, which is only a part of the complete data. More specifically, the data employed here are from 41 heats. Considering the steady state simulation, a few parameters were fixed during the computation. Table 9 shows the parameters exploited for modeling.
Table 9 Industrial parameters used in the simulations

<table>
<thead>
<tr>
<th></th>
<th>Lance Height (m)</th>
<th>Oxygen Flow rate (Nm³/min)</th>
<th>Oxygen Temp. (°C)</th>
<th>Blowing time (min)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Values used in the modeling</td>
<td>1.7</td>
<td>385</td>
<td>0</td>
<td>17</td>
</tr>
</tbody>
</table>

Since the blowing time for the converter process is 17 minutes, the decarburization rate can be calculated using equation (18). Based on the data from the 41 heats, \( m_{steel} \) and \( m_{metal} \) are 129.32 and 118.96 ton; \([wt\%C]_{metal}\) and \([wt\%C]_{steel}\) are 4.68 and 0.06 wt%, respectively. Thus, the value of \( R_{de} \) is 5.39 kg/s.

5.2.1.3 Estimation of CO formation
In the current work it is assumed that carbon first reacts with oxygen and then directly generates CO. Since the decarburization rate is already known, the CO generation rate can also be calculated by use of equations (19) and (20).

\[
C + \frac{1}{2}O_2 = CO \tag{19}
\]

\[
R_{CO} = \frac{R_{de} \cdot M_{CO}}{M_C} \tag{20}
\]

where \( R_{CO} \) indicates the CO generation rate (kg/s). The parameters \( M_{CO} \) and \( M_C \) represent the molar mass of CO and C (g/mol). In the present work, they are 28 and 12 g/mol, respectively. From the relation above, it can be estimated that the generated CO is 12.58 kg/s.

5.2.1.4 Estimation of O₂ reacted due to decarburization
Since it is assumed that CO is generated from the reaction between carbon and oxygen, the consumed oxygen can be estimated as follows by use of equation (21):

\[
R_{O_2} = \frac{R_{de} \cdot M_{O_2}}{2M_C} \tag{21}
\]

where \( R_{O_2} \) is the oxygen consumption rate (g/mol) and \( M_{O_2} \) is the molar mass of O₂, 32 g/mol. The calculation shows that the oxygen is consumed by the carbon with a mass rate of 7.19 kg/s.

5.2.1.5 Off-gas analysis
The off-gas data were registered in a flue above the converter mouth. Totally 41 heats were analyzed and the change of gas concentration with time is illustrated for one heat in Figure 30. Since the whole steel making process is similar for all 41 heats, the gas concentration profiles for only four heats are shown here. The figure shows the change of the off-gas mass concentration under the oxygen blowing. It can be seen that just before
the oxygen blowing, the nitrogen content is high. Moreover, that the oxygen gas exists in the flue since the flue is now filled with air. When the blowing starts, the nitrogen and the oxygen content sharply decrease and CO₂ appears in the flue prior to the detected CO. This is due to that the initially generated CO in the decarburization reaction immediately reacts with the injected oxygen before it leaves the converter. After a while, the CO content begins to increase rapidly and the oxygen gas disappears. This means that all oxygen either reacted during decarburization or was exhausted for other reasons, such as due to the post combustion. An almost leveled–off curve can be noticed after a few minutes, when the CO and the nitrogen content values are fairly stable. This situation is regarded as a steady state. Consequently, the data for this region were analyzed and compared to the modeling results.

![Figure 30](image)

**Figure 30** Measured off-gas concentration as a function of time

The post combustion ratio, namely the CO₂ content in the current work is of great interest. For the stable region where the CO₂ content remains the same, it can be observed that the average CO₂ mass fraction is slightly less than 20 percent. In addition, since there is nitrogen in the gas it can be confirmed that post combustion also occurs in the flue gas.

