# Study of Computational Issues in Simulation of Transient Flow in Continuous Casting

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#### Abstract

The attachment probability of inclusions on a bubble surface is investigated based on fundamental fluid flow simulations, incorporating the inclusion trajectory and sliding time of each individual inclusion along the bubble surface as a function of particle and bubble size. Then, the turbulent fluid flow in a typical continuous casting mold, trajectories of bubbles and their path length in the mold are calculated. The inclusion removal by bubble transport in the mold is calculated based on the obtained attachment probability of inclusion on bubble and the computed path length of the bubbles. The results are important to estimate the significance of different inclusion removal mechanisms. This work is part of a comprehensive effort to optimize steelmaking and casting operations to lower defects.

#### Introduction

Computational fluid dynamics (CFD) is becoming a powerful tool to study turbulent fluid flow in complex metallurgical processes, such as the continuous casting of steel slabs. These fundamentally-based mathematical models have advantages over other tools, such as water models and plant experiments, owing to their ability to quickly and accurately visualize and quantify flow patterns and related phenomena such as free surface motion, multiphase particle transport and entrapment, and heat transfer. Furthermore, their use is rapidly accelerating, due to the tremendous increases in computer hardware and software, which doubles in power about every 1.5 years. [1]

Although CFD models are growing in power and complexity, accurate results are often difficult to achieve. This can be due to modeling assumptions in the turbulence model, inappropriate assumption of flow symmetry, insufficient domain size, oversimplified inlet conditions, inadequate mesh refinement, convergence problems, poor choice of boundary conditions such as wall laws and outlet conditions, and many others. Many different modelling choices are available, and the best choice is often problem dependent. Thus, the present work was undertaken to investigate some of the issues affecting the numerical accuracy of CFD models in the context of turbulent flow in the nozzle and mold during the continuous casting of steel slabs. Based on the results of many simulations of the same system with different models, guidelines are offered for choosing the simulation domain, symmetry assumption, inlet conditions, mesh refinement, and turbulence model. This work should be useful for developing future models of continuous casting, or similar flow systems, and in evaluating the accuracy of the results.

#### **Previous Work**

In spite of the widespread application of CFD models to continuous casting, and the many different modeling options that are available, relatively few studies have systematically investigated the numerical accuracy of CFD models of this system. The accuracy of CFD models has been investigated systematically in other systems [2-4]. Najjar et al [5, 6] studied the effects of inlet conditions and wall laws on velocity distribution in a continuous slab casting mold fed from a bifurcated nozzle using a 2-D finite-element K- $\varepsilon$  model. They developed guidelines for achieving efficient convergence, consisting of larger relaxation factors for early iterations to accelerate reduction of the initial error, followed by smaller relaxation factors to maintain stable convergence. A new wall law so found to produce better accuracy than the standard wall law for this flow problem involving jet impingement and recirculation. Inlet conditions, including those for turbulence parameters, had a huge influence on the flow pattern. Hershey et al [7] found that uncoupling the nozzle and mold simulations was reasonable, as it produced only small differences in the flow pattern near the recirculation region near the upper ports.

Thomas et al [8] compared 4 different methods for studying fluid flow in slab casting. Two different modelling approaches both matched well with measurements in a water model and in an actual steel caster. The standard K- $\epsilon$  model was able to simulate the time averaged 3-D flow pattern with almost equal accuracy to a fully-transient, large eddy simulation with a fine mesh, as compared with Particle Image Velocimetry measurements and measurements in an operating steel slab casting mold. However, the K- $\epsilon$  model was less accurate for time-related phenomena, such as the turbulent kinetic energy distribution and flow oscillations. These and other related phenomena, such as the distribution of superheat, the transport and removal of inclusion particles, and the multiphase interactions between the top surface of the steel and the flux layers above are much more important than the fluid flow itself. The accuracy of CFD predictions of these phenomena has not been compared quantitatively.

This work focuses on single-phase fluid flow and heat transfer in a continuous caster of stainless thin slabs [9] pictured in Fig. 1 for the conditions given in Table 1. Previous work [10, 11] has demonstrated that predictions of an LES model of transient flow in this caster matches well with measurements in a water model, including the flow velocities, [10] top surface contour, and particle flotation rates.[11] The present work investigates computational issues involved in obtaining accurate predictions of this system, including the time averaged flow pattern, transient behaviour, and heat transfer in the molten pool.

