

Full-Scale Large Eddy Simulation of a 185 t Ladle Optimizing a Hybrid Eulerian Grid and a Discrete Bubble Mapping Approach

Tim Haas,* Christian Schubert, Moritz Eickhoff, and Herbert Pfeifer

Numerical simulation is a vital tool for the continuous improvement of all steelmaking processes. In previous works, the authors have dedicated different approaches to optimize modeling of fluid flow in the ladle. This includes a sensitivity analysis of validation techniques, assembling of a validation database, and a model optimization on the water model scale. Herein, the final part of this project is presented at which the optimized model is scaled to the real process. Associated problems are identified and solutions are proposed. To achieve a tradeoff between large eddy simulation (LES) grid requirements and current computational capacities, a hybrid meshing strategy is optimized. To overcome the intrinsic drawbacks of the Euler–Lagrange model, a mapping approach for phase decoupling is implemented and made publicly available on GitHub. The upscaling of semi-empiric submodels is discussed. Good agreement with experimental mixing time measurements is found, indicating the success of upscaling. A first time-averaged flow field of a full-scale 185 t ladle with the LES model is presented. Due to the extreme computing requirements, these results may currently be used as a benchmark, but the trend toward increasing computing capacities may make LES models state of the art in the future.

times and lower energy consumption must be ensured. From a social point of view, environmental aspects are increasingly gaining importance. The steel industry must respond to these growing challenges by continuously improving all processes and equipment. Since measurements in metallurgical aggregates are quite cumbersome, numerical models have proven to be a vital tool for these continuous improvements.

Ever since the first numerical model of a ladle was introduced by Szekely et al.,^[1] more than 200 flow models have been proposed. The reviews by Mazumdar and Guthrie^[2] and more recently by Liu et al.^[3] summarize the most important developments. Due to significantly increasing computational capabilities and improved mathematical models, there is a distinct trend toward more complex and accurate models. Turbulence has been computed almost exclusively using the Reynolds-Averaged Navier-Stokes (RANS) standard k- ϵ model except for some very early

1. Introduction

The ladle furnace is the most important aggregate in secondary steelmaking. Its metallurgical tasks include melt transport, addition and homogenization of alloying elements, adjustment of a homogeneous casting temperature, and the removal of nonmetallic inclusions. However, the demands on process control are constantly increasing. Customers are expecting steadily decreasing levels of nonmetallic inclusions. Economically, shorter batch

works. It is only in recent years that large eddy simulation (LES) based models are gaining importance. Li et al.^[4,5] and Haas et al.^[6,7] showed on the water model scale that transient phenomena can be represented and higher accuracy is achieved compared to RANS models. Other works used the LES model for local phenomena such as slag emulsification.^[8–10] A first full-scale LES model was presented by Li and Pistorius,^[11,12] though this work focused on transient phenomena, not averaging the flow field. Thus, the computed physical time was low.

For gas bubble modeling, the early quasi single-phase model has been almost completely replaced by the Euler–Euler (E-E) or Euler–Lagrangian (E-L) model. In particular, the latter has found the most application in recent years. In some cases, the bubble's phase boundary has been modeled directly with the volume of fluid (VOF) model.^[13] However, the numerical grid resolution is much too low for an appropriate computation of the phase boundary.^[14] The E-L approach has some model intrinsic drawbacks like that the bubbles are considered as point masses and do not occupy any volume on the Eulerian grid. Two different methods have been proposed to overcome this. Chen et al.^[15] coupled the Lagrangian and the Eulerian phase by adjusting the local Eulerian properties in dependence of the void fraction computed by the Lagrangian bubbles. However, that method, which might be called E-L-mixture coupling, might cause stability issues since

T. Haas, C. Schubert, M. Eickhoff, H. Pfeifer
Department for Industrial Furnaces and Heat Engineering
RWTH Aachen University
Kopernikusstraße 10, D-52074 Aachen, Germany
E-mail: haas@iob.rwth-aachen.de

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it produces steep density gradients. In addition, bubbles still need to be small compared to the Eulerian grid. Li et al.^[16] proposed a E-L-VOF coupling at which bubbles smaller than the grid are modeled by the Lagrangian approach and are transformed into a VOF phase in case the bubble diameter exceeds the grid spacing. Liu et al.^[17] employed the same approach. However, the grid resolution is far too coarse to appropriately model the VOF phase.

Despite the trend toward more complex and more accurate models, a common feature of all presented models is that good agreement with validation data was reported. The discrepancy between more elaborate models on the one hand and the same “good” results on the other underlines the need for more accurate and detailed validation. With the goal of a structured optimization of numerical models, the authors of this work met this by different approaches.

First, a comprehensive sensitivity analysis of the most frequently used validation methods was carried out.^[18] It could be shown that a structured optimization of numerical models is only possible by combining flow measurements and bubble swarm tracking. Since this information cannot be determined accurately enough in the real process, this implies that the numerical model should first be optimized on a water model scale.

For this purpose, a new measurement method, BubCNN, was developed to identify gas bubbles on high-speed videos using convolutional neural networks (CNNs).^[19] In combination with a tracking algorithm, not only the bubble size but also the bubble rising velocity could be determined. These measurements were combined with particle image velocimetry (PIV) in the single-phase and multiphase regions to form a validation database.^[20] In addition to a comprehensive experimental documentation, this database includes a detailed uncertainty estimate of the employed measurement techniques. In order to assess the model’s accuracy using all validation data available in the database simultaneously and to use a quantitative rather than a qualitative metric, a validation score was derived. The overall score is composed of various subscores that reveal additional optimization potentials:

1.1. Toroid (Max. Score: 10)

The “toroid” subscore compares the predicted and measured position of the point where the radial flow near the surface is redirected into a downward axial flow. Thereby, the prediction accuracy of the general flow structure and the position of possible dead zones are assessed.

1.2. Means (Max. Score: 20)

The “means” subscore compares the numerically calculated mean values of the velocity components and their fluctuation with the measured values on the plane of symmetry. This evaluates the extent to which the numerical model predicts the strength of the flow and thus is able to predict mixing, refractory wear, or removal of inclusions.

1.3. Monitors (Max. Score: 40)

The “monitors” subscore is a refinement of the previous subscores. Here the flow direction and the velocity components, as well as their fluctuation are compared at eight defined control points on the plane of symmetry as well as on the plane perpendicular to it. Thereby conclusions can be drawn about the prediction accuracy of the flow structure and the flow velocity.

1.4. Bubbles (Max. Score: 15)

The “bubble” subscore compares the calculated and measured mean bubble rising velocity and the width of the bubble plume at five different heights. It allows a detailed optimization of all bubble-related submodels that play a major role in the formation of the flow as well as heat and mass transfer in the ladle.

1.5. Plume (Max. Score: 15)

The “plume” subscore evaluates the prediction accuracy of the numerical model with respect to the axial velocity and the width of the flow profile of the continuous phase in the plume zone. Like the bubble subscore, it allows an optimization of all bubble-related submodels.

With this validation score, the numerical model was first optimized for the water model.^[7] An important result was that the accuracy is significantly higher when the LES turbulence model is used. In this case, the anisotropy of turbulence in the bubble column can be represented which increases the accuracy significantly.

In this work, the final step of this structured optimization is presented. Here, the numerical model optimized for the water model is scaled to the real process. However, there are further sources of inaccuracy as well as modeling problems associated with this upscaling which are discussed later. Associated challenges are finding a tradeoff between grid requirements of the LES model and current computational capacity, overcoming the intrinsic problems of the E-L method on fine grids by proposing a two-way coupling between Eulerian and Lagrangian reference frames, discussing the transferability of semi-empirical models from the air–water system to argon–steel and finally verifying the upscaling by suitable plant data.