### 5.2.1.6 Emissivity Measurement

A ThermoVision camera was held with its lens against the inner lining of the convert through a window gap during the measurement. The emissivity of the lining was estimated by the software using equation (22):

\[
\varepsilon_e = \frac{E_{lining}}{E_{black}}
\]

(22)

where \( E_{lining} \) and \( E_{black} \) are the energy emitted by an object and by a blackbody at the same temperature. After the data treatment in ThermaCAM Researcher, the emissivity of the inner wall can be calculated for a chosen reference temperature of 1500°C. Based on these data, an average value of 0.7 was adopted in the modeling.
5.2.1.7 Lining properties
A MgO-C 10~12 wt% brick is employed for the inner lining of the converter. The density of this brick is already known to be 3000 kg/m³. The specific heat and the thermal conductivity of the MgO-C refractory for different carbon contents at different temperatures were obtained. The higher the carbon content is, the higher the specific heat and the thermal conductivity are. On the other hand, the increase of the temperature gives rise to two opposite trends regarding the specific heat and the thermal conductivity. With a higher temperature, the specific heat of the refractory becomes higher while the heat conductivity becomes lower. In the present work, the refractory parameters for the modeling were chosen for a carbon content of 10 wt% and a temperature of 1500 °C. Therefore, a specific heat value is 1415 J/(kg·K) and a thermal conductivity value of 5.3 W/(m·K) were used in the modeling.

5.2.1.8 The Oxygen transferred to slag
When oxygen starts to impinge on the hot metal surface in a converter, slag and foam start to form. Because of the strong impacting force, the oxygen plunges into the steel under the formation of a cavity through the reaction in equation (2). Consequently, the oxygen jet has a sufficient contact with the steel surface and the carbon from the hot metal is removed gradually. However, from equation (19), for the oxygen consumed during the decarburization ($R_{O_2} = 7.19 \text{ kg/s}$), it is known that all the oxygen does not react with the carbon in the hot metal. Instead, it either goes to the slag in the form of compounds, such as FeO, or remains for the post combustion with CO according to equation (1). In the present work, it is already known that only 78 wt% of oxygen is consumed for decarburization. Hence, it is assumed that 20 wt% of the total oxygen injected reacts with Fe or other elements and then form oxides moving into the slag; besides, the remaining 2 wt% oxygen reacts with CO for post combustion.

5.2.2 Simulation results

5.2.2.1 Stream function
Figure 31 shows the streamlines of the flow pattern. It can be seen that the whole flow is represented by streamlines reflecting the direction in which the fluid travels. For the top part of the converter it shows that the gas flow goes upwards to the converter mouth. On the other hand, it can also be noticed that, near the decarburization zone, a recirculation zone arises due to both the decarburization sink and the steel and the slag that block the oxygen jet to move further down. Here, a hot zone appears probably at the location where a big amount of post combustion takes place. Moreover, the temperature around this zone is higher than that of the top zone of the converter. This is the result of the heat being released by the reaction between CO and O₂. Another less obvious recirculation zone stays close to the inlet of the oxygen jet and its shape is not as circular as the first one below. The formation of this zone is induced by the entrapment effect of the oxygen jet bringing the CO gas near it. This implies that the post combustion between CO and O₂ also occurs in this region. Also, the exothermal heat generated due to equation (1) results in a high temperature, as is described later.
5.2.2.2 Temperature

The temperature distribution above the steel bath in the converter is displayed in Figure 32. Since the oxygen is injected at zero degrees Celsius, the temperature is homogeneously distributed in the oxygen stream. However, owing to the decarburization and recirculation zones, a part of CO generated by decarburization is mixed with the O₂. This generates a considerable amount of heat due to the exothermal reaction between CO and O₂. This, in turn, creates a high temperature spot. Furthermore, a more homogeneous temperature region than the hot spot can be seen in the lower part of the domain beside the hot spot. This indicates that, a steady post combustion region could exist just above the steel bath and close to the oxygen impinging area (hot spot). Another interesting region is the high temperature part close to the oxygen gas inlet. This high temperature region is a result of the entrainment of generated CO into the high speed oxygen jet. This implies that a part of the oxygen blown into the converter will be used for post combustion directly with entrained CO, before it impacts on the steel bath. In addition, on the right side above the slag the temperature is lower than that close to the oxygen jet and the steel bath. The reason can be explained by that one of the combusting gases, oxygen, is a little bit far away from this region. Therefore, no obvious post combustion is discerned.
5.2.2.3 Carbon dioxide

