

**Final Report for Blue Waters, Fall, 2015:**

# Fluid-Flow and Stress Analysis of Steel Continuous Casting

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## **2. Project Abstract**

Many defects in steel products are caused by transient fluid flow, such as level fluctuations capturing slag inclusions at the top surface of the mold. This project aims to develop advanced computational models of the continuous casting of steel, including multiphase turbulent fluid flow, MagnetoHydroDynamics, particle transport, interfacial behavior, heat transfer, solidification, and thermal-mechanical behavior; to apply these models to better understand the multiphysics phenomena related to defect formation; and to evaluate ways to improve this important commercial process, such as finding safe operating windows of adjustable casting conditions. In the past year, advanced multiphase flow simulations have been conducted to gain new insights into transient defect formation. The inhouse multi-GPU code CUFLOW has been developed and tested on Blue Waters XK node, with Nvidia K20x GPU co-processors, and shows good speed up. Recent testing of commercial code, ANSYS FLUENT also shows good scaling on Blue Waters. Blue Waters is needed to shorten simulation times (currently several months on workstations), to enable better mesh refinement, for more accurate multiphase flow simulation. Future plans will extend this research to thermal-stress analysis of crack formation on Blue Waters.

## **3. Field of Science**

Engineering (specifically – mechanical engineering and materials process engineering)

Fluid, Particulate, and Hydraulic Systems (continuous casting of steel)

Computer and Computation Research (Large-Eddy Simulation of multiphase flow with electromagnetics)

## 4. Description or Research Activities and Results

### 4.1 Key Challenges

Continuous casting produces over 95% of steel in the world today, so small improvements to this important commercial process have large impact. Many defects in final steel products originate during this process, including bubbles, slag and inclusions, captured due to non-optimal flow in the mold, and oxidized/segregated longitudinal cracks due to inadequate mold taper. Continuous casting is difficult to optimize, owing to the hostile environment of the molten steel, and the many process variables which affect these problems, including the nozzle and mold geometry, casting speed, nozzle submergence depth, gas injection, and electromagnetic forces. Thus, computational models present an ideal tool to improve this process, if they are accurate enough.

This work aims to improve understanding of this complex process using comprehensive computational models, made better by the increased computing power of Blue Waters. Specifically, high-resolution multiphase flow simulations will calculate the turbulent flow pattern, interface motion, and particle transport to capture phenomena, including the transport and entrapment of bubbles and inclusions, detrimental fluctuations of mold flux/molten steel interface, and mold slag entrainment. Furthermore, effect of casting conditions such as electromagnetic force (induced by static- and moving-magnetic fields), nozzle port angle, and nozzle submergence depth will be investigated. Secondly, a transient thermo-fluid model will be applied to simulate the initial solidification in the meniscus region and to investigate the formation mechanism of defects such as hooks and oscillation marks. In addition, transient, explicit, thermal-elastic-viscoplastic finite-element analysis of the thermal-mechanical behavior of the solidifying steel shell will be performed at the micro-scale, including complicated microstructural features such as dendrites, which govern the formation of hot-tear cracks. Previous work suggests that very refined numerical meshes are needed for quantitative predictions of these behaviors. When combined with the long time scales needed, the computational cost is very large (several months for one LES simulation on a workstation [1]). This presents an ideal opportunity for high-performance computing, such as the Blue Waters computer system.

To facilitate easy technology transfer, the widely-used commercial software tools (FLUENT and ABAQUS/Explicit) will be used to supplement our in-house code, CUFLOW. Both software developers have efficient implementations on the Blue Waters system, with promising scale-up for our specific numerical methodologies, which we are exploiting, with the help of experts on both codes (both in-house co-PIs, and collaborators at the software companies).

This project is supported by the Continuous Casting Consortium at the University of Illinois (which currently has 11 member companies who provide funding and experimental measurements, and freely share the results of the research with each other and with the public), and by two active NSF grants (NSF CMMI-13-00907 and CMMI 11-30882).