2. Numerical Model

2.1. Geometry

The modeled system is a 185 t ladle, operated at an argon flow rate of 200 NL min^{−1}. Its dimensions are given in **Figure 1**. Employed fluid properties are summarized in **Table 1**. The system is considered isothermal. Numerical models that investigated the temperature distribution in the melt suggest that this assumption is reasonable. Mukhopadhyay et al.^[21] reported a maximum temperature gradient of 2 °C after 1.5 min of stirring that totally vanished after 3 min. Ganguly and Chakraborty^[22] reported that a argon flow rate of 0.5 NL min^{−1} is sufficient to remove any thermal stratification in a 105 t ladle. The total energy loss of the melt during ladle treatment is also neglected, since the

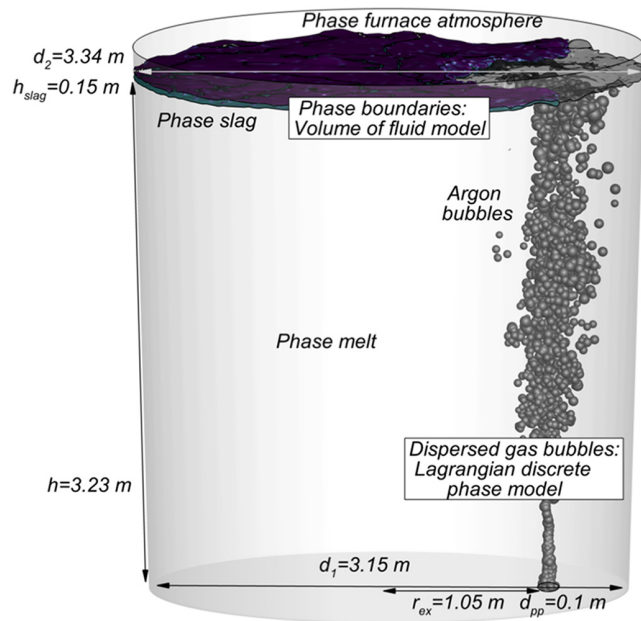


Figure 1. Dimensions, phases, and modeling approaches of the numerical model.

Table 1. Employed physical properties.

			Melt	Slag	Furnace [Atmosphere]
Temperature	T	°C	1600	1600	1600
Density	ρ_F	kg m ⁻³	6932	2700	1.2
Viscosity	μ_F	kg ms ⁻¹	5.06×10^{-3}	1	1.78×10^{-5}
Surface tension	σ	N m ⁻¹	1.5	1.5	

calculated time is short enough so that this overall temperature loss is very small. A no-slip boundary condition is applied to all walls, and the opening is modeled by a wall with a no-shear condition. For the computations, a structured hexahedral grid is created. Specifics are discussed in Section 3.

The ladle comprises three continuous phases and one dispersed phase which requires two different multiphase modeling approaches. The continuous phases, steel, slag, and furnace atmosphere are modeled with the Eulerian approach. Their phase boundaries, indicated by a volume fraction F_n in the range between 0 and 1, are dynamically modeled with the VOF interface tracking method^[23]

$$\frac{\partial F_n}{\partial t} + \frac{\partial}{\partial x_i} (F_n u_i) = 0 \quad (1)$$

In cells that contain a phase boundary, the effect of surface tension is modeled by an additional source term in the momentum equations.

The conservation equations for the continuous Eulerian phases are discretized by the nondiffusive bounded central difference scheme.

2.2. Bubbles

The dispersed argon bubbles are modeled with the E-L approach. The bubbles' trajectories are computed by a coupled solution of Equation (2) and (3) by a fifth order Runge Kutta scheme.

$$\frac{\partial x_B}{\partial t} = u_B \quad (2)$$

$$\begin{aligned} \frac{\partial u_B}{\partial t} &= \frac{1}{m_B} \sum_i F_{B,i} \\ &= \underbrace{g V_B (\rho_F - \rho_B)}_{F_B} + \underbrace{\frac{1}{2} c_D \rho_F \frac{\pi d_B^2}{4} (u_B - u_F)^2}_{F_D} \\ &\quad + \underbrace{c_L \frac{\pi d_B^3}{6} \rho_F (u_B - u_F) \times (\nabla \times u_F)}_{F_L} + \underbrace{c_{VM} \rho_F V_B \left(\frac{du_F}{dt} - \frac{du_B}{dt} \right)}_{F_{VM}} \end{aligned} \quad (3)$$

As can be seen from Equation (3), the bubble trajectories are governed by a force balance that include the buoyancy force F_B , the drag force F_D , the lift force F_L and the virtual mass force F_{VM} . These forces are determined by fluid and bubble properties and the drag coefficient, c_D , lift coefficient c_L , and the virtual mass coefficient c_{VM} . In the water model study,^[7] it was found that most accurate results are obtained by employing the drag coefficient model for fully contaminated systems, Equation (4), by Tomiyama et al.,^[24] the lift coefficient model, Equation (5), by Tomiyama et al.^[25] with the expansion by Frank et al.^[26] and a constant virtual mass coefficient of 0.5.

$$c_D = \max \left[\frac{24}{Re_B} \left(1 + 0.15 Re_B^{0.687} \right), \frac{8}{3} \frac{Eo}{Eo + 4} \right] \quad (4)$$

$$c_L = \begin{cases} \min[0.288 \tanh(0.121 Re_B; f(Eo_d))] Eo_d \leq 4 \\ f(Eo_d) & 4 < Eo_d \leq 10 \\ -0.27 & Eo_d > 10 \\ f(Eo_d) = 0.00105 Eo_d^3 - 0.0159 Eo_d^2 + 0.474 \end{cases} \quad (5)$$

In Equation (5), Eo_d is the modified Eotvos number that considers the deformation of larger bubbles into ellipsoids rather than spheroids

$$Eo_d = \frac{g(\rho_F - \rho_B) d_h^2}{\sigma} \quad (6)$$

To estimate the deformation, Tomiyama et al.^[24] proposed to use the correlation by Wellek et al.^[27]

$$d_h = d_B (1 + 0.163 Eo^{0.757})^{1/3} \quad (7)$$

This model was originally derived for liquid droplets though have shown to be suited for contaminated bubbles as well. Whether it describes bubble deformation in liquid steel is difficult to assess as will be discussed in the subsequent chapter. Bubbles are released with a log-normal diameter distribution between 10 and 50 mm and a mean of 25 mm into the computational domain. The real bubble size distribution in the melt is largely unknown and is a major source of model uncertainty in

upscaling the model. It is discussed extensively in the next chapter. Some previous experimental studies^[28,29] suggest that bubble coagulation and breakup have an influence on the flow. However, the governing mechanisms of coagulation and breakup are not fully understood and still require additional research, especially in liquid metals.^[30] Thus, these phenomena are not considered in the presented model as the uncertain of such empiric submodels are considered too high at this stage.

On their rising path, the bubbles grow slightly, while its density decreases because of a declining static pressure according to

$$d_B(z) = d_{B,0} \left(\frac{\rho_F g H_{\text{Fill}} + p_0}{\rho_F g (H_{\text{Fill}} - z) + p_0} \right)^{1/3} \quad (8)$$

$$\rho_B(z) = \rho_{B,0} \frac{\rho_F g (H_{\text{Fill}} - z) + p_0}{\rho_F g H_{\text{Fill}} + p_0} \quad (9)$$

Implemented by a user-defined function (UDF) described in detail later, all bubbles are removed from the computational domain as they reach the phase boundary of furnace atmosphere, which is indicated by an atmosphere volume fraction F_n above 0.25.

The momentum exchange between bubbles and fluid is modeled by an additional volume force in the momentum conservation equations

$$F_{\text{Ex}} = \sum_i F_{d,i} \dot{m}_B \Delta t \quad (10)$$

However, coupling between the bubbles and the fluid properties is one of the major scaling problems, since the bubbles are large compared to the grid width. The solution for that problem is discussed in the next chapter in detail.

2.3. Turbulence

In the previous optimization of the numerical model on the water model scale,^[7] it was shown that the accuracy can be significantly increased when the LES turbulence model is employed. In this model, originally proposed by Smagorinsky,^[31] the Navier Stokes equations are filtered using a spatial low-pass filter. The filtered parts of the turbulence spectrum are directly modeled, while the remainder, the smaller scale turbulences that tend to be more isotropic in nature, are modeled with a subgrid model. In implicit filtering, which is used by Ansys Fluent and most commercial solvers, no explicit filter function is used, but the filtering is maintained implicitly via the discretization of the Navier Stokes equations resulting in Equation (11)

$$\frac{\Delta(\rho u_i)}{\Delta t} + \frac{\Delta(\rho u_i u_j)}{\Delta x_j} = -\frac{\Delta p}{\Delta x_i} + \frac{\Delta}{\Delta x_j} \left[\mu \left(\frac{\Delta u_i}{\Delta x_j} + \frac{\Delta u_j}{\Delta x_i} - \frac{2}{3} \delta_{ij} \frac{\Delta u_k}{\Delta x_k} \right) \right] + \rho f_i \quad (11)$$