The amount of carbon dioxide is the most straightforward index to judge the post combustion ratio. The more carbon dioxide that is generated, the more post combustion takes place and the more reaction heat can be released. Figure 32 shows the carbon dioxide contours in the converter. At the left side above the slag it can be noticed that almost no CO$_2$ is generated, because there is a distance between this region and the oxygen source. From the left bottom of the domain, a different phenomenon can be observed. Due to the decarburization sink at the corner, CO and O$_2$ are mixed and thus they react to produce a substantial amount of CO$_2$. In addition, the recirculation region close to the steel bath also contributes with CO gas to the post combustion in the decarburization zone. This explains the small region at the left bottom corner of Figure 32, with a high CO$_2$ concentration. Moreover, another region with a high CO$_2$ concentration develops near the oxygen inlet. Here, much post combustion occurs due to the entrapment of CO which is generated from the decarburization by the oxygen jet. For other parts in the converter, it can be perceived that the CO$_2$ concentration continuously decreases from the center to the wall of the converter. This is due to that the distance to the combustion agent oxygen becomes longer at a position nearer to the wall.
5.2.3 Metallurgical discussion

In order to evaluate the off-gas data from the modeling results, the analyzed and processed data from a great amount of the off-gas information for the converter are compiled and compared in Figure 34. Figure 34 shows a comparison between the industrial data and the modeling data with respect to the CO$_2$ concentration in the off-gas. In Figure 34, it can be seen that this value is 16.7% and that it stays in conformity to the industrial data, which fluctuate from 15 wt% to 20 wt%. These values are deemed to be realistic from a production point of view. Furthermore, the modeling result is comparable to data presented the reviewed literature, which showed an average CO$_2$ concentration of less than 25% and larger than 13% from an oxygen blowing time of 6 minutes to 12 minutes [37].
From this result it can be concluded that the present BOF converter model can predict the gas mass fraction in a realizable manner. However, since the off-gas probe located in the flue lies a distance away from the converter mouth, a model of the off-gas flue should be established in the future so that the off-gas data can be more precisely studied and correlated to the available converter modeling data.

Table 10 Changes of off-gas properties with converter temperature

<table>
<thead>
<tr>
<th>Temp. of CO (°C)</th>
<th>Outlet off-gas temperature (°C)</th>
<th>CO₂ mass fraction (wt%)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1500</td>
<td>1585</td>
<td>16.71</td>
</tr>
<tr>
<td>1600</td>
<td>1685</td>
<td>16.73</td>
</tr>
<tr>
<td>1700</td>
<td>1780</td>
<td>16.75</td>
</tr>
</tbody>
</table>

The effect of the converter temperature on the off-gas is also of great interest. Apart from the modeling case with an inlet CO temperature of 1500 °C, other temperatures of 1600 °C and 1700 °C were also tested during the simulation. In reality, the formation of FeO as well as other slag oxides and the temperature change in the converter have a mutual influence on each other. Hence, an assumption was made that only the heat or energy released by the post combustion was considered in the model. Table 10 shows the influence of different CO inlet temperatures on the gas information at the outlet. It can be seen that when the CO temperature increases from 1500 °C to 1700 °C, the outlet temperature correspondingly increases from 1585 °C to 1780 °C. However, the post combustion is not affected as much as the converter mouth temperature is. The CO₂ content only increases by 0.24 wt% while the outlet temperature is increased by 12.30 wt%. This indicates that the high temperature in the converter has no direct
influence on the gas composition change brought by exothermic reactions during post combustion.