	Table I. Parameters and properties for steel caster simulation.		
	Mold (domain) thickness	132	mm
	Mold width	984	mm
	Model domain width	492	mm
Stopper Rod	Nozzle domain length (to port top)	687	mm
	Strand domain length	1.2	m
SEN	Model domain length (total)	1.76	m
	Nozzle bore diameter	70	mm
Free-Slip Bounary 132mm	Side Nozzle port height	75	mm
Casting Speed = 25.4mm/s	Side Nozzle port width	32	mm
	Bottom Nozzle port diameter	32	mm
	SEN submergence depth	127	mm
	Casting speed	25.4	mm·s <sup>-1</sup>
	Casting temperature	1832	K
	Steel composition	Stainless	
No-Slip Boundary D	Steel liquidus temperature	1775	K
Pressure Boundary	Reference temperature, $T_0$	1775	K
	Laminar viscosity	0.00555	kg·m <sup>-1</sup> ·s <sup>-1</sup>
	Thermal conductivity	26	$W \cdot m^{-1} \cdot K^{-1}$
	Density	7020	kg∙m <sup>-3</sup>
Condition at Bottom	Specific heat	680	J·kg <sup>-1</sup> ·K <sup>-1</sup>
	Thermal expansion coefficient	$1.0 \times 10^{-4}$	K <sup>-1</sup>
09.4mm	Gravity acceleration	9.8	m·s <sup>-2</sup>
90411111	Reynolds number (at side ports)	$2.8 \times 10^{5}$	

Figure 1. Schematic of the nozzle and mold domains.

#### Flow Model Equations

The models in this work solve the three-dimensional Navier-Stokes equations which govern the conservation of mass and fluid momentum:

$$\frac{\partial v_i}{\partial x_i} = 0 \tag{1}$$

$$\rho\left(\frac{\partial}{\partial t}v_i + \frac{\partial}{\partial x_j}v_jv_i\right) = -\frac{\partial P}{\partial x_i} + \frac{\partial}{\partial x_j}\mu_{eff}\left(\frac{\partial v_j}{\partial x_i} + \frac{\partial v_i}{\partial x_j}\right)$$
(2)

where:

$$\mu_{eff} = \mu_0 + \mu_t \tag{3}$$

In the large eddy simulations (LES), the time-dependent unknown velocities, vi, represent the large scale eddies, as the effect of the small scale eddies is approximated with a sub-grid scale (SGS) model. In some simulations, the turbulent vis-

cosity,  $\mu_t$ , is set to zero, which can be interpreted as coarse-grid DNS (direct numerical simulations). Numerical diffusion from the discretization scheme and coarse grid can be interpreted as creating some artificial turbulent viscosity in these simulations.

In the SGS-K model [12], turbulent viscosity is approximated by:

$$\mu_t = 0.05\rho K_G^{1/2} \Delta \tag{4}$$

where

$$\Delta = (\Delta_x \Delta_y \Delta_z)^{1/3} \tag{5}$$

and  $\Delta_i$  is the grid spacing in the x, y, or z direction. The SGS kinetic energy  $K_G$  is found by solving the following extra transport equation:

$$\rho\left(\frac{\partial K_G}{\partial t} + v_j \frac{\partial K_G}{\partial x_j}\right) = \frac{1}{2}\mu_i \left(\frac{\partial v_i}{\partial x_j} \frac{\partial v_i}{\partial x_j} + \frac{\partial v_i}{\partial x_j} \frac{\partial v_j}{\partial x_i}\right) - \rho \frac{K_G^{3/2}}{\Delta} + \frac{\partial}{\partial x_i} \left[\left(\mu_0 + 0.1\rho K_G^{1/2} \Delta\right) \frac{\partial K_G}{\partial x_i}\right]$$
(6)

In the standard K- $\varepsilon$  model simulations, only the time-averaged velocity field is solved and the turbulent viscosity is defined by:

$$\mu_t = c_{\mu} \rho \frac{K^2}{\varepsilon} \tag{7}$$

where  $c_{\mu}=0.09$ . This approach requires solving two additional partial differential equations for the transport of turbulent kinetic energy, K (m<sup>2</sup>/s<sup>2</sup>), and its dissipation,  $\epsilon$  (m<sup>2</sup>/s<sup>3</sup>).