However, this approach leads to the fact that on grids larger than the Kolmogorov length scale the energy dissipation from large eddies to eddies smaller than the grid is not sufficiently represented, i.e., unphysically little energy is dissipated. Therefore, a model is needed that approximates the energy dissipation of the subgrid scale eddies. Commonly, the dissipation

is considered by the subgrid Reynolds stresses that are added to Equation (11). In the previous study,^[7] it was found that the dynamic Smagorinsky model, Equation (12), is slightly more accurate than the one-equation model by Deardorff.^[32] Following the mixing-length concept, Smagorinsky^[31] proposed for the turbulent viscosity

$$\mu_{\text{sgs}} = \rho_F C_s^2 \Delta^2 \sqrt{S^2} \quad (12)$$

Though it is the most often employed subgrid model, this static Smagorinsky model has two decisive disadvantages. First, the model constant C_s must be defined a priori. Its value can vary greatly depending on the flow and is fundamentally different in multiphase zones.^[33] Another disadvantage is that the Smagorinsky model is a pure sink for energy, which is only true in the statistical mean. Locally, smaller vortices can transfer their energy to larger scales, known as backscattering. In this work, an approach that eliminates these two disadvantages is used, the dynamic subgrid model by Germano modified by Lilly.^[34] Here, two filter operations are performed with different filter width. The first filter width is the grid width and the second usually twice the grid width. From this, the energy exchange between the scales can be approximated and thus the model constant C_s can be dynamically adapted locally. It can also become negative that takes the backscatter effect into account.

2.4. Numerical Details

The time step size is determined by the Courant–Friedrichs–Lewy (CFL) criterion

$$\text{CFL} = \frac{\Delta t u_{\text{max}}}{\Delta x_{\text{min}}} < 1 \quad (13)$$

That implies that the time step size is determined by the plume zone where the velocity and the grid resolution are highest. After grid optimization, described in the next section, a time step size of 0.002 s is used. The simulations are carried out using Ansys Fluent 2019 R3. After 90 s, the flow is considered to be in a quasi-stationary state and sampling for averaging is started. The average is computed based on 150 s physical computation time. The computation runs on a cluster that includes 64 cores (2 × AMD EPYC 7502 32-Core Processor, 512 GB RAM). Still, the whole computation takes about 9 months.

3. Upscaling Challenges

By the parameter study in the water model,^[7] optimal submodels were found to reproduce the validation data numerically. However, a direct transfer of the water model's numerical model to the industrial scale ladle cannot be done. There are three major challenges that need to be considered: the computational costs, the opposing grid requirements of the E-L multiphase model and the LES turbulence model, and the scaling of semi-empirical bubble closures. Finally, it is difficult to verify the accuracy of upscaling.^[18] These different aspects and solution strategies are discussed later.

3.1. Grid Optimization

Due to a scaling factor of $\lambda = 0.2$, a fine grid could be employed in the water model study. For the industrial scale, however, maintaining the same resolution would increase the computational costs by a factor of about 125. This exceeds memory of most facilities and takes far too long runtimes for any practical relevance. Therefore, a fine resolution like in the water model is not feasible. Instead, a hybrid meshing approach has to be found, which allows a high accuracy and at the same time reasonable computing times. Here, four different zones in the ladle must be distinguished.

3.1.1. Plume

High turbulent intensity and the highest flow velocities occur in the plume zone, so that the grid needs to be very fine. At the same time, this zone determines the time step size. In the water model study, it was found that a resolution of about 4 mm is sufficient to obtain a high accordance with validation data.

3.1.2. Phase Boundaries

At the free surface, the flow direction is changed several times and high flow velocities and gradients occur. In addition, for a realistic resolution of the phase boundary, the VOF model requires a certain resolution.

3.1.3. Near-Wall

Unlike RANS models, the LES model does not have a wall law. Therefore, the near-wall zone must be resolved very finely. However, the theoretical requirements of $y^+ = 1$ cannot usually be met. Since the wall friction plays only a minor role for the fluid flow in the ladle, the above criterion does not necessarily have to be met.

3.1.4. Flow

The bulk flow zone takes up the largest volume in the ladle and is characterized by a relatively slow, less turbulent flow. Thus, a grid coarsening might be applied.

A problem in finding an optimal grid resolution is that with implicitly filtered LES it is not possible to distinguish between model and discretization errors. This implies that, in contrast to RANS, there is no grid-independent LES solution because this would be a direct numerical simulation (DNS).

To determine the minimum grid requirements in the different zones, there is an a priori and an a posteriori approach. With the a priori approach, a RANS calculation is performed first. From this calculation, the turbulent length scale l_0 at which turbulence production equals its dissipation can be derived from the turbulent kinetic energy and dissipation transport equations. To model about 80% of the turbulence spectrum directly, a grid width of $\Delta x \sim l_0/5$ should be employed. **Figure 2** shows the turbulent length scale from a RANS simulation of the water model as a contour plot (a) and on isolines (b).

The a priori estimate suggests that the grid in the bulk zone can be up to $\Delta x \leq 50$ mm. The resolution in the plume zone depends on the height and reaches from about $\Delta x \approx 1$ mm in the vicinity of the injector to $\Delta x \approx 20$ mm close to the surface. The free surface seems to require no special refinement in comparison to the bulk flow, whereas the near-wall resolution should be $\Delta x \leq 1$ mm.

A problem with this method is that it is strictly speaking only valid for single-phase flows and isotropic turbulence. For multiphase flows, the problem arises that the turbulence model not only influences the strength of the flow but also the structure of the flow field.

For the a posteriori approach, a LES calculation is first performed. Afterward, the quality of the grid can be evaluated by an appropriate measure such as the index of resolution quality for LES (LES_{IQ}) proposed by Celik et al.^[35]

$$LES_{IQ} = \frac{1}{1 + 0.05 \left[\frac{(\mu_F + \mu_{sgs})}{\mu_F} \right]^{0.53}} \quad (14)$$

With a value above 0.75, the resolution can be considered adequate, though this does not necessarily mean that the model is accurate, nor vice versa. Similar to a comparison of the resolved and modeled turbulent kinetic energy, the index of resolution has two major inaccuracies. First, the numerical error depends not only on the grid resolution but also on the numerical scheme used, which is not considered in the evaluation. Especially in case of an odd first-order scheme (upwind), the numerical error is much larger than in case of a central differencing scheme (second order). The second major inaccuracy is related to the fact that the turbulent viscosity depends not only on the model constant C_s and the filter width but also on the resolved strain rate S . This is often underestimated, especially in areas close to the wall, which can lead to a significant underestimation of the turbulent viscosity.^[35] From a practical perspective, a drawback of the a posteriori approach is that the LES computation has to get into a pseudo-stationary state before the index of quality can be assessed. Thus, it is far more time consuming than the a priori approach.

In this article, both approaches are compared. Due to the faster computation times and the possibility to assess the model accuracy simultaneously, the most efficient hybrid grid for the water model is investigated. The models accuracies, assessed by the validation score, are summarized in **Table 2**. The results are then transferred to the industrial scale and finally evaluated.

Figure 3 shows the a posteriori index of quality criterion for a grid that fulfills the requirements predicted with the a priori criterion. In the bulk zone, a resolution of $\Delta x = 32$ mm is employed, while in the near-wall and the plume zone, a grid width of $\Delta x = 4$ mm is used. It is apparent that the resolution in the main flow is far too coarse. As a result, the model's accuracy, in particular in the bulk zone, is significantly reduced, as shown in **Table 2**. The a priori criterion alone is therefore unsuitable for the given problem to predict a minimum grid resolution. Thus, this approach is discarded, and the a posteriori approach is used hereafter.