5.3 AOD modeling

5.3.1 Simulation results

In order to visualize the effects of post combustion in an AOD converter, the contours of gas temperature and concentration are shown. If the inlet gas temperature is 1600 °C, the gas containing CO and argon will rise from the steel surface. Moreover, the CO will post-combust with the oxygen contained in the leakage air, which is sucked into the off-gas flue. The Gauge pressures of -800 to 0 Pa were tested at the end of the off-gas flue. The results from the cases with Gauge pressures of -800, -500 and -50 Pa are compared and discussed below.

The post combustion in the off-gas with a large outlet fan gauge pressure of -800 Pa was investigated. Figure 35 shows the temperature distribution of the gas phase in the whole system for a fan gauge pressure of -800 Pa. It can be seen that a gas mixture containing argon and CO is released with a high temperature into the converter chamber. At the off-gas flue inlet, cool air is sucked in due to the lower pressure in the off-gas flue system. Furthermore, a temperature gradient can be observed around a position near the AOD mouth in the flue. This implies that the gases coming from the AOD are being mixed with cool air, which is sucked in during this passage. However, from a kinetic point of view, if the flow of the cool leakage air into the flue is too high, the gas mixture temperature will be largely decreased and post combustion will be suppressed. The plot of the cross section contours shows a uniform temperature distribution with a high temperature in the center and a low temperature away from the center. These findings show that no post combustion occurs when a fan gauge pressure of -800 Pa is used.
When the fan gauge pressure is further changed to -50 Pa, the situation becomes different. Figure 36 shows the temperature distribution of the AOD system. It can be seen that the temperature distribution is no longer the same as in the cases with a fan gauge pressure of -800 or -500 Pa. This implies that post combustion occurs near the flue inlet for this certain fan outlet pressure. Furthermore, for the assumption that adiabatic walls with no heat loss exist, the highest temperature region can be seen around the upper elbow of the flue where the temperature reaches 2694 K. This indicates that the post combustion mainly happens here. Figures 37 and 38 show the CO and nitrogen gas composition in the computational domain. The concentration of these two gases decreases when moving upwards in the off-gas channel. The nitrogen concentration decreases because this fan pressure causes less air to be sucked into the system, compared to the previous two cases. Also, owing to the post combustion that consumes CO, the CO content also decreases. A direct view of the CO\(_2\) concentration change can be observed in Figure 39 for the AOD domain. It can be seen that the CO starts a post combustion reaction with oxygen immediately after the AOD mouth. In addition, the concentration of the post combustion product, CO\(_2\), reaches its maximal value of 39 wt% after the first elbow of the flue. From the three cases of three fan gauge pressures of -800, -500 and -50 Pa, it can be concluded that the fan gauge pressure of the flue has a significant influence on the post combustion ratio. Furthermore, a high fan pressure difference favors a quick removal of the off-gas without a heavy post-combustion. For all the three cases being discussed, no post combustion was found in the internal part of the AOD. This means that no leakage air is sucked into the AOD chamber in the model with the chosen boundary conditions. Also, with the assumption that all the decarburizing oxygen is consumed before it leaves the steel bath, there will be no oxygen which can be used for post combustion in the AOD chamber.
Figure 36 Temperature contours for a fan gauge pressure of -50 Pa

Figure 37 CO content contours for a fan gauge pressure of -50 Pa
Figure 38 N\textsubscript{2} content contours for a fan gauge pressure of -50 Pa

Figure 39 CO\textsubscript{2} content contours for a fan gauge pressure of -50 Pa
5.3.2 Metallurgical discussion

Figure 40 Argon and nitrogen content at the flue outlet as a function of the outlet gauge pressure