In the low-Re K- $\epsilon$  model, the turbulence is gradually diminished towards laminar flow in the low velocity regions such as near the walls, by redefining  $c_{\mu}$  as a function of the local turbulent Reynold's number, Re<sub>T</sub>,

$$c_{\mu} = 0.09 \exp\left(\frac{-3.4}{\left(1 + \text{Re}_{T}/50\right)^{2}}\right)$$
 (8)

$$\operatorname{Re}_{T} = \frac{\rho K^{2}}{\mu \varepsilon}$$
(9)

In addition, extra terms appear in the K and  $\varepsilon$  transport equations, as defined elsewhere. [13, 14]

# **Boundary Conditions**

*Inlet:* The liquid pool is fed by a trifurcated nozzle, which has an important influence on the flow pattern. [8] Thus nozzle simulations were conducted to acquire accurate inlet conditions to the mold. For uncoupled simulations, unsteady flow velocities leaving the nozzle ports were collected at regular time intervals and recycled periodically as the inlet conditions for the liquid pool simulations. As shown in Fig. 1, the 1.1-m long nozzle extends from the tundish bottom and is fed through the annulus formed by a 64.4% open stopper rod, down a 70-mm diameter round bore upper nozzle that tapered into a thin trifurcated outlet region. The flow pattern computed in the complete nozzle is shown in Fig. 2, showing close-ups near the stopper rod, and the nozzle exit ports. Simplified simulations of just half of the nozzle were also performed, starting from a uniform velocity profile 293mm below the stopper rod. Some simulations with this nozzle were also coupled with the mold domain in the same grid.

*Outlet:* For simulation efficiency, the computational domain of the water model simulated in this work is obtained by truncating the 2.6m long physical domain at a plane 1.2m below the top surface. This generates an artificial outlet plane. A simulation is also performed of the real thin-slab caster, which differs by gradually tapering the liquid pool that is contained within the solidifying shell, and truncating it at 2.4m below the top surface. A constant pressure boundary condition, with zero gradient of other variables, was used at the outlet planes where the flow becomes nearly uniform.

*Top Surface and Symmetry Plane(s):* The effect of assuming symmetry is investigated by comparing full pool, half pool, and quarter pool simulations. A free-slip condition was imposed at symmetry plane(s) to represent center plane(s). Specifically, the normal velocity and the normal gradients of pressure and the other two velocity components were set to zero. The same condition was imposed on the top surface. The predictions of this work (presented later) match previous measurements

where

[10] that the top surface is relatively quiescent, so a model for free surface deformation is not necessary to accurately model the flow.

*Narrow Face and Wide Face Walls:* Water models and steel casters have very different walls. Water models have stationary straight plastic side walls representing the solidification front. Thus all three velocity components were set to zero at the wall boundaries. Flow in the steel caster was modeled up to, but not including, the front of the downward moving mushy zone, [15] where solidification occurs to take away mass from the molten steel pool. In addition to tapering the domain walls, the mass transfer across the solidification front was modeled with the following velocity boundary conditions [10]:



Figure 2. Computed flow velocities in nozzle near (a) stopper rod and (b) exit ports.

$$\mathbf{v}_{x} = \left(\frac{\rho_{s}}{\rho_{l}} - 1\right) \sin \theta \cos \theta V_{casting} \tag{10a}$$

$$\mathbf{v}_{z} = \left(\frac{\rho_{s}}{\rho_{l}}\sin^{2}\theta + \cos^{2}\theta\right) V_{casting}$$
(10b)

where  $\rho_s$  and  $\rho_l$  are the solid and liquid densities, the casting speed is  $V_{casting}$ , and the solidification front makes an angle  $\theta$  with the casting direction that decreases with distance below the meniscus.