The equidistant grids with a resolution of $\Delta x = 4$ mm and $\Delta x = 6$ mm from the previous water model study^[7] serve as

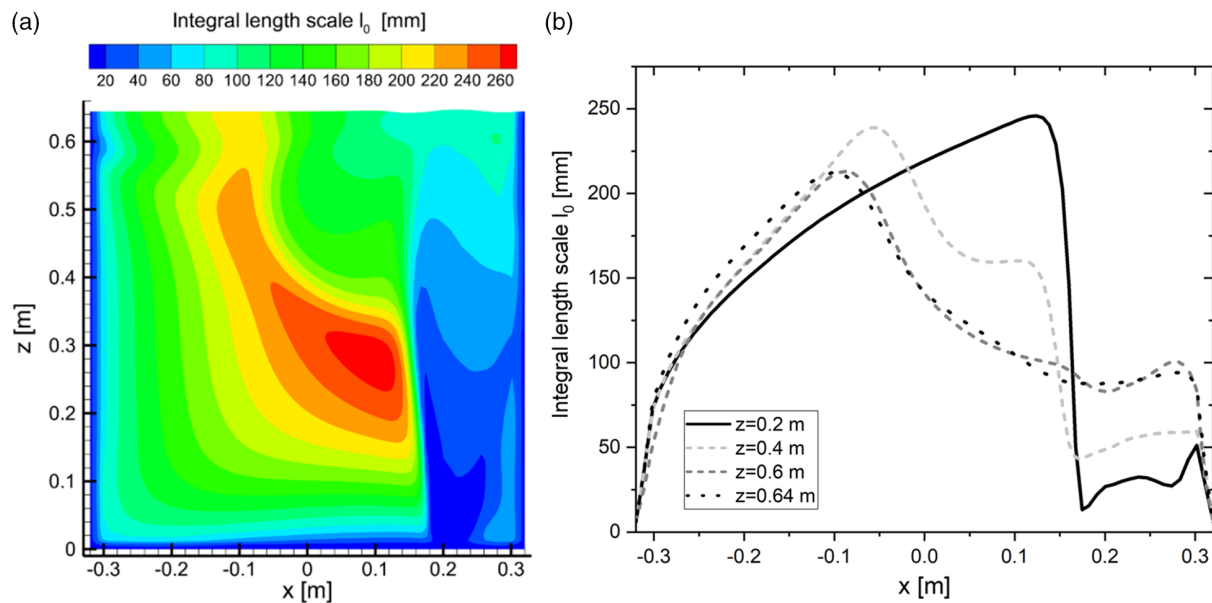


Figure 2. A priori estimation of the required grid resolution by the integral length scale from RANS as a) a contour plot and b) as isolines.

Table 2. Validation score for different tested grids.

	Δx_{plume} [mm]	Δx_{wall} [mm]	$\Delta x_{\text{surface}}$ [mm]	Δx_{bulk} [mm]	#cells	Validation-score (T/M/Mt/P/B/ Σ) ^{a)}
Bench	4	4	4	4	4 050 000	9.8/19.2/33.1/12.6/13.1/87.6
Bench II	6	6	6	6	1 205 892	9.6/17.7/31.8/12.6/13.3/85.1
A priori	4	4	32	32	279 232	8.6/13.4/13.8/11.8/13.8/61.1
Plume refinement	3	12	12	12	235 613	8.4/18.8/29.7/12.1/13.8/82.7
Plume+boundary refinement	3	12	6	12	301 896	8.7/19.5/32.3/12.1/13.8/86.2
Plume+boundary+wall refinement	3	6	6	12	441 777	9.2/19.2/30.1/12.2/13.5/85.0

^{a)}T= toroid, M = means, Mt= monitors, P = plume, B = bubbles, Σ = total score.

benchmarks for the subsequent a posteriori grid optimization. With a cell count of ≈ 4 million and 1.2 million, these grids obtained a validation score of 87.6 and 85.1, respectively, as summarized in Table 2. A plot of the LES index of quality of the $\Delta x = 6$ mm grid is shown in Figure 4a. The grid resolution in the bulk zone results in a very high index of quality that suggests a grid coarsening. For the phase boundary zone and the near-wall zone similar conclusions can be made. In the plume zone, however, the index of quality drops below 0.75 locally, suggesting a grid refinement. These considerations lead to the hybrid grid shown in Figure 4b. Since the plume spreads radially with height, the grid is refined stepwise to $\Delta x = 3$ mm. In the remaining zones, the grid is coarsened to $\Delta x = 12$ mm. This reduces the number of cells to about 250 000. However, the resolution requirements in the plume zone are met very well with these measures, but there is a violation in the phase boundary zone. In the near-wall zone, the index of quality drops below 0.75 at one point and approaches this value in other areas. Thus, the validation score drops to 82.7.

Therefore, in the following, the grid resolution in the phase boundary zone is increased again to $\Delta x = 6$ mm. This increases

the number of cells to about 300 000, but increases the validation score to 86.2, which is even higher than the benchmark with an equidistant $\Delta x = 6$ mm grid. In the final step, the resolution of the near-wall zone is increased to $\Delta x = 6$ mm. This increases the number of cells to 440 000, while the validation score decreases slightly to 85.0. Therefore, it is concluded that in the water model, an ideal tradeoff between accuracy and computational cost is found with a hybrid grid, where the bulk and near-wall zones are discretized with a $\Delta x = 12$ mm grid, while in the phase boundary zone a grid resolution of $\Delta x = 6$ mm is employed. In the plume zone, the grid is further refined to $\Delta x = 3$ mm.

Figure 5 shows the index of quality for the grid used for the full-scale model. The grid consists of 34 597 907 cells. It can be seen that the index of quality locally drops below 0.75. This is particularly noticeable in the plume zone, so that an even finer grid would be necessary here. However, it takes more than 3 months of computing time to reach the quasi-stationary state and the capacity limit of the computing cluster is reached, so that calculations are nevertheless continued with this grid. With increasing computing capacities in the future, however, the grid should be refined in order to further increase the model's accuracy.

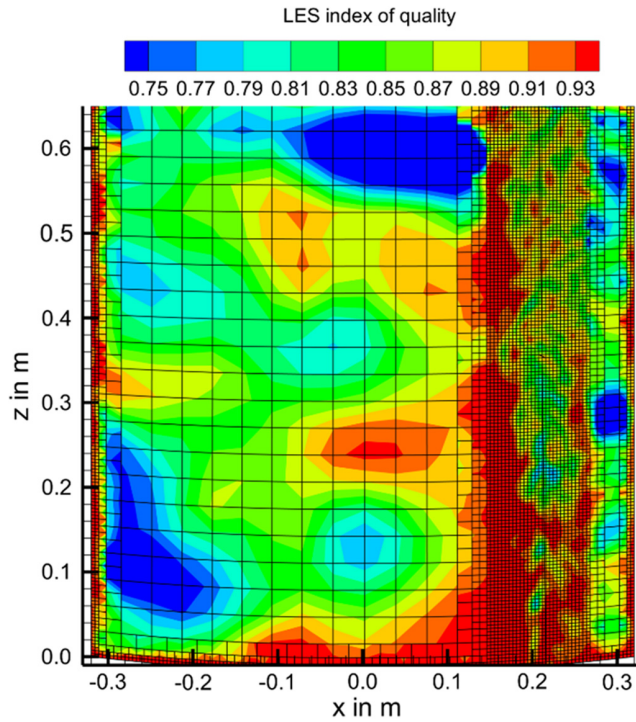


Figure 3. LES index of quality for a grid proposed by the a priori approach ($\Delta x_{\text{bulk}} = 32 \text{ mm}$, $\Delta x_{\text{surface}} = 32 \text{ mm}$, $\Delta x_{\text{plume}} = 4 \text{ mm}$, $\Delta x_{\text{wall}} = 4 \text{ mm}$).

3.2. Lagrange Phase Mapping

Another problem is that the standard E-L model, preimplemented in Ansys Fluent, is based on the particle source in cell (PSI) approach by Crowe et al.^[36] In this implementation, it is

assumed that the bubbles are small compared to the grid and therefore exchanges flow properties and momentum only with the cell in which the bubble center are located. In the presented work, however, the LES model requires a grid as fine as possible, in particular in the turbulent plume zone, violating the PSI condition. In the water model, the bubbles are in a similar size range as the sufficient grid width for LES, so that good results can still be achieved with node-based average, preimplemented in Ansys Fluent. Even if the bubble size in the industrial ladle is unknown, it can be assumed that most bubbles are significantly larger than the width of the grid ($d_B/\Delta x \sim 10$), so that node-based averaging is no longer permissible. However, the grid is still too coarse to use the VOF model. To overcome this problem, the Eulerian and Lagrangian reference frames are decoupled by implementing the particle in a ball model.^[37] In that, interpolation between the reference frames is maintained by an exchange function

$$\phi_{\text{ex}}(j) = \frac{1}{V_{\text{cell}}} \sum \phi_{\text{ex,tot}} \int_{\Omega_j} \omega(b) d\Omega \quad (15)$$

where $\omega(b)$ is a template function

$$\int_{\Omega_j} \omega(b) d\Omega = \int_{\Omega_{j,x}} \int_{\Omega_{j,y}} \int_{\Omega_{j,z}} \omega(x_n - x_b) \omega(y_n - y_b) \omega(z_n - z_b) dx dy dz \quad (16)$$

