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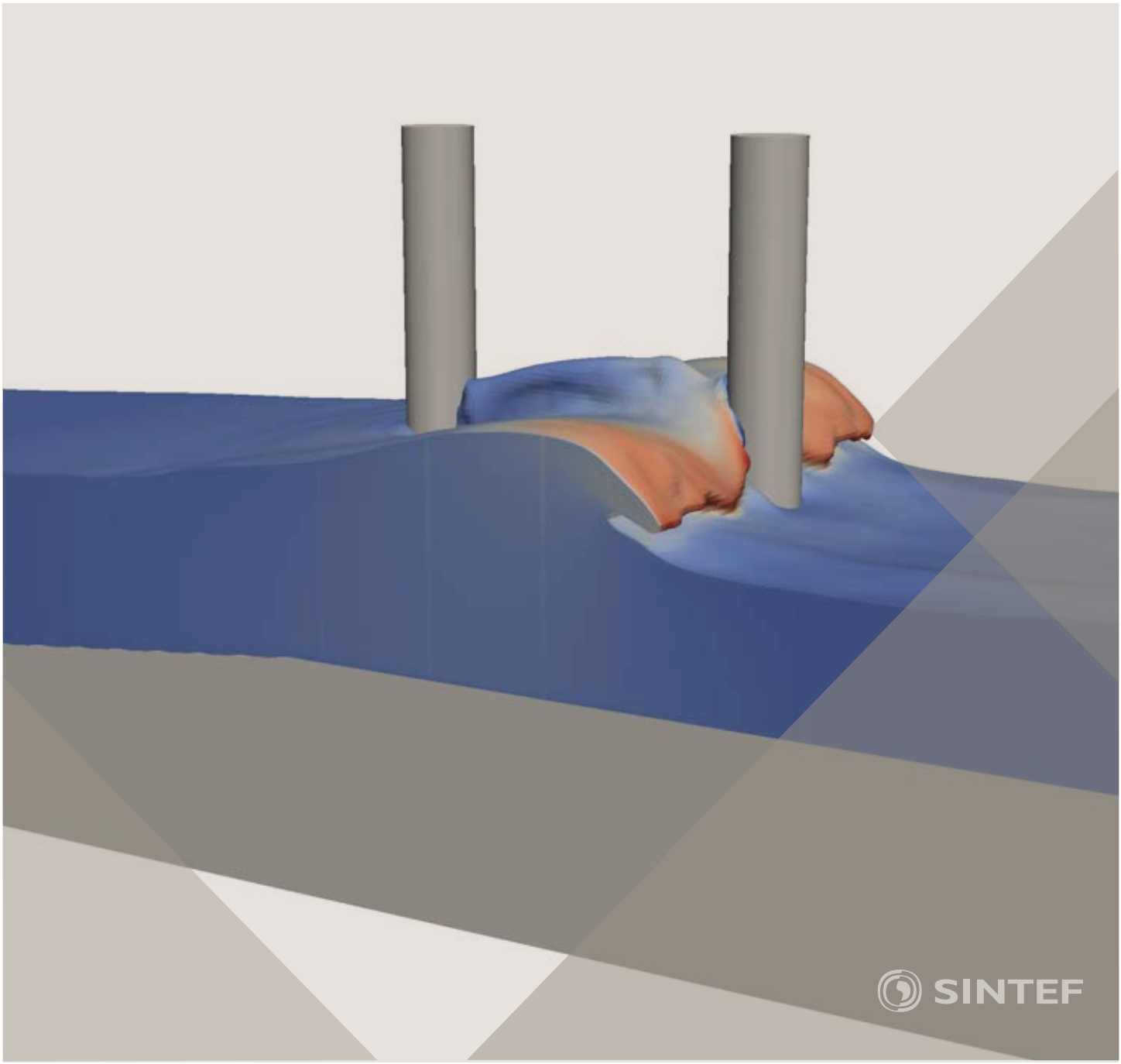
Proceedings of the 12th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries

Progress in Applied CFD – CFD2017



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Editors:
Jan Erik Olsen and Stein Tore Johansen

Progress in Applied CFD – CFD2017

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PREFACE

This book contains all manuscripts approved by the reviewers and the organizing committee of the 12th International Conference on Computational Fluid Dynamics in the Oil & Gas, Metallurgical and Process Industries. The conference was hosted by SINTEF in Trondheim in May/June 2017 and is also known as CFD2017 for short. The conference series was initiated by CSIRO and Phil Schwarz in 1997. So far the conference has been alternating between CSIRO in Melbourne and SINTEF in Trondheim. The conferences focuses on the application of CFD in the oil and gas industries, metal production, mineral processing, power generation, chemicals and other process industries. In addition pragmatic modelling concepts and bio-mechanical applications have become an important part of the conference. The papers in this book demonstrate the current progress in applied CFD.