## 4.2 *Why It Matters*

This project aims to safe operating windows in the continuous casting process, pictured in Fig. 1 [2], by avoiding defects forming in the mold related to fluid flow, and crack formation in the solidifying steel shell. By using Blue Waters, bubble rising dynamics with and without static magnetic fields, have been quantified to minimize inclusion defects [Accomplishments A-1]. In addition, we have investigated transient mold flow patterns and their effect on surface flows with several nozzle port angles, to find optimal nozzle angle for the considered casting condition [Accomplishments A-2]. Based on understanding from these studies, we plan to further improve the models and conduct simulations of more difficult casting scenarios, to gain deeper insight into the relation between the transient fluid flow phenomena and defect formation during continuous slab casting. First, we plan to model bubble behaviors such as formation, breakup, coalescence, and accumulation, which are affected by turbulent flows in nozzle and mold, in order to track the size distribution and to investigate more realistic bubble transport. The bubble size distribution is needed as input data for coupled multiphase transient LES model simulations. Transient slag/molten steel interface motion will be also calculated by applying a transient VOF model. From the VOF modeling, mechanisms of surface and internal defects caused by surface slag entrainments and slag/molten steel interface instability, can be investigated. Furthermore, the effects of magnetic forces (both static or “braking” fields and moving or “stirring” fields, pictured in Fig. 2) [3] on multiphase flow will be further studied with changing casting speed, coil current, and nozzle submergence depth. Of particular interest is the top surface flow in the mold, which can lead to surface defects if the transient level fluctuations are too large, or slag entrainment if the surface velocities are too large. Then, the transport and entrapment of inclusion particles will be computed from the previously-calculated transient flow fields. Large eddy simulations (LES) will be performed for different: magnetic field strengths and locations, argon gas injection rates, and nozzle geometries (which are all easy and inexpensive to change in practice). The results will be analyzed in order to find safe operating windows for different casting conditions, (such as slab width, and casting speed).

Previous investigations [1] show that in order to resolve the flow details in the caster, a fine mesh should be used. For example, our previous simulation with 7.6 million cells properly resolved the

thin Hartmann layer [4], and quantitatively matched the flow pattern measured in a laboratory-scale model [4], while a 1.2-million-cell mesh used in another numerical study of the same experiment produced a qualitatively-different flow pattern [5]. In this project, to study the inclusion transport and capture in the caster, a fine mesh is needed to accurately predict the velocities of the fluid and particle when it is close to the dendritic solidification front. The computational domain should include the complete slide gate, submergence nozzle (SEN) and mold, to incorporate asymmetric effects from upstream. The large physical size of the commercial caster requires that the computational domain include 1.495 m<sup>3</sup> (mold thickness 230 mm, mold width 1300 mm and length of the domain is 5000 mm). The average cell size used in these simulations should be ~64 mm<sup>3</sup> (cube with edge length 4 mm) so around 23.4 million cells will be required.

Argon gas is often injected into the nozzle, (to avoid air aspiration, reoxidation, and clogging problems), but it also forms bubbles which greatly affect the transient flow pattern in the mold and particle entrapment [6]. To include the coupled effects of argon gas bubbles on the multiphase flow, simulations will be conducted using a “Discrete Phase Model” DPM modeling approach, which tracks the trajectory of each single bubble through the domain, and its coupled effect (via corresponding source terms in both the fluid momentum and particle transport equations) on the local fluid velocity. Although very accurate, this approach is very computationally intensive in both tracking and storing the location of each of several thousand gas bubbles. The LES MHD simulations with fine mesh resolution are very computational expensive. Our previous simulations required several months of computation for just a 15-second simulation [4] with less resolution than preferred, and less time simulated than needed to capture low-frequency behaviors, which are often most important [7,8].

The region where the steel shell first starts to solidify is called the meniscus region due to its shape. Defects formed during initial solidification in the meniscus region will be carried down with the shell and end up in final product. While steel flow in most of the caster is dominated by the incoming steel jet from the SEN, flow in the meniscus region is also affected by the oscillating mold and the slag layer floating on top of the steel. In order to investigate surface defects such as oscillation marks and hooks, a detailed model of the meniscus region is needed. A coupled thermo-fluid transient model has been developed which includes both the steel and slag phase using the

“volume of fluid” method. Steel solidification is achieved by latent heat removal and solidified steel will be pulled down at casting speed. Previous studies conducted on a lab PC shows that a very fine mesh is needed to capture the shape of solidified steel shell tip and the gap between steel shell and the mold. In addition, due to the complicated nature of this model, (coupled flow-thermo-VOF-solidification), a very small time step size of  $10^{-5}$  second is needed. A single run on a lab PC requires more than 2 weeks of wall clock time, which our projections show should reduce to a single day with only 4 Blue Waters nodes.

To avoid cracking defects and catastrophic breakouts during casting requires quantifying the thermal-mechanical behavior of the solidifying steel shell in the mold. The taper (slope) of the mold walls, which are subject to significant thermal distortion during operation, should match the shape of the shrinking solidifying shell, as it moves down through the mold. In addition to being influenced by fluid flow, heat transfer is controlled by the size of the interfacial gap between the shell and the mold, so the macroscale thermal and stress calculations are intimately coupled. Cracks can form along the austenite grain boundaries, if the grains grow too large, which can be simulated by a microscale model of individual austenite grain [9], in order to find failure criteria for the macroscale model. By aiming to capture physical phenomena involving detailed behavior on the small scale of the microstructure, the finite-element model cannot run on a personal computer and requires advanced computation, such as available with Blue Waters.