The principle of two-way coupling is shown in **Figure 6**. For the sake of simplicity, it is depicted in two dimensions. During forward coupling (a), the flow properties of the influenced area, stored in the Eulerian cell nodes, are weight averaged with the mapping function according to Deen et al.^[38] and applied to the Lagrangian bubble

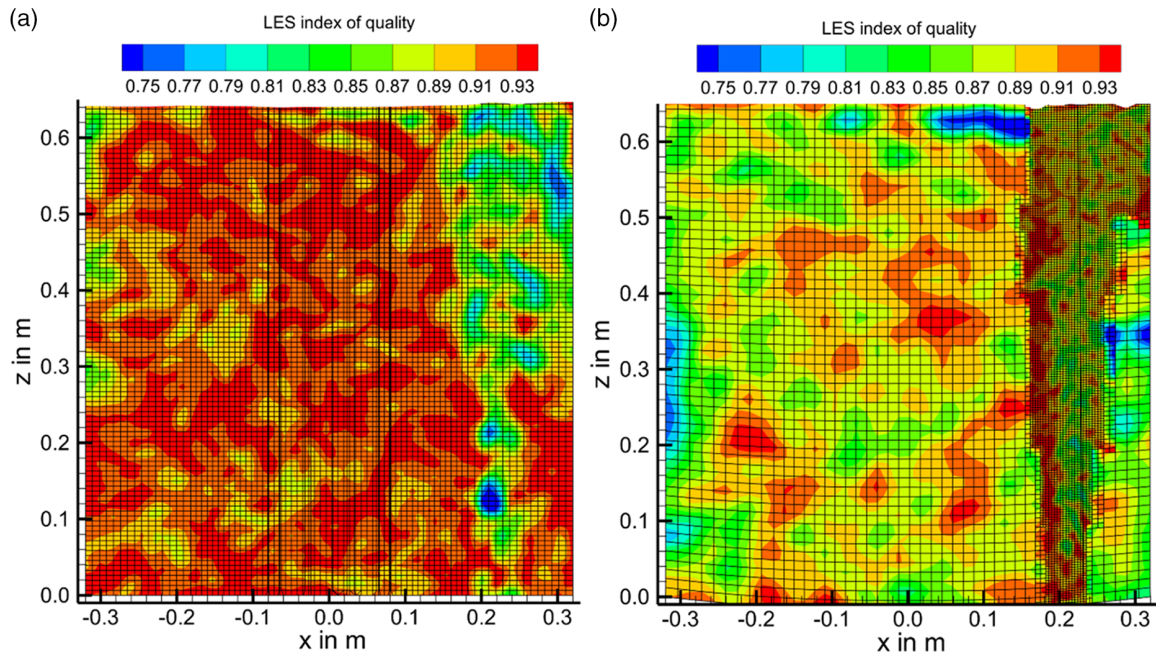


Figure 4. LES index of quality for a uniform $\Delta x = 6 \text{ mm}$ and $\Delta z = 6 \text{ mm}$ grid.

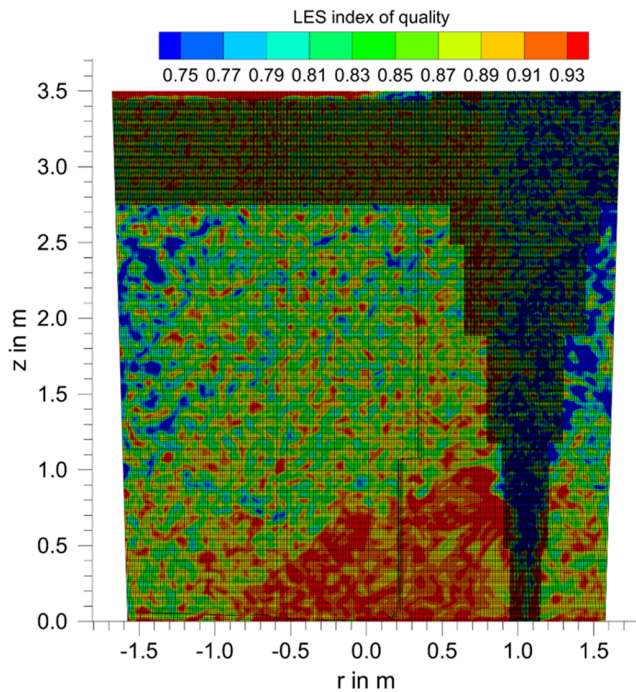


Figure 5. LES index of quality for the industrial scale grid.

$$\omega(x_i - x_{b,i}) = \frac{15}{16} \left[\frac{(x_i - x_{b,i})^4}{n^5} - \frac{2(x_i - x_{b,i})^2}{n^3} + \frac{1}{n} \right], \quad (17)$$

$$-n \leq x_i - x_{b,i} \leq n$$

where n is the mapping window. Lau et al.^[39] investigated the optimum size of the mapping window and found that values of $n = 2R_B$, $3R_B$, and $4R_B$ all had advantages or disadvantages that depend on the axial position in the plume. In this work, a mapping window size of $4R_B$ is employed.

In backward coupling (b), the exchanged momentum of the bubbles is transferred to the Eulerian grid with the same mapping function. This makes the E-L approach independent of the numerical grid.

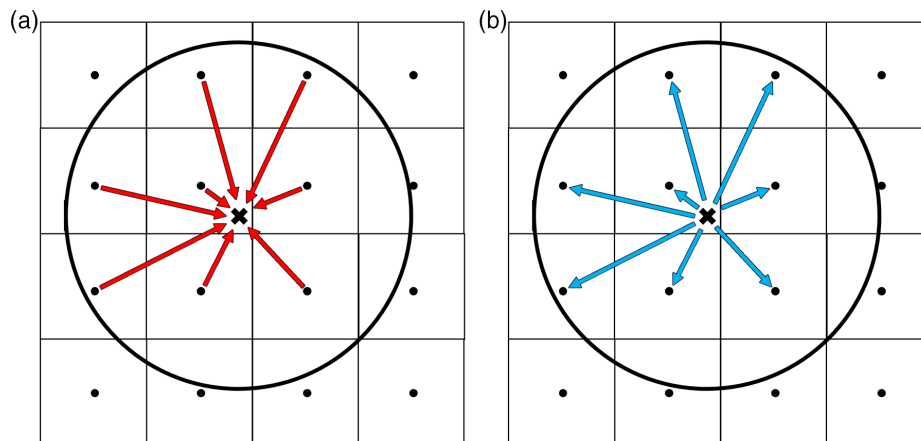


Figure 6. a) Forward and b) backward mapping between Lagrangian bubble and Eulerian grid.

A comparison of the different approaches is shown in **Figure 7**. The rising velocity for both, a single 6 mm bubble (a) and a 20 mm bubble (b) on an equidistant grid with $\Delta x = 2$ mm is shown. In the first case, the PSI approach overestimates the rising velocity by about 100%. In addition, there is a strong fluctuation of the rising velocity. This phenomenon, known as pseudo-turbulence,^[40] occurs when the center of the bubble crosses a cell boundary. With the preimplemented node-based averaging, this phenomenon no longer occurs, but the rising velocity is still overestimated by about 40%. In contrast, with two-way coupling, the rising velocity is almost the same as the analytical solution. The differences can be explained by the fact that the analytical solution assumes a quiescent fluid, whereas in the numerical solution, the bubble induces a flow. In case of a 20 mm bubble, the PSI method diverges directly. Node-based averaging also diverges very quickly. The grid-independent two-way coupling, in contrast, is stable and yields realistic rising velocities.

The implementation in Fluent is maintained by UDFs. The sequence of the program is shown in **Figure 8**. The functions of the individual UDFs, identified by its Fluent specific names, are described in the Appendix. The source code is publicly available on GitHub: https://github.com/Tim-Haas/DPM-Euler_coupling_for_Ansys_Fluent.