The conference papers undergo a review process involving two experts. Only papers accepted by the reviewers are included in the proceedings. 108 contributions were presented at the conference together with six keynote presentations. A majority of these contributions are presented by their manuscript in this collection (a few were granted to present without an accompanying manuscript).

The organizing committee would like to thank everyone who has helped with review of manuscripts, all those who helped to promote the conference and all authors who have submitted scientific contributions. We are also grateful for the support from the conference sponsors: ANSYS, SFI Metal Production and NanoSim.

Stein Tore Johansen & Jan Erik Olsen

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CONTENTS

VALIDATION OF A RAPID SLAG VISCOSITY MEASUREMENT BY CFD

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ABSTRACT

Slag viscosity is an important property in daily process practice, as well as for modelling flows in metallurgical processes accurately. Measuring slag viscosities is a challenging task, and usually requires a specific high-temperature furnace set-up, which needs to be gas tight and still allow for e.g. torque measurements on a well-aligned rotating viscometer spindle. The inclined plane technique is an alternative, requiring little time and no complex instruments. A slag sample, heated in a crucible or from an industrial furnace, is poured onto an inclined steel plate, and runs down while solidifying, to form a ribbon of a certain length. The ribbon length has been experimentally proven to be correlated rather accurately to the high temperature viscosity. However, as the viscosity increases sharply during cooling, the ribbon length should also depend on the temperature dependence of the viscosity. To study these effects, a CFD model has been built in this project. This model also allows to understand the effect of slag weight, steel plate thickness, temperature, and inclination, which could influence the results. The model is based on a VOF description for the slag surface and uses accurate heat capacity and viscosity functions based on thermodynamic calculations. This approach allows to increase the reliability of the fast slag viscosity measurement.

Keywords: CFD, metallurgy, viscosity, slag

NOMENCLATURE.

Greek Symbols

α Angle of inclined plane, [°] or Volume fraction, [-].
Γ Diffusion coefficient, [m²/s].
η Viscosity, [Pa s] or [Poise].
ρ Mass density, [kg/m^3].
ϕ A conserved scalar

Latin Symbols

A Parameter of Wayman-Frenkel relationship, [Pa.s/K].
B Parameter of Wayman-Frenkel relationship, [K].
c_p Heat capacity, [J/kg.K]
L Ribbon length, [m].
$\dot{m}_{pq}$ Mass transfer from phase p to phase q, [kg/m³].
n Number of phases, [-].
S_ϕ A source term of conserved scalar ϕ
T Temperature, [K] or [°C].
v Velocity, [m/s].
X Molecular fraction, [-].

Sub/superscripts

p Phase p.
q Phase q.

INTRODUCTION

Within the metal producing industry, slag control is often instrumental for the efficiency of the production. Controlling the slag composition is key to have a good metal yield in any smelting or refining activity (Reis, 2014). Next to composition, which defines the chemical equilibria of reactions, also the physical property viscosity has a direct impact on the production process. To remove a slag from the furnace, it is commonly tapped as a liquid. This procedure requires a slag with a low viscosity, allowing it to flow. A low viscosity has the additional advantage that the metal-slag reactions will encounter less kinetic difficulties, e.g. due to better mixing. However, a low viscosity slag with a high reactivity towards the furnace lining could accelerate the refractory wear (Chen, 2016). Viscosity is thus a very important, although hard to measure, property of the slag. This research project explores the possibilities of an experimental measurement called the inclined plane technique. The measurement is tested in a lab environment and is modelled by CFD, which allows for a sensitivity analysis. It is clear that when this technique is installed in an industrial environment, some initial validation is needed. From this study with both CFD and experiments, a first indication of the most influential parameters is obtained.