An in-depth investigation on the influence of different fan pressures was conducted. **Figure 40** shows the argon and nitrogen concentration at the end of the off-gas system in the AOD. A mass-weighted average value was adopted for the investigation of the information at the off-gas flue outlet. Since nitrogen is contained in the air and argon is present in the process gas mixture, these two curves on the figure represent the proportion of the air and the AOD gas mixture in the system. It can be seen that the nitrogen concentration decreases from 71 wt% to 14 wt% when the fan gauge pressure changes from -800 to 0 Pa. Furthermore, the argon concentration, on the contrary, increases from 2.6 wt% to 27.2 wt%. This can be explained such that a zero value gauge pressure results in less air from the environment into the flue, which leads to a decreased nitrogen concentration. In addition, an increased argon concentration is brought by a decreased nitrogen concentration. It can also be noticed that around a fan gauge pressure of -530 Pa, the nitrogen and argon content decreases and increases sharply, respectively. This implies that the leakage air into the flue decreases sharply with an increased pressure difference and that post combustion starts to appear around this pressure value.

The results have shown that no post combustion can be seen in the AOD chamber. This is mainly due to the large mass flow rate of the gas mixture from the steel bath and this specific geometry design. The paper by Tang et al. showed that the entrapped air into the AOD chamber can only be observed when a small flow rate of the gas mixture of 5 Nm3/min is adopted at the reduction stage [24]. However, for the current paper aiming at the decarburization stage, a much larger gas mixture flow rate was employed. Thus, this
resulted in no post combustion in the chamber. This knowledge is important if continuous measurements of temperature are carried out in the converter.

**Figure 41** Profiles of temperature and CO$_2$ content as a function of the outlet gauge pressure at the flue outlet

*Figure 41* shows the temperature change and CO$_2$ concentration change at the flue outlet for different fan pressures. It can be seen that for a fan gauge pressure of -800 Pa, the temperature of the gas at the flue outlet (421 K) is much lower than the AOD gas mixture temperature (1873 K). Furthermore, almost no trace of CO$_2$ can be seen. This is due to too much cool air being mixed into the off-gas flow. Thus, it prevents the post combustion from taking place. Moreover, the Arrhenius reaction rate starts to determine the reaction rate for low temperatures in most part of the domain. This is due to that it cannot be assumed that different reacting species react immediately when they meet each other. When the fan gauge pressure changes from a value of -800 to -550 Pa, it can be observed that the temperature increases slightly from 421 to 451 K. This is due to that less air is sucked into the flue at lower fan gauge pressures. In addition, the CO$_2$ concentration increase is even less obvious. Therefore, it can be concluded that no post combustion can be observed at these fan gauge pressures. However, when the fan gauge pressure is changed to -530 Pa, a high temperature (1445 K) and a high CO$_2$ concentration (15.07 wt%) are seen in the figure. This indicates that post combustion occurs, which brings a large amount of heat that contributes to the increase of the temperature value. On the other hand, when the fan gauge pressure is changed from -100 to 0 Pa, the temperature and CO$_2$ value decreases sharply. This can be explained such that even though post combustion occurs, there is not enough oxygen to facilitate a large increase in temperature. The temperature is higher than for the cases with higher gauge pressures, due to the fact that less cold air is sucked in and mixed with the process gases. This results in a low CO$_2$ content and a low temperature at the flue outlet. Furthermore,
this figure also implies that a critical gauge pressure value exists. This can give rise to the maximum post combustion is around -150 Pa for the current system.