In the standard K- $\varepsilon$  model simulations, standard wall functions were used to represent the high gradients of velocity, kinetic energy, and dissipation near the walls. [13] The normal distance from the wall to the first node, *n*, is expressed in non-dimensional form, y<sup>+</sup>, defined as

$$y^{+} = \frac{\rho C_{\mu}^{0.25} K^{0.5}}{\mu} n \tag{11}$$

The tangential velocity profile  $V_t$  as a function of  $y^+$  is

$$V_{t} = \begin{cases} -\left(C_{\mu}K\right)^{0.5} y^{+}, & \text{for } y^{+} < y_{o}^{+} \\ \frac{-\left(C_{\mu}K\right)^{0.5}}{\kappa} \log\left(Ey^{+}\right), & \text{for } y^{+} \ge y_{o}^{+} \end{cases}$$
(12)

where E=9.0 is the roughness constant,  $\kappa$ =0.41 is the Von-Karman constant and  $y_0^+$  is the cross over point between the viscous sub-layer and the logarithmic region.

The wall law for the K equation (K- $\epsilon$  model) is simply a zero gradient condition at the wall. Turbulence dissipation at the wall is calculated from K using the relation: [13]

$$\varepsilon_{(y^{+}=0)} = \frac{C_{\mu}^{0.75} K^{1.5}}{\kappa n}$$
(13)

The LES and low Re K- $\varepsilon$  models do not use wall functions, and simply set the velocity components and turbulence parameters K and  $\varepsilon$  to zero at the walls.

## **Solution Procedure**

In the LES computations, the time-dependent three-dimensional Navier-Stokes equations are discretized using the Harlow-Welch fractional step procedure. [16] Second-order central differencing is used for the convection terms and the Crank-Nicolson scheme [17] is used for the diffusion terms. The Adams-Bashforth scheme [18] is used to discretize in time with second order accuracy. The pressure Poisson equation is solved using an algebraic multi-grid (AMG) solver [19] on an unstructured Cartesian grid. The other computations used the solver in CFX [13].

## **Computational Details**

The computational domain is presented in Fig. 1. The geometry, casting conditions, material properties and computational parameters are given in Table I. There is no argon gas in any of the simulations in order to match the real caster, where calcium treatment was used to avoid nozzle clogging. The LES computations employed the in-house CFD code, UIFLOW [20]. The K- $\varepsilon$  model results [14] were computed with the commercial package CFX. [13]

For computational efficiency, the domain was divided into nozzle and liquid pool regions for most simulations. A full nozzle LES simulation with a 0.6 million cell mesh took 10 days on a Pentium IV 1.7GHz CPU for a 9.45s simulation. Transient velocities exiting the trifurcated nozzle ports were stored every 0.025s and used as inflow conditions to the liquid pool. An LES simulation of the full mold region (no symmetry assumption) with 1.3 million cells took 29.5 CPU-s per time step or 24 days for 70,000 time steps (70s of real time). Most K- $\varepsilon$  models employed a 0.3 million node grid and required only a few hours to run. Further computational details are given elsewhere. [10, 11, 14, 21].

#### Flow Velocity Results

Before a computational model is applied to investigate the problem of interest, it should first be validated by comparison with a known solution, to verify that the computational method is accurate, and that the grid is sufficiently refined. It should then be compared with measurements of a similar system, to validate that the modelling approach, domain, boundary conditions, and properties are all reasonable.



Figure 3. Time-averaged velocity fields at the center plane y=0 obtained from LES with  $20x10^3$  (left),  $400x10^3$  (middle) and  $800x10^3$  (right) computational cells.

The codes used in this work were first run to match analytical solutions of simple test problems such as flow in round and square pipes.[20] The next step of numerical validation is to demonstrate "grid independence", by comparing the results of simulations on successively finer computational meshes for the specific problem of interest.

## **Effect of Grid Resolution**

To investigate the effect of mesh refinement, LES computations were performed on six different grids, containing 0.02, 0.08, 0.10, 0.20, 0.40, and 0.80 million cells. Assuming symmetry between the right and left sides, the computational domain was one half of the physical domain. All simulations were performed with the SGS K-model and ignored buoy-ancyeffects. The inlet conditions for these simulations were taken from a 100s half-nozzle simulation corresponding with the finest grid, stored every 0.001s.

The grids were all stretched with a factor of 1.01-1.03 to produce finer cells near the boundaries where they are most needed for accuracy, owing to the high local changes in gradient. This produced cell-center spacings from the wall at the critical region of jet impingement of 6mm, 3mm, 2.5mm, 2.5mm, 1.5mm and 1.5mm, for the 6 different grids respectively.