MODEL DESCRIPTION

Inclined plane technique

The inclined plane technique is a relatively simple and robust set-up. This gives the opportunity to use the measurement both in industrial as well as in lab environments. In this method, a certain amount of a slag is placed in a graphite or platinum crucible and heated to a temperature above the melting temperature. Industrially, it can be taken directly from the furnace or from the slag stream during tapping. The molten slag is then quickly poured onto a V-shaped stainless steel plate, set at a certain inclination (the inclined plane).

The slag flows down the inclined plane until it solidifies and forms a slag ribbon. The experimental set-up used by Dey and Riaz (2012) is shown in Figure 1. The length of the slag ribbon (L) has been found to be a exponentially related to the viscosity (η) (Dey, 2012; Mills, 1997). To estimate the slag viscosity by the Inclined Plane Method, a (L, η) curve must be constructed first. The (L, η) curve can be constructed experimentally by measuring the ribbon length of slags with known viscosities. Subsequently, when the (L, η) curve is available, a slag sample with unknown viscosity is poured and then its ribbon length is measured. With the measured ribbon length and the available (L, η) curve, the viscosity of the studied slag can be estimated. This gives a quantitative technique to evaluate the flow properties of slag.

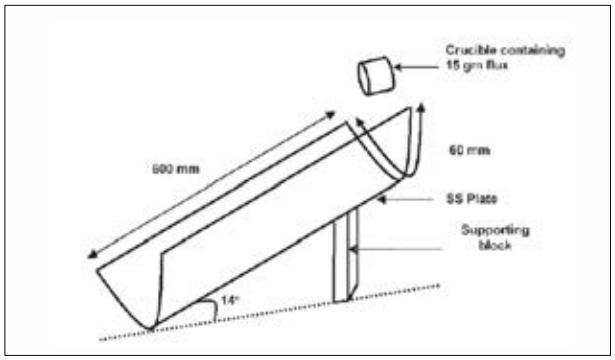

Figure 1: Schematic representation of set-up for the inclined plane technique (After Dey, 2012)

The experimental technique was evaluated and proven to be a fast technique with a good repeatability of the results. In this experimental phase, the angle of the set-up, the amount of material and initial temperature were considered as parameters, as shown in Table 1. Complementing this, the aim of the CFD calculations is to evaluate the robustness of the technique towards the experimental parameters, and towards parameters which are harder to vary experimentally, such as the thickness of the inclined plate, the temperature dependence of the viscosity and the initial temperature of this plate.

Table 1: Experimental parameters

Series	T(°C)	Inclination	Mass of slag	Composition
1	1300	12.5°	15g	1-6
2	1350	12.5°	15g	1-6
3	1400	12.5°	15g	1-6
4	1300	25°	15g	1-3
5	1300	12.5°	30g	1-3

Viscosity model

In literature, several models are described for the viscosity of a slag as a function of composition and temperature. In general, slags are formed by a solution of oxides and silicates. For the sake of viscosity, generally three types of oxides, namely acidic oxides, basic oxides and amphoteric oxides, are considered (Slag Atlas, 1995).

Figure 2: Picture of the experimental set-up

Acidic oxides such as SiO_2, P_2O_5, B_2O_3 possess stiff, highly covalent metal-oxygen bonds. SiO_2 forms tetrahedral anionic molecules of SiO_4^{4-} (silicate) which polymerize with each other to form more complicated polymer structures and even 3D networks, leading to high viscosities (Slag Atlas, 1995 and Kekkonen, 2012). With addition of basic oxides such as CaO, Na_2O, MgO with ionic metal-oxygen bonds, which do not require defined bond angles, the network breaks down, and consequently the viscosity of the slag decreases. The magnitude of the network-breaking effect depends strongly on the components and their proportions present in the slag. Amphoteric oxides, such as Al_2O_3, Fe_2O_3, may act either as a network former or a breaker, depending on the composition of the slag (Kekkonen, 2012).

The temperature dependence of slag viscosity is mostly expressed in the form of the Wayman-Frenkel relationship (Equation 1) in which A and B are viscosity parameters and T is the temperature in K.