3.3. Scaling of Semi-Empiric Models

In the water model study,^[7] semi-empirical models were found to describe the force balance on the bubbles in such a way that very good agreement is found between the numerical model and validation data. However, the transferability of these interfacial force correlations to the system steel-argon is difficult to verify. Moreover, the bubble size distribution is unknown in the real process. To overcome the uncertainty introduced by extrapolating existing models to different liquid–gas systems, a comprehensive literature review was carried out.^[30] For the drag force, there are a few experimental measurements in liquid metals and DNS calculations that suggest that the existing models can be extrapolated. For the lift force, validation for liquid metal systems is completely lacking, and studies in systems with small Morton numbers are very rare. Furthermore, there are very little

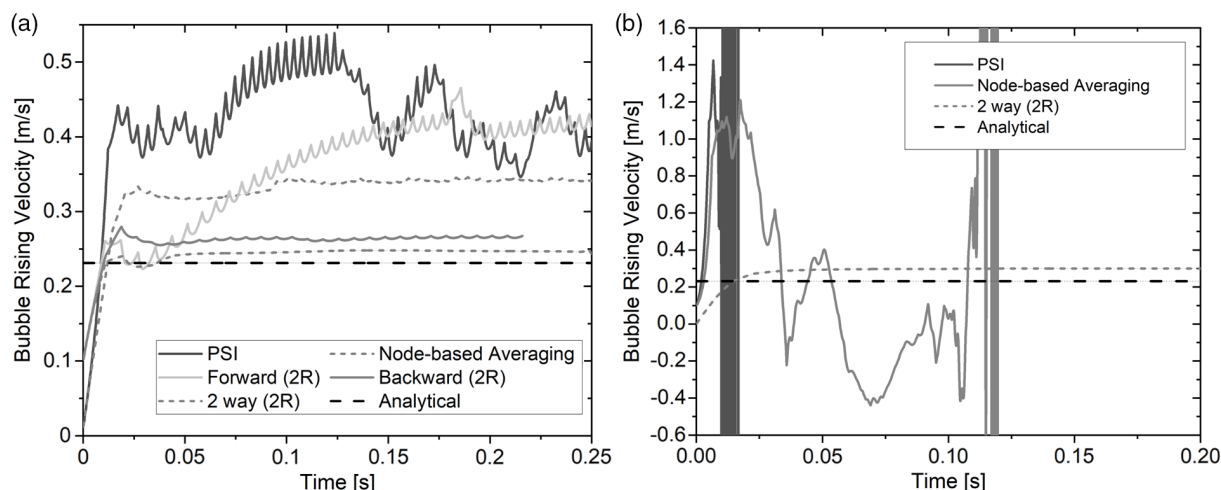


Figure 7. Comparison of different E-L approaches with analytical rising velocity for a) a 6 mm and b) a 20 mm, bubble on an equidistant 2 mm grid.

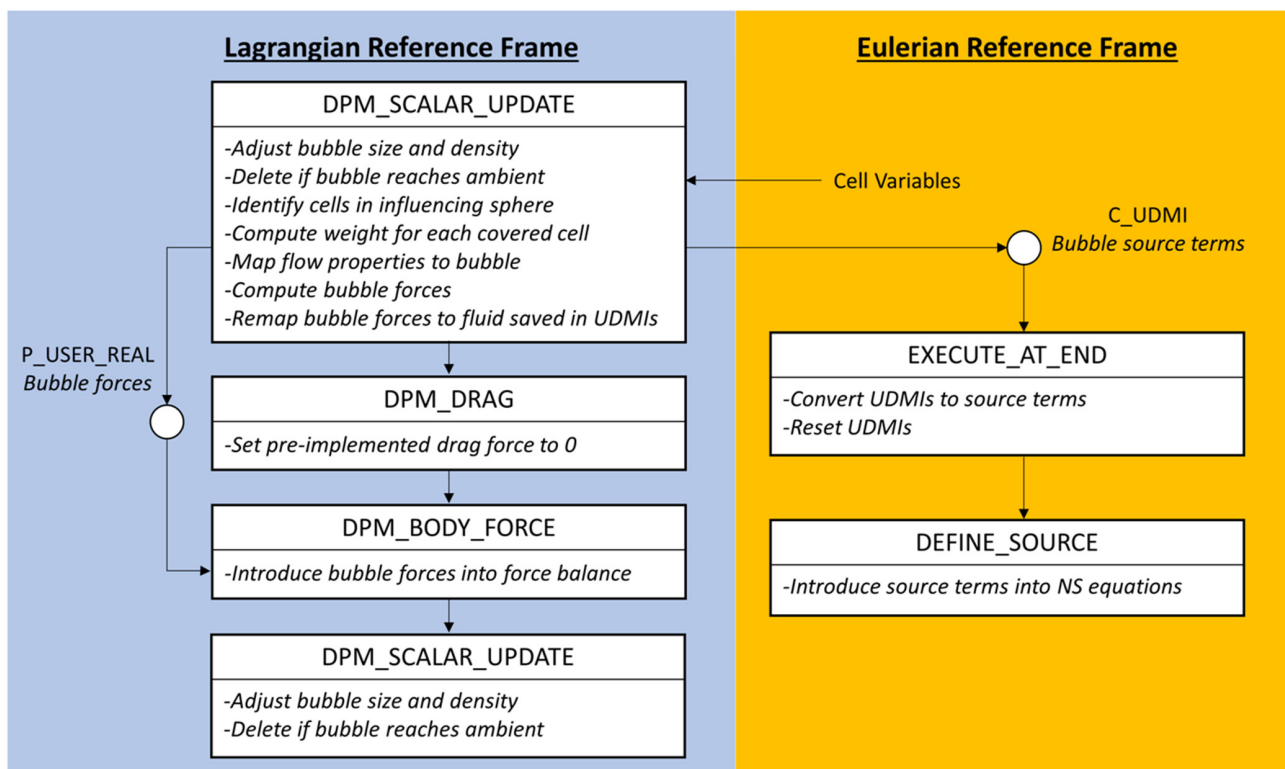


Figure 8. UDF sequence for E-L two-way coupling.

experimental data for bubble deformation in liquid metals, so it is difficult to evaluate which of the widely differing models should be used. However, since deformation has a large effect on the lift force, the scaling here is particularly uncertain. In addition, it can be observed in aqueous systems that impurities have a very strong influence on all bubble forces. Whether this applies to liquid metals too and whether impurities are present in the ladle cannot be answered; however, since there is no data basis

for this. Last, the bubble size distribution, which has a great influence on the model accuracy, is largely unknown in the real process. Here, either measurements in liquid metals at single nozzles with small flow rates can be transferred to porous plugs or measurements at porous plugs in water models can be transferred to liquid metal systems. However, both approaches are rather uncertain, so that the bubble size distribution can only be estimated with a very high degree of uncertainty. For the given

reasons, the upscaling of existing semi-empirical models is a major source of model uncertainty. More elaborate measurement techniques such as X-ray or thermal neutron imaging^[41–44] and DNS might decrease that uncertainty in the future.

3.4. Verification with Literature Data

As pointed out in the sensitivity analysis of validation techniques,^[18] the validation of a numerical model in the industrial ladle itself is very difficult. Currently, mixing time measurements are the most sensitive and accurate choice. Even if this technique has problems, such as high measurement uncertainties, it is still better suited than the alternative evaluation of the slag eye opening area. In this work, to verify upscaling of the numerical model, the mixing time measurements by Lachmund et al.^[45] are used. Lachmund et al.^[45] published two mixing time measurements with the same setup, decreasing the measurement uncertainty at least a little. The numerical model tries to reproduce the experimental conditions as closely as possible in order to reduce possible uncertainties by simplifications. For this purpose, the ferromanganese alloy particles are first treated as melting particles in the Lagrangian reference frame. The particle size distribution and feeding rate are taken from Lachmund et al.^[45] The tracer particles are injected at $x = -1.113$, $y = 0$, and $z = 3.03$, staggered with a radius of 0.25 m. The melting time is calculated for each particle with the model of Aoki et al.^[46] by Equation (18), and the employed physical properties are given in Table 3

$$t_1 = \frac{c_p \rho_A d_A}{\pi h} \frac{T_S - T_0}{T_M - T_S} \quad (18)$$

The heat transport coefficient h is given by Equation (19)

$$h = \frac{\text{Nu } k_F}{d_A} \quad (19)$$

The Nusselt and the Prandtl number are given by Equation (20) and (21)

$$\text{Nu} = 2 + (0.4 \text{Re}^{0.5} + 0.06 \text{Re}^{0.66}) \text{Pr}^{0.4} \quad (20)$$

$$\text{Pr} = \frac{c_{pM} \mu}{k_M} \quad (21)$$

After the residence time of an individual particle has reached the specific melting time, the particle temporarily becomes a source term of a scalar transport equation before it is removed.

Table 3. Employed physical properties to calculate the alloy particle's melting time.

–	–	FeMn ^[51]	Melt
T_S	°C	1250	1536
c_p	J kgK ^{−1}	800	820
k_M	J smK ^{−1}	50	40.3
ρ	kg m ^{−3}	7290	6932
T_0	°C	25	–
T_M	°C	–	1600

Table 4. Monitoring points.