Flow patterns in the center plane of three different grids are compared in Fig. 3. The jet traverses across the domain to impinge on the narrow face, where it turns upward to the top surface and back towards the SEN in a classic double roll flow pattern. The two finest grids are almost identical, showing that grid independence has been achieved. The coarse grid shows an important deviation in jet direction that would have a large adverse effect on secondary calculations, such as particle motion.

To quantify the difference between grids on an equal basis, the velocities computed for each grid were first interpolated onto a  $64 \times 128$  uniform-spaced grid. Errors for both the time-average and rms velocity were calculated as an average at the center plane y = 0 as follows:

$$Error = \sqrt{\frac{\sum_{i=1}^{N} \left[ \left( \mathbf{V}_{x,i} - \mathbf{V}_{x,i}^{\text{exact}} \right)^{2} + \left( \mathbf{V}_{y,i} - \mathbf{V}_{y,i}^{\text{exact}} \right)^{2} + \left( \mathbf{V}_{z,i} - \mathbf{V}_{z,i}^{\text{exact}} \right)^{2} \right]}{N}$$
(14)

where the exact solution was estimated using the results from the finest grid (0.8 million cells).

The time average error results are presented in Fig. 4a. This error increases exponentially with increasing grid spacing, which corresponds with decreasing number of cells in the grid. The error between the two finest grids averages only  $\sim 0.03$ m/s, although this represents a 17% difference, relative to the mean velocity in the domain,  $\sim 0.18$ m/s. Coarser grids have errors that are much larger than a glance at the velocity vectors would indicate.

The rms velocity error results are presented in Fig. 4b. This error also increases greatly with coarsening grid size. These results indicate that the mesh resolution prediction of velocity fluctuations is accurate within  $\sim 0.02$  m/s or  $\sim 17\%$ . The fluctuating velocity component is almost half of the mean velocity component, indicating that turbulence is very strong. Overall, the fine mesh (0.8 million nodes) is believed to produce reasonable results for engineering purposes.



Figure 4. Effect of grid refinement on error in (a) time-averaged and (b) rms velocities.

## Validation with Measurements

In addition to numerical validation and demonstration of sufficient mesh refinement, computational models also require comparison with experimental measurements, to ensure that the modelling assumptions are sound. This has been done extensively in previous work [10, 11, 22]. An example is shown in Fig. 5, which compares the velocities computed along the top surface with measurements from videos of die injection into the water model. These particular results are of practical importance because the maximum surface velocity should fall within a critical range (suggested by Kubota to be 0.2-0.4m/s)[23, 24] in order to avoid defects. The measurements are instantaneous, so are expected to fall within the range of velocities computed at this position. The rough agreement suggests that these computational models are able to predict flow in this process.

## **Effect of Turbulence Model**

The results in Fig. 5 also compare the predictions of different turbulence models. The difference between different models is on the same order as the difference between the models and the measurements. As reported in previous work, [8] the K- $\epsilon$  model gives qualitatively the same time-averaged results as the LES models. This figure also suggests that the effect of adding an SGS-K model [12] is relatively small. Closer analysis of the velocity vector field confirms this, except in regions very close to the nozzle port exits, where the high velocity gradients generate extra turbulent energy, which causes the SGS-K model jet to spread a little more. The general similarity indicates that either the unresolved small turbulent eddies are not very important, or that false diffusion from numerical discretization errors dominates over the sub-grid scale effects.



Figure 5. Top surface velocity predictions with different turbulence models.

## Effect of Asymmetry Assumption

The continuous casting process in Fig. 1 appears at first glance to contain two-fold symmetry, about the centerplanes between the wide and narrow faces. The effect of invoking these symmetry assumptions was investigated by performing simulations on a quarter-domain, half-domain, and a full-domain with no symmetry assumed. The results are compared in Fig. 6.