Wayman-Frenkel relationship

$$\eta = AT\exp(\frac{B}{T}) \quad (1)$$

CFD model specifications

Geometry and mesh of 2D model

The flow of the liquid slag in a V-shaped gutter is simplified to a 2D geometry to decrease the calculation time. The third dimension is modelled as a symmetry plane which corresponds with an infinite long plate over which a wave of liquid slag flows. Clearly, this has consequences for the cooling of the slag which will be discussed further when comparing the 2D to 3D situation. For now, the aim is to verify the influence of some parameters on the length of the formed ribbon which can qualitatively be understood from the 2D case. The mesh contains 30668 quad elements. A small cell size of $2.5*10^{-7}$ m² and 2nd order upwind schemes are used to capture the strong temperature and viscosity gradients present. The steel plate is meshed as well to capture the heat transfer in the solid domain. The mesh dependency of the ribbon length is illustrated in Table 2. A variation of -6% in the final ribbon length is significant and indicates that mesh effects are present. However, these deviations are within the experimental error margin.

Table 2: Validation of mesh dependency

Series	Mesh elements [-]	Final ribbon length [m]
1	13137	0,1577
2	30668	0,1547
3	54627	0,1449

Governing equations

Modelling the inclined plane technique is a multiphase problem with steep viscosity and temperature gradients. By using the volume of fluid (VOF) approach only one set of continuity equations must be solved for each iteration (Ansys, 2017). In its most general form the conservation of a scalar can be written as in Equation 2 (Ferziger, 2002 and Versteeg, 2007).

General transport equation

$$\frac{\partial \rho \phi}{\partial t} + div(\rho \phi \mathbf{v}) = div(\Gamma grad \phi) + S_\phi \qquad (2)$$

with $\mathbf{v}$ the velocity vector, S_ϕ the source term of conserved parameter ϕ and Γ the diffusion coefficient. The conserved variable ϕ can be taken equal to 1, equal to the velocity in x, y, z direction or equal to the temperature. The conservation equations of mass, x-momentum, y-momentum, z-momentum or energy will be found respectively (Versteeg, 2007). Equation 3 gives as an example the continuity equation for mass conservation.

Continuity equation

$$\frac{\partial \rho}{\partial t} + div(\rho \mathbf{v}) = div(\Gamma grad(1)) + S_\phi = 0 \qquad (3)$$

Additionally, in the Eulerian VOF description the interface is tracked by solving an additional continuity equation of the volume fraction for one or more phases (Ansys, 2017). The continuity equation for phase q in a simulation with n phases is given in Equation 4 (Ansys, 2017).

$$\frac{1}{\rho_q}\left[\frac{\partial \rho_q \alpha_q}{\partial t} + div(\rho_q \alpha_q \mathbf{v}_q)\right] = \frac{1}{\rho_q}\left[\sum_{p=1}^{n}\left(\dot{m}_{pq} - \dot{m}_{qp}\right) + S_{\alpha q}\right] \qquad (4)$$

with $\dot{m}_{pq}$ being the mass transfer from phase p to phase q. The interface is reconstructed from the volume fractions. For this model the Compressive Interface Capturing Scheme for Arbitrary Meshes (CISCAM) is used due to its ability to cope with large differences in viscosity (Ansys, 2017).

Material properties and boundary conditions

The material properties used in the CFD model are given in Table 3 (Ansys, 2017 and Bale et al., 2016 and Slag Atlas, 1995). The slag properties correspond to the reference slag M1 of Dey and Riaz (2012).

Table 3: Material properties used for modelling

Property	Air	Slag	Steel
c_p [J/kgK]	1006	1273	502
ρ [kg/m³]	1.225	2580	8030
α [W/mK]	0.024	0.8	16.3
σ [N/m]	-	0.4 (with air)	-
η [Pa.s]	$1.78*10^{-5}$	UDF (see below)	-

The viscosity of the slag phase is implemented in Fluent 18.0 using a user defined function (UDF). The temperature dependence of the viscosity is calculated with the Riboud model. This model gives the coefficients of the Wayman-Frenkel relation based on the composition for the slag (Slag Atlas, 1995). These estimated coefficients are then used in the UDF to calculate the viscosity in each cell depending on the cell temperature. The viscosity calculated by the UDF is limited to 1000 Pa.s. This limitation is necessary to avoid the extreme gradients for lower temperatures. Without this limitation, the viscosities predicted by the Wayman-Frenkel equation cause the solver to diverge. This behaviour is observed for both the 2D and 3D situation. A limit of 1000 Pa.s is not expected to have an influence on the end result as the achieved solution displays no further movement of the slag.