Monitoring point	x	y	z
M1	1.05	0	1
M2	1.05	0	2.5
M3	0	1	1
M4	0	1.5	3
M5	−0.5	0	0.25
M6	−0.5	−0.75	1
M7	−1.3	−1	2.5
M8	−1.3	1	2.5
M9	−1.3	0	3

Similar to the work of Aoki et al.,^[46] the concentration of tracer is measured at nine monitoring points whose coordinates are given in Table 4.

It has been shown experimentally that the measured mixing times can vary greatly. Aoki et al.^[46] showed that this also applies to the numerically calculated mixing times. It can be assumed that this applies in particular to LES model, since the unsteadiness of flow is considered. Therefore, tracer particles are added to the model at five different times, and five different scalar transport equations are solved to reduce the uncertainty due to temporal variation.

4. Results

The calculation runs for 240 s, whereby the first 90 s are calculated so that the flow gets into a quasi-stationary state. After that, averaging and the addition of tracer particles started. The calculation time is about 9 months.

Figure 9 shows the comparison of a numerically calculated tracer concentration and the measurements of Lachmund et al.^[45] There is a very high agreement between numerical and experimental data. The deviation is in the range of the measurement uncertainty which can be roughly characterized by the differences of the two experimental measurement series. Thus, it can be concluded that the upscaling was successful.

The flow field on the symmetry plane ($y = 0$), averaged over 150 s, is shown in Figure 10. The scale is truncated to 0.35 m s^{−1} to visualize the velocity differences in the bulk flow. As expected, the highest flow velocity of about 1.5 m s^{−1} can be observed in the plume zone. The maximum flow velocity in the phase boundary zone is about 0.5 m s^{−1} close to the slag eye. In the near-wall zone, a maximum velocity magnitude of about 0.5 m s^{−1} can be observed between plume and wall. In the bulk zone, the maximum velocity is about 0.3 m s^{−1}. Due to the increased dynamic pressure at the spout, a slag eye with an average diameter of 1.2 m is formed. In comparison, Ramasetti et al.^[47] measured for the same flow rate in a 150 t ladle with a slightly thicker slag layer of 0.25 m an opening area of 1.08 m². Given that the opening area increases with decreasing slag thickness, this agreement is reasonable. At the spout, the flow is redirected. Compared to the water model, however, the flow toroid is significantly closer to

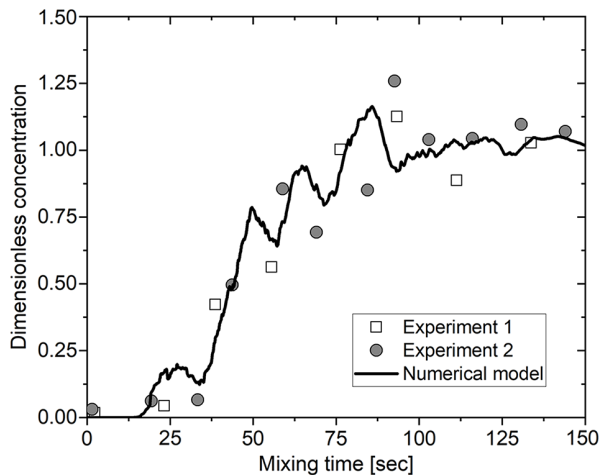


Figure 9. Comparison between numerically computed and experimentally measured tracer concentration.

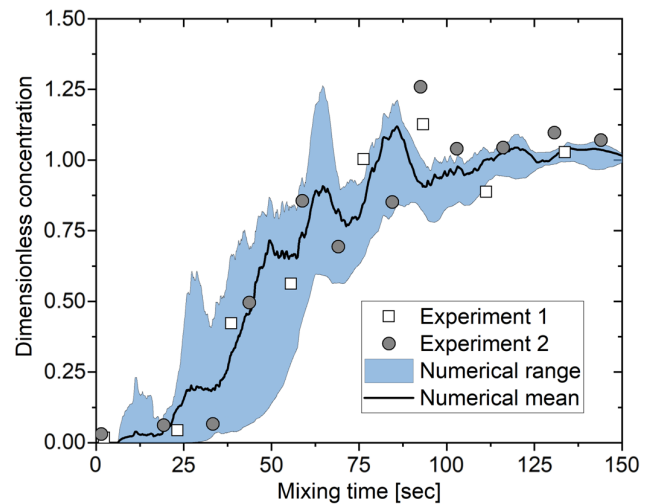


Figure 11. Range of numerically calculated mixing times.

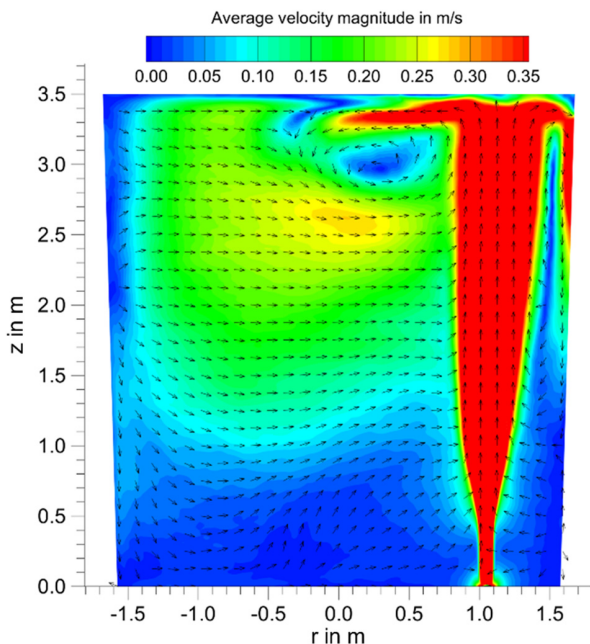


Figure 10. Flow field on symmetry plane ($y = 0$), averaged over 150 s.

the plume. This can probably be explained by a damping effect of the slag layer, which was also found experimentally.^[48–50]

5. Discussion

Within the scope of this work, a numerical model of the flow in the ladle, previously optimized on the water model scale, was scaled to the industrial scale. Several problems and their solutions were discussed.

A very good agreement with experimental concentration measurements by Lachmund et al.^[45] was found. However, it should be taken into account that, as shown in the sensitivity analysis of different validation techniques,^[18] concentration

measurements are characterized by a high measurement uncertainty. **Figure 11** shows the range of values of the different numerically calculated concentrations where the calculations differ at the time of tracer addition. The mentioned measurement uncertainty is well recognizable here.

Due to the good agreement between the numerical and experimental results, it can be concluded that the scaling was successful. However, a quantitative estimation of the model uncertainty, as in the water model, is not possible from these data. Since the computation capacities are still limited and thus the grid resolution does not everywhere meet the requirements of an LES calculation, a somewhat larger model uncertainty than in the water model can be assumed. This is further increased by the uncertainty of scaling of semi-empirical models whose verification is still insufficient. However, due to increasing computational capacities, it should be possible in the future to compute models with higher grid resolutions so that an LES index of quality of at least 0.75 is reached everywhere. Eventually, the grid resolution will be fine enough to realistically model the bubbles with the VOF model. Due to the currently very high computational costs, an LES calculation is currently mainly interesting for the academic sector as a benchmark. With increasing computing capacities, however, it can become state of the art in the industry.

6. Conclusion

In this work, a numerical model that was previously optimized at the water model scale was scaled to the real process. Different challenges and their solutions were discussed. For the numerical grid, a hybrid meshing approach was developed where the resolution is locally refined or coarsened, and its applicability was assessed by the a posteriori approach. In this way, a tradeoff between accuracy and maximum computational capacity was optimized. The intrinsic problems of the E-L model were overcome by implementing a mapping strategy in Ansys Fluent to decouple the phases. This method has been made publicly available on GitHub. The scaling of semi-empirical models was

discussed extensively in a previous publication.^[30] By these measures, good agreement was found with experimental concentration measurements by Lachmund et al.^[45] However, because of measurement uncertainties, it can only be concluded that the scale up was successful. However, it is difficult to estimate the accuracy of the model.

High-resolution LES models are currently still primarily of academic interest due to the extreme computation times. In the future, however, they may become state of the art due to further increasing computing capacities.