Table 11 Temperature effects on the outlet gas properties

<table>
<thead>
<tr>
<th>Fan Gauge pressure (Pa)</th>
<th>Inlet temperature (°C)</th>
<th>Outlet temperature (°C)</th>
<th>CO₂ (wt%)</th>
<th>N₂ (wt%)</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>1500</td>
<td>2173</td>
<td>24.02</td>
<td>29.26</td>
</tr>
<tr>
<td>-50</td>
<td>1600</td>
<td>2212</td>
<td>24.06</td>
<td>29.30</td>
</tr>
<tr>
<td></td>
<td>1700</td>
<td>2260</td>
<td>24.12</td>
<td>29.38</td>
</tr>
<tr>
<td>-800</td>
<td>1600</td>
<td>138</td>
<td>0.0011</td>
<td>71.14</td>
</tr>
<tr>
<td></td>
<td>1700</td>
<td>158</td>
<td>0.0015</td>
<td>70.98</td>
</tr>
</tbody>
</table>

Different temperatures of the gas mixture were also tried to explore their effects on the post combustion. Table 11 shows the outlet temperatures and the mass concentrations of CO₂ and N₂ for different temperatures of the inlet gas. Since no slag or the formation of CO was considered in this model, the inlet gas temperature will not be affected by the off-gas generation. It can be seen from the table that two fan gauge pressures were tested. More specifically, the gauge pressure of -50 Pa was proven to give rise to much post combustion in the flue while the gauge pressure of -800 Pa led to no post combustion. Three inlet gas temperatures of 1500, 1600 and 1700 °C were adopted for the investigation, since these temperatures commonly prevail in the AOD converter. When the inlet gas temperature is increased from 1500 °C to 1700 °C, it can be observed that the outlet temperature increases correspondingly. This is true for both two fan gauge pressures from 2173 to 2260 °C and 138 to 158 °C, respectively. Nevertheless, no obvious variations in the gas concentrations of CO₂ and N₂ for both two gauge pressures were seen in the table. This implies that a temperature change of the post-combusting gases in the AOD converter would not yield much different results with respect to the post combustion in the off-gas flue.

Finally, it is important to point out that it might be difficult to always have a stable operation of the flue fans. This means that the level of post combustion will change, even if the level of decarburization is constant. If this is not considered, temperature measurements in the off-gas flue will be less trustworthy.
6. Concluding Discussion

This thesis focuses on some important process aspects in the following decarburization processes: VOD, BOF/LD and AOD. The simulation results of the two De Laval nozzles from a VOD process from Supplement 1 and 2 have been shown in the previous chapter. Besides, the post combustion phenomena in the BOF/LD and AOD process were illustrated in Supplement 3 and 4. From the introduction chapter, it can be seen the simple connection between different supplements (Figure 2). In this chapter, Figure 42 shows a detailed performed work which was done in each supplement. In addition, the supplement connection will be further discussed for these four supplements from a metallurgic point of view.

![Diagram of steelmaking decarburization processes]

**Figure 42** Overall summaries of the detailed work as well as the connections among all the four supplements

The results for the modeling of a VOD nozzle jets can also be used as a base to study other converter processes. More specifically, different nozzle models can be created for the investigation of flow properties for various top-blowing converters with different chamber pressures and blowing jet velocities, such as, BOF/LD converter, AOD converter with a top-blowing lance, etc.

Apart from the oxygen flow itself, the entrapment of the generated CO and the post combustion inside a converter should also be investigated. In Supplement 3, a BOF/LD converter was modeled to study the post combustion phenomenon inside the converter. In this supplement, the focus was thus on the CO entrapment into the oxygen flow. Radiation was modeled as well as turbulence, which was created by a high speed oxygen flow. A slag zone was created in the lower part of the converter but phenomena inside the slag were not modeled. Off-Gas composition from the industry was utilized for
verification of the predictions. From the modeling result it can be concluded that the converter model created in Supplement 3 functions well with regard to the prediction of the gas mass fraction. More specifically, a mass-weighted average value is obtained by the modeling calculation at the outlet of the converter.