The outer walls of the solid domain (steel plate) are modelled by a convection wall with a heat transfer coefficient of 15 W/(m^{2}K) and a free stream temperature of 21 °C. The outer walls of the fluid domain are set to a fixed temperature of 21 °C. In the contact area between liquid and solid, the temperatures are coupled. “No slip” boundaries are used on all boundaries of the fluid domain.

The initial parameters of the base case are given in Table 4. The inclination is implemented by the orientation of the gravity. This allows the inclination to be changed more easily because the world reference and mesh can remain the same. The initial slag area corresponds to a cross section of the 3D case with 15g of slag.

Table 4: Initial conditions of base case

Inclination	12.5°
Initial temperature of steel plate	21°C
Initial temperature of air	21°C
Initial temperature of slag	1300°C
Initial area of slag	$48.1*10^{-6}$ m²
Time step	0.0005s (except first 1000 iterations where it is 0.0001s)

In the experiments, the slag solidifies when it runs down the plate. In the simulations, the slag is said to be solidified when the slag ribbon length remains constant for at least one second.

RESULTS

Inclined plane technique test results

It is expected that the temperature of the liquid slag has a direct influence on the slag viscosity following the Wayman-Frenkel relation. In the experiments, it is indeed seen that a higher initial temperature results in a longer ribbon length (Figure 3). The compositions in Figure 3 correspond to earlier work by Dey and Riaz (2012). For all tested compositions, the influence of temperature seems to have an equal effect. From Figure 4, it is learned that the initial temperature has no influence on the relation between ribbon length and the viscosity, indicating that temperature information is not necessary to measure the viscosity with this technique. This means, the technique can be used to measure the viscosity at any experimental temperature, without knowing the temperature.

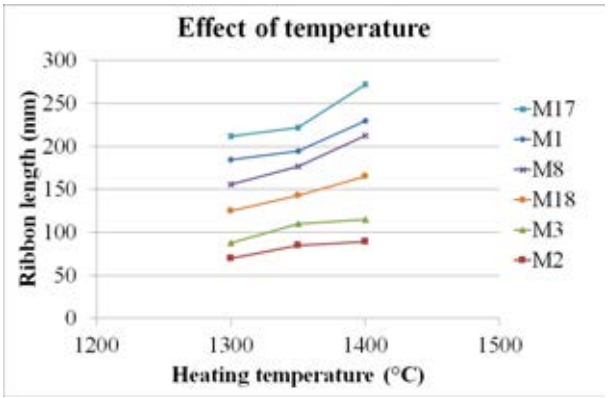

Figure 3: Increasing the initial temperature results in a larger ribbon length, corresponding to the viscosity dependence on temperature and composition

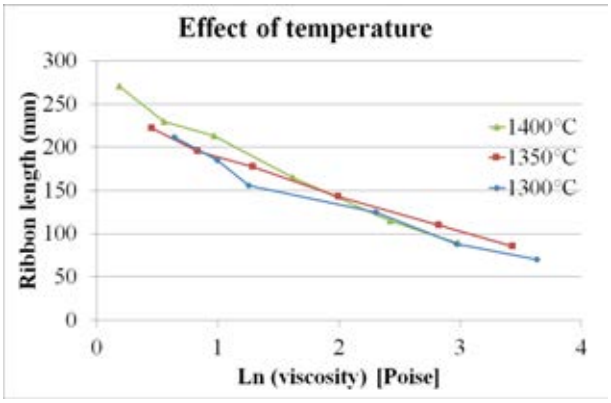

Figure 4: Ribbon length displays a linear relation with the logarithm of the viscosity over different initial temperatures

The second slag-related parameter for this test is the amount of material used for the inclined plane measurement. Obviously, when more material is present, a longer ribbon is expected. For three compositions, tests with both 15 g and 30 g are performed. An overview of the resulting ribbon lengths is given in Figure 5. These results indicate that a correction factor for the amount of slag will indeed be necessary. Roughly estimated from the limited number of experiments, doubling the weight of slag leads to a 50% longer ribbon. The amount of slag can be weighed after cooling, so correcting the length after the measurement is feasible in an industrial set-up. A calibration is needed and expected to be possible, but from the limited amount of trials in this test series, it is not yet clear how many data points are needed for an accurate weight correction.