Appendix

A1. Implementation Details of E-L Two-Way Coupling

The UDF DPM_SCALAR_UPDATE is called twice in a time step for each bubble. To distinguish the calls, the solver passes the Boolean flag “init” to the UDF. (Table A1)

In both cases, the UDF adjusts the bubble diameter and density depending on the axial position according to Equation (8) and (9). In addition, it checks whether the bubble has reached the phase boundary of furnace atmosphere, and in this case, the bubble is removed and the UDF is terminated. In case that the UDF is called for the first time (init = 1) for a particular bubble, mapping is performed. For each bubble, the system searches for all cells that are in the bubble's area of influence, a sphere with the diameter of the mapping window. A problem is that Fluent converts every computational grid into an unstructured grid. This means that even with structured, hexahedral grids, there is not a directly accessible connection between neighboring cells. For example, it is not possible to switch from a cell to neighboring cells by increasing a pointer value. An extremely uneconomical approach would be to loop over all cells for each bubble and check whether they are located in the area of influence of the bubble. Instead, a face loop cascade is conducted to find cells within the influencing sphere of a bubble and store them in an array. The procedure is shown in Figure 12, for the sake of simplicity it is given for 2D. The cascade starts at the cell in which the bubble center is located in. A loop is performed over the cell faces, six in case of a hexahedral grid. For all adjacent cells, it is checked whether they are within the bubble's influence area but not already present in the cell array. If this condition is fulfilled, the array is extended by this cell. Afterward, the procedure is repeated by looping over all faces of a cell added to the cell array in the previous cascade step. This cascade is repeated until no further cells are added to the array. A problem can arise with parallel calculations due to the partitioning of the computing domain. Each computation core handles only the cells that are located in its computational area. Partially, the area of influence of the bubbles may extend into an adjacent partitioning. However, the core cannot access these cells, so these cells are simply ignored in this case.

In the next step, the weighting factor is calculated for each identified cell using Equation (17). Due to the partitioning problem and rounding errors, the sum of all weighting factors can become less than one. Therefore, the weighting is calculated

Table A1. List of abbreviations.

Symbol	Description
c_D	Drag coefficient
c_L	Lift coefficient
c_{VM}	Virtual mass coefficient
c_p	Specific heat capacity, [J kgK ⁻¹]
C_S	Model parameter
d_A	Diameter of tracer alloy particle, m
$d_{B,0}$	Initial bubble diameter, m
d_B	Bubble diameter at height (z), [m]
d_h	Length of bubble major axis, [m]
E_o	Eotvos number
$E_{o,d}$	Modified Eotvos number
F_B	Buoyancy force, [N]
$F_{B,i}$	Mass-based force i on bubble, [N]
F_D	Frag force, [N]
F_L	Lift force, [N]
F_n	Volume fraction of phase [n]
f_i	Volume force source term, [N m ⁻³]
g	Gravity, 9.81 m s ⁻²
h	Heat transport coefficient, [W m ⁻² K ⁻¹]
H_{Fill}	Filling height, [m]
k_F	Thermal conductivity, [J smK ⁻¹]
L_S	Mixing length for subgrid scales, [m]
m_B	Bubble mass, [kg]
$\dot{m}_B$	Bubble mass flow, [kg s ⁻¹]
Nu	Nusselt number
n	Radius of influencing sphere of a bubble,[m]
Pr	Prandtl number
p	Pressure, [N m ⁻²]
p_0	Atmospheric pressure, [N m ⁻²]
R_B	Bubble radius, [m]
Re_B	Bubble Reynolds number
S	Resolved strain rate
T	Temperature, [°C]
T_F	Temperature of the fluid, [°C]
T_s	Solidification temperature, [°C]
T_0	Initial temperature of tracer particle, [°C]
t_i	Tracer particle melting time, [s]
Δt	Time step size, [s]
$\vec{u}_B$	Bubble velocity, [m s ⁻¹]
$\vec{u}_F$	Fluid velocity, [m s ⁻¹]
$\vec{u}_i$	Fluid velocity component i, [m s ⁻¹]
V_{cell}	Volume of a Eulerian cell, [m ³]
$\vec{x}_B$	Coordinate of bubble
Δx	Cell width, [m]
μ_F	Fluid viscosity, [Ns m ⁻²]
μ_{SGS}	Subgrid turbulent viscosity, [Ns m ⁻²]

Table A1. Continued.

Symbol	Description
ρ_A	Density of tracer alloy, [kg m^{-3}]
ρ_B	Bubble density, [kg m^{-3}]
$\rho_{B,0}$	Bubble density, [kg m^{-3}]
ρ_F	Fluid density, [kg m^{-3}]
σ	Surface tension, [N m^{-1}]
δ_i	Kronecker delta
ϕ_{ex}	Exchanged quantity
ω	Template function
Abbreviation	Description
B	Bubble score
CFL	Courant–Friedrichs–Lewy number
CNN	Convolutional neural network
DNS	Direct numerical simulation
E-E	Euler–Euler multiphase approach
E-L	Euler–Lagrange multiphase approach
LES	Large eddy simulation
LES_{IQ}	LES index of quality
M	Means score
M_t	Monitors score
P	Plume score
PSI	Particle source in cell approach
RANS	Reynolds-average Navier-Stokes
T	Toroid score
UDF	User-defined function
UDMI	User-defined memory
VOF	Volume of fluid model

for all cells except the first one using Equation (17). In the cell that contains the center of the bubble, the difference between one and the sum of all other weights is taken as weighting factor. This prevents that a part of the bubble momentum is lost. For forward mapping, the flow properties are multiplied by the weighting factor for each cell in the area of influence and these values are summed up. With these values, the forces acting from the fluid onto the bubble are calculated employing Equation (3). Among the drag and lift models used in this work, other models are implemented too. The total force is decomposed in its x -, y -, and z -components and saved in P_USER_REAL structs for each bubble. Finally, the bubble force components are mapped back to all cells within the influencing sphere by employing the weighting factors again. These decomposed forces are stored in each cell in user defined memories (UDMIs).

In the UDF DPM_DRAG, the drag force implemented in Fluent is set to zero by setting the drag coefficient to zero. This is necessary because the standard implementation in Fluent always considers the drag force according to the PSI approach automatically and takes it as source term of the momentum equations.

In the UDF DPM_BODY_FORCE, the bubble forces computed within DPM_SCALAR_UPDATE are passed to the bubble force balance by P_USER_REAL structs. Because the UDF DPM_BODY_FORCE is called several times in a DPM iteration, it is more efficient to calculate the forces once in DPM_SCALAR_UPDATE and to transfer into DPM_BODY_FORCE only these already calculated forces to the bubble.

After the DPM iteration has finished, the UDMIs that store the bubble momentum are transferred to temporary UDMIs and are then reset. This is necessary because one cell could be in the area of influence of several bubbles. Thus, the bubble momentum is just added to the current value in the UDMI to avoid overwriting the momentum of other bubbles.

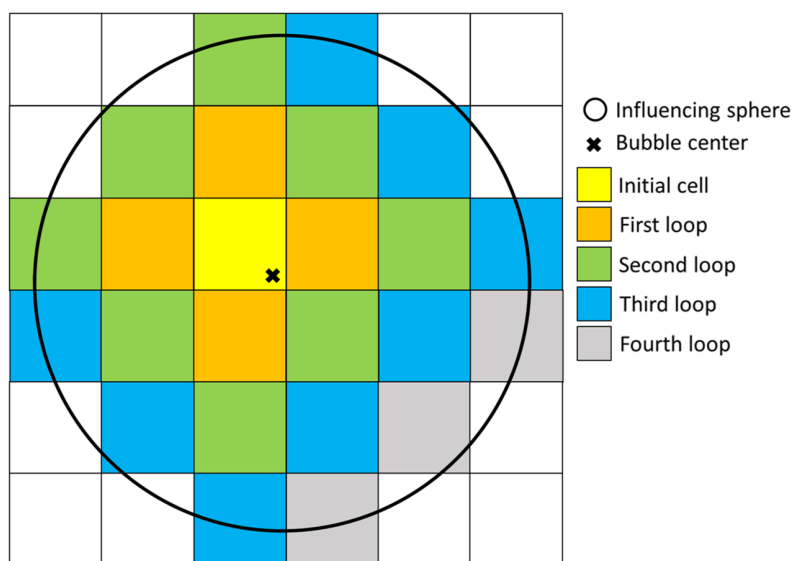


Figure 12. Face loop cascade to identify cells within the influencing sphere of a bubble.

Finally, the bubble momentum is introduced into the momentum equation of Eulerian cells by including the values stored in the temporary UMDIs as a source term.

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

Research data are not shared.

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