The present research on the post combustion in a BOF/LD shows an approach of a verification of modeling results by means of off-gas data. The similar approach can be utilized on the investigation of the post combustion in other steelmaking decarburization processes, such as AOD, VOD, etc. However, since the post combustion also occurs in an off-gas flue, the study of gas flows in the off-gas flue should be carried out. Therefore, a model of a converter together with an off-gas flue was created in Supplement 4. Since the methodology of the off-gas modeling can be transferred between different decarburization processes, a model of an AOD converter together with an off-gas flue was created instead of a BOF/LD converter in Supplement 4. Radiation and turbulence were modeled together with post combustion. Boundary conditions were obtained from the industry; different fan pressures at the flue outlet were tested to explore the relation between pressures and post combustion. Considering the temperature effects on the process gases of BOF/LD and AOD in Supplement 3 and 4, it was concluded that no obvious effects brought by the high process temperatures on the post combustion can be observed.

To summarize, the four supplements mainly focus on the gas flow and its collateral effects on steelmaking processes as illustrated in Figure 42. Different steelmaking processes were studied due to the projects’ requirements. The gas flow out of VOD nozzles was studied in Supplement 1 and 2. The investigation of a gas phase above the steel bath in a BOF/LD converter was performed in Supplement 3. Furthermore, the gas condition in an AOD flue was explored in Supplement 4. It was obtained from the Supplement 1 and 2 that different nozzles can be equipped for different ambient pressures to optimize the oxygen flow with respect to the impinging effects. This conclusion is significant for the BOF/LD process in Supplement 3, where the post combustion phenomena were studied and compared to industrial off-gas data. Specifically, the injected oxygen speed changes with different nozzle types, which results in different CO gas entrapments. This will bring about an influence on the post combustion because the kinetic and thermodynamic conditions in the system will be changed. Furthermore, the results from Supplement 4 show that post combustion takes place in the off-gas flue; besides, the values of different fan gauge pressures affect also the post combustion. This implies that in Supplement 3, the industrial off-gas data should be further investigated to validate whether they are representative of the off-gas at the converter mouth. In a sentence, the present work shows a possible and initial approach to investigate the gas flows in different positions and stages of different steelmaking decarburization processes.
7. Conclusions

The present work helps to comprehend the gas flows in different metallurgical processes. The flow field of two VOD nozzles was displayed in Supplement 1 and 2. Temperature effects on the jet velocity and dynamic pressure for both nozzles were illustrated. From the nozzle theory calculation and the numerical simulation results the conclusions of the work are summarized as follows:

- A good correlation can be found from the nozzle-theory calculations and simulations. The flow would appear over-expanded or under-expanded if the calculated diameter is smaller or larger than the real one, respectively. A lower ambient pressure yields a higher flow velocity through the domain, but result in heavier flow fluctuations. Besides, the flow pattern of Nozzle B appears better than that of Nozzle A at a low ambient pressure.
- A lower ambient pressure produces a higher jet velocity and a dynamic pressure with a narrower jet width. However, a too low ambient pressure drives the flow in acute fluctuation. This has a negative impact on the jet velocity and dynamic pressure. Also, nozzle B gives rise to a higher jet velocity and dynamic pressure than Nozzle A for low ambient pressures. Moreover, slightly lower ambient pressures improve the velocity and dynamic pressures of the jet for both nozzles.
- A high ambient temperature yields a high jet dynamic pressure before the blowing distance 1m; nevertheless, it does not benefit the improvement of the dynamic pressure much near the end of the domain. It could be found that a reasonably decreased ambient pressure can to a larger extent increase the dynamic pressures of the jet than an increased ambient temperature. Furthermore, a changing temperature has a stronger effect on the jet dynamic pressure for Nozzle A than for Nozzle B.
- The knowledge of temperature and pressure effects should be used when designing a nozzle. Also, in the absence of a variable nozzle geometry, the effects of altering the temperature and pressure outside the nozzle design parameters can be known.
- No indication shows that higher ambient temperatures support higher total jet forces. The jet force profile at a blowing distance of 1.3m conforms favorably to a Multi-Gaussian fitting ($R^2>0.9999$).