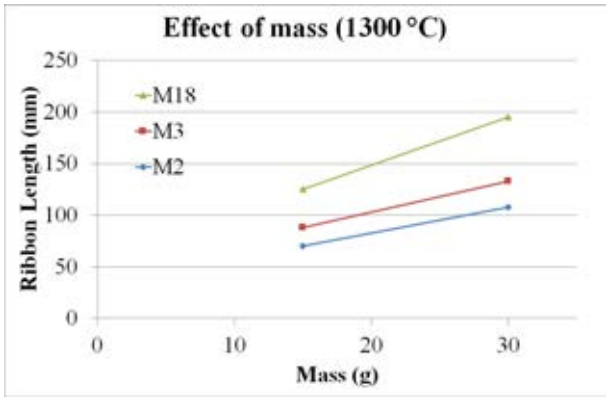

Figure 5: An increasing slag amount results in a longer ribbon

CFD model results

All results are compared to the base case as described earlier in the model specifications (Table 4). The flow of the base case is illustrated in Figure 6. The first frame, the red rectangle, illustrates the initial position of the slag phase. During the simulations, the slag will stream down the plate and form the slag ribbon. The last frame illustrates how the final slag ribbon looks like. This shape agrees with the experimental observed solidified slag ribbons. During the simulation, the temperature decreases, due to the contact with the steel plate. Consequently, the viscosity increases. The velocity of slag slows down due to this increasing viscosity. This can also be observed in Figure 7. In this figure, the length evolution of three different calculations is compared, in which the temperature dependence of the viscosity is changed as shown in Figure 8. The steeper the dependency of the slag viscosity on the temperature, the faster the velocity of the slag decreases, resulting in a shorter ribbon.

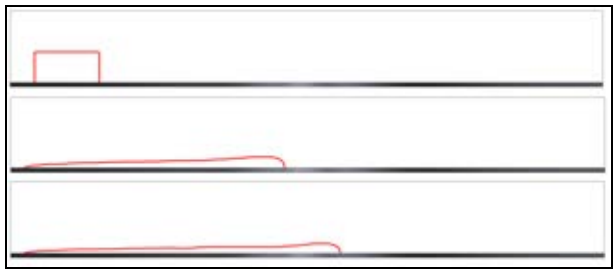

Figure 6: Contour evolution of the slag phase in the base case. From up to down: 0.0s, 0.5s and 1.0s

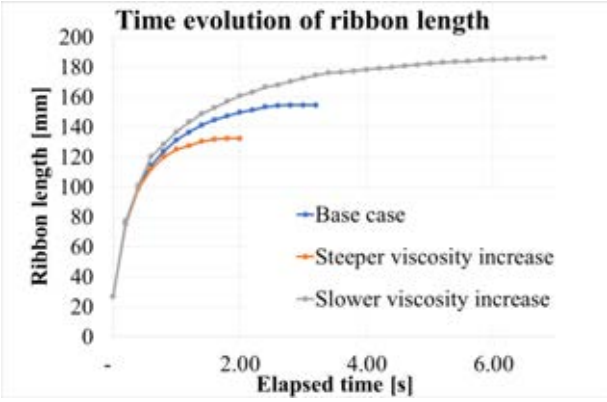

Figure 7: Time evolution of different temperature dependent cases

Figure 6 and Figure 7 prove that the maximum viscosity used in the UDF is sufficiently high to approximate the solidification. The ribbon length and shape of the slag phase all remain stable. For these length scales and forces, a liquid with a viscosity of 1000 Pa.s is practically solid.

Two types of parameters have been studied: set-up variations and material properties variations. The set-up variations include:

- increasing the inclination to 25°,
- increasing the initial temperature of the steel plate to 100 °C and 200 °C,
- increasing thickness of the steel plate to 5 mm,
- increasing the volume of slag by 59%, which corresponds to doubling a 3D cubic volume equally in all directions.