The full-domain simulation was performed on a 0.74-million cell grid, so has larger cell spacing than the other meshes. However, the differences between the right and left sides of the domain are more significant than the differences between grids. The asymmetries between sides are minor for the time-average flow pattern for this nozzle, but have very detrimental effects on quality in other cases. Large instantaneous variations between sides can only be observed in transient simulations with a full-domain model. Of even greater importance is the exaggerated spreading of the jet in the quarter simulation. This unreasonable result is believed to be caused by the prevention of jet oscillation across the symmetry plane. In the half and full domains, the jet is observed to swirl and oscillate both vertically and horizontally as it traverses the mold. The K- $\epsilon$ model results do not suffer from this problem, as the K- $\epsilon$  results in Fig. 5, were also produced on a quarter domain. Fig. 7 compares the computed speed  $(v_x^2 + v_z^2)^{0.5}$  along a vertical line in the caster centerplane, midway between the SEN center and the narrow face. This figure quantifies that the differences between velocity predictions using different model domains are small, except for the poor quarter-domain results. Fig. 8 compares the transient velocity fluctuations predicted using the different domains. The results with the half-domain are similar to the each half of the full-domain model. These rms velocity predictions appear to have roughly equal accuracy as the velocity predictions themselves.



Figure 6. Effect of symmetry assumption on time-averaged velocity fields for simulation domains with (a) both halves (b) half (left) and quarter (right) of the mold region.



Figure 7. Time-averaged velocities along vertical line 152mm from SEN outlet, from LES.

### **Effect of Inlet Conditions**

Previous work has established that inlet conditions have a great effect on the flow pattern [22], so modeling should be extended upstream to simulate flow in the nozzle. The time-averaged velocities in the nozzle were presented in Fig. 2 for a 9.5s simulation with the 0.6 million node mesh of the complete nozzle. A slight asymmetry is observed at the top of the nozzle, where flow accelerates past the stopper rod flow control. This does not persist to the lower region of the nozzle, however, as flow disturbances diminish with distance downstream. For this reason, flow entering the mold from a shortened 0.1-million half-nozzle domain (neglecting the stopper rod) was similar. In both cases, most of the flow exits the lower portion of the nozzles, owing to the oversized outlet ports (ratio of total port area to bore area at top of ports is 1.54). The downward angle of the two side jets varies in time from  $\sim 30^{\circ}$  to  $45^{\circ}$ . Results from further simplifications of the nozzle were unacceptably different [22].

Uncoupling of the nozzle and mold domains was found in previous work [7] to have negligible adverse effect, which was confirmed in the present work. The combined effects of simplifying the nozzle and coupling the nozzle and mold domains on flow entering the mold is seen in Fig. 9 to be small. The very slight uplifting of flow near the edges of the side ports is believed to be due to the hindrance of flow oscillations inside the nozzle by the half-nozzle domain. The combined effect on flow in the mold of this difference in inlet conditions and the difference between the coarse-grid full mold and fine-grid half-mold simulations is shown in Fig. 10 to be small.



Figure 9. Comparison of time-averaged velocity vectors exiting nozzle ports obtained from (a) coupled simplified nozzle and (b) uncoupled complete nozzle simulations.



Figure 10. Comparison of time-averaged velocities obtained from nozzle-mold coupled and uncoupled mold simulation along a vertical line 152mm from the SEN outlet plane.

#### Conclusions

Computational models of turbulent flow have been applied to investigate computational issues in simulation of metallurgical processes. The time-averaged flow pattern is the easiest result to approximate with reasonable accuracy, even with a relatively coarse grid and simplified model. Actual velocity errors are larger than they might appear on a vector plot, however.

Transient phenomena are better modelled with Large Eddy Simulation, but care must taken in choosing the domain and grid. The domain should be extended sufficiently upstream to produce reasonable results in the region of interest. Uncoupling the domains of adjacent regions, such as performing separate calculations of flow in the nozzle and mold, has little effect if the flow between regions does not include much recirculation.

Invoking symmetry by modelling only a quarter of the process is reasonable for time-averaged models, such as K- $\epsilon$ . However, the transient LES models were found to be sensitive to disruption of the real flow oscillations which can produce inaccurate results. For example, a quarter-mold simulation that prevented transverse jet oscillation resulted in exaggerated vertical oscillation, excessive jet spreading, and poor accuracy.

Secondary phenomena such as the prediction of superheat transport are more difficult to model accurately and the results from different models vary widely. Inadequate grid refinement produces very large errors, particularly for the low-Re K- $\epsilon$  model. Further work is needed on turbulence models, wall laws, and grid refinement for heat transfer prediction, especially for processes involving solidification.

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