A mathematical model of a LD converter was created for the purpose of investigating the phenomenon of post combustion in Supplement 3. A large amount of industrial data of the converter process was collected. These data were systematically analyzed and used in the mathematical modeling. Thanks to the simulation, contour plots were shown to display the temperature and gas distribution in the converter. The positions of the region where most of the post combustion takes place were clearly shown.

- An agreement was found between the real industrial off-gas data and the modeling results. Specifically, the off-gas data at the model outlet (16.7 wt%) conformed well to the industrial data of the off-gas composition (15-20 wt%).
Based on the assumption that the formation of slag oxides is not considered in the present work, the change of the converter internal temperature at a constant decarburization rate didn’t show obvious influences (Standard deviation<0.02) on the gas composition at the converter outlet. The gas temperature at the outlet increases correspondingly with an increasing temperature (from 1500 to 1700 °C) inside the converter.

The post combustion in an AOD system with a negative fan gauge pressure in its flue was studied in Supplement 4. The study was done using mathematical modeling based on industrial data. Different fan gauge pressures at the flue outlet were tested and it was proved that a changing fan gauge pressure will affect the post combustion in the off-gas flue. Furthermore, the effect of the AOD chamber temperature on the post combustion was also studied. The specific conclusions can be summarized as follows:

- No post combustion could be discerned in the inner part of the AOD converter.
- A critical fan gauge pressure (around ~150 Pa) was confirmed to generate the highest post-combustion value in the flue. Beyond this critical gauge pressure value, a higher or lower fan gauge pressure would decrease the CO combustion efficiency in the flue. This can be caused by too much cold air being sucked into the flue and too little oxygen supplied for the post combustion with CO, respectively.
- A critical fan gauge pressure (approx. -550 Pa) exists for the post combustion to take place in the current AOD. A larger pressure difference than the critical value prevents the post combustion from happening.
- If it is assumed that the temperature change in the converter does not alter the slag formation and the CO generation due to the decarburization, a changed temperature from 1500 to 1700 °C of the post-combusting gas of CO will not influence on the post combustion itself.
- When analyzing the temperature in the flue (e.g. off-gas analysis equipment), it is really important to have a good control of the flue fan system, since the post combustion is so strongly dependent on the leakage air.

Considering these four supplements, it can be concluded that:

- In top-blown systems, such as VOD, BOF/LD and sometimes AOD processes, a good understanding of the nozzle geometry is important in order to have a high bowing efficiency. Besides, temperatures and chamber pressures are also important parameters with respect to the process control.
- The temperatures in BOF/LD and AOD processes have little effect on the post combustion reactions since the temperature range of both processes is so high that the post combustion reactions are not limited by the gas temperature.
8. Future Work

The flow properties of two De Laval nozzles from production were investigated through mathematical modeling. The post combustion in a BOF/LD converter and an AOD flue was also studied using mathematical modeling. From the current research results, it was found that the lack of realistic boundary conditions made the direct comparison between the modeling results and industrial results difficult. It should be mentioned that the current models can be only regarded as the first step toward more comprehensive models. In order to develop the research work, the following points are suggested as future work:

- Continuously optimize the mathematical models with different turbulence models, combustion models and radiation models.
- Numerical modeling should be used to find the optimal nozzle geometry for a VOD operation with respect to the entire pressure cycle. This also proposes a possibility of the usage of geometry-changing nozzles in real VOD vessels.
- Verification methods should be developed to perform measurements towards a gas flow by use of physical modeling.
- For the BOF/LD converter, in addition to the continuous quality improvement for the mathematical model, an off-gas flue and a real oxygen lance nozzle can be attached to the converter model to further investigate the off-gas parameters.
- For the AOD flue, different gas proportions for different decarburizations stages should be investigated.
9. References


[34] I. Sumi, Y. Kishimoto, Y. Kikuchi and H. Igarashi: ISIJ Int., Vol. 46 (2006), No. 9, pp. 1312-1317


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