The material variations include:

- increasing/decreasing the slope of the Wayman-Frenkel relationship with a factor 2 while keeping the viscosity constant at 1300 °C (increased/decreased temperature dependency with the same start viscosity, dashed black lines in Figure 8),
- increasing the initial temperature of the slag to 1400 °C,
- doubling the initial viscosity with same temperature dependency (solid black line in Figure 8).

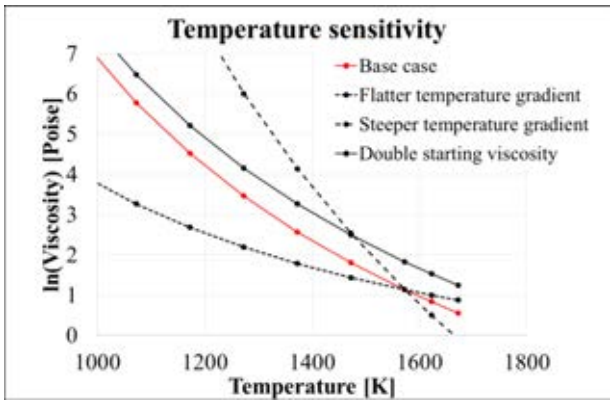

Figure 8: Temperature dependency of different cases. Red line is the base case scenario, the black lines represent changes in temperature dependency

The effect of the set-up parameters is summarized in Figure 9. By modelling the inclined plane, it can be concluded that the effect of both thickness and initial temperature of the plate are negligible for the final ribbon length. Consequently, doing sequential experiments, effectively increasing the initial temperature of the plate, will not largely influence the measured ribbon length. On the other hand, the angle of the plate and amount of material are to be calibrated for to obtain the actual viscosity from the ribbon length. In the model, the final length scales linearly with the amount of slag. This contradicts earlier experimental observations. This is due to neglecting the V-shape of the plate in the 2D model. In reality the system would react differently to an increasing amount of poured material. A 3D model seems prerequisite to correctly model the effect of a volume change.

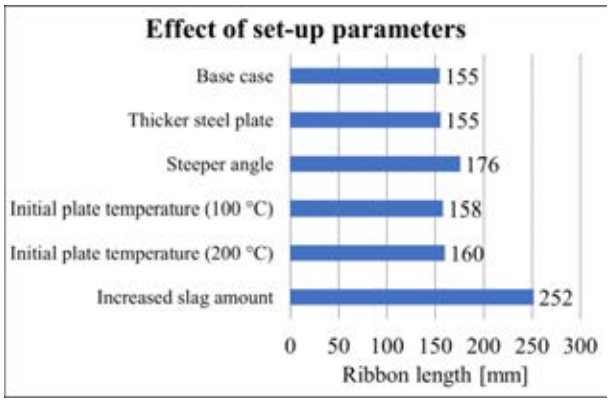

Figure 9: Effect of set-up parameters on ribbon length

The effect of the material property variations is summarized in Figure 10. The temperature dependency of the different cases is illustrated by Figure 8. Simulations with the same temperature dependency follow the experimentally observed linear relationship of Figure 4. However, Figure 10 indicates that the linear relationship between the final ribbon length and the viscosity is not depending on only the starting viscosity. In fact, the viscosity dependency on the temperature could cause serious deviations on the experimentally observed linear relationship.

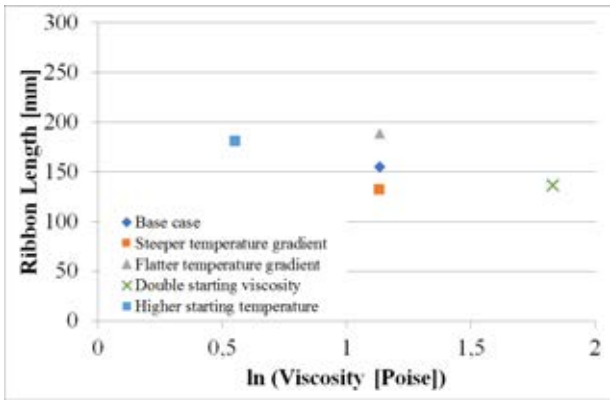

Figure 10: Effect of viscosity parameters on ribbon length

The inclined plane method therefore has the most comparative value if the temperature dependency for

different samples is similar. This will be the case in an industrial set-up where the same type of slag is always produced. This is also valid for the tested samples, for which the change in viscosity as a function of temperature is given in Figure 11. The Riboud model theoretically predicts the temperature dependency from the composition of the slag (Slag Atlas, 1995):

$$B = 31140 - 23896X_{CaO} - 46356X_{CaF_2} - 39159X_{Na_2O} + 68833X_{Al_2O_3} \quad (5)$$

with X being the molecular fraction of the different compounds. Consequently, the predicted values will change rather limited unless the molar fraction of aluminium is largely affected. For example, an increase of the molar fraction of alumina by 10% in the base case (with a decrease of calcium fluoride) will only lead to a change in temperature dependency of around 3%.

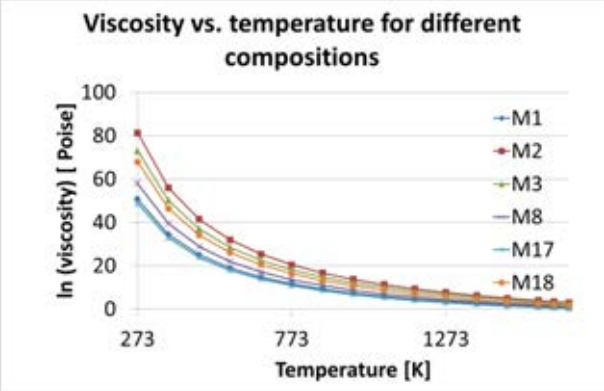

Figure 11: Viscosity dependencies on temperature for the different composition of the test campaign

Future Research

To validate the current model to the experimental data and to predict absolute ribbon lengths, a 3D model is necessary. Certain effects where neglected in the 2D model such as the stream of the slag to the centre of the gutter, a larger contact area with the steel plate, and a larger heat sink in the steel plate next to the sample. These effects make any quantitative and predictive model impossible when working in 2D.

Unfortunately, artefacts exist when working with high viscosity liquids in Fluent 18.0 with the current approach. The slag phase does not fully make contact with the metal plate, but a certain volume fraction of air remains present at the interface. This distorts the heat transfer. Currently this problem can also be recreated in 2D by increasing the viscosity. The effect is not present in the simulations used in this paper.

In Figure 12 a first result of the 3D model is given. Although the shape and movement of the slag look realistic, some optimisation steps are necessary to increase the credibility of the result, especially concerning the heat transfer at the boundary conditions.

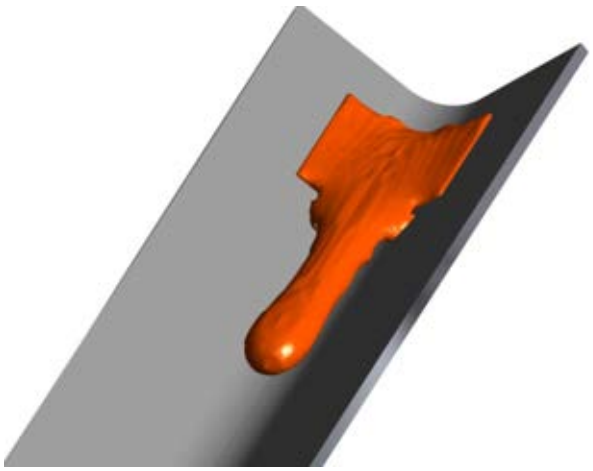

Figure 12: Illustration of 3D model

CONCLUSION

In this work, CFD was used to complement the outcome of a testing campaign to validate the inclined plane set-up as a technique to measure slag viscosity. CFD allowed to verify the influence of several material and set-up parameters which are difficult to test in lab environment. It was concluded that the inclined plane technique is a reliable and robust technique, which looks promising to be used in an industrial environment for fast measurements of viscosity. CFD showed that sequential testing does not pose too large deviations due to heating of the equipment and it proved that if the composition changes are not too large, a quantitative comparison of ribbon lengths and related viscosities is possible. Given the positive outcome of this study, further effort will be done to calibrate the measurement to make it available for industry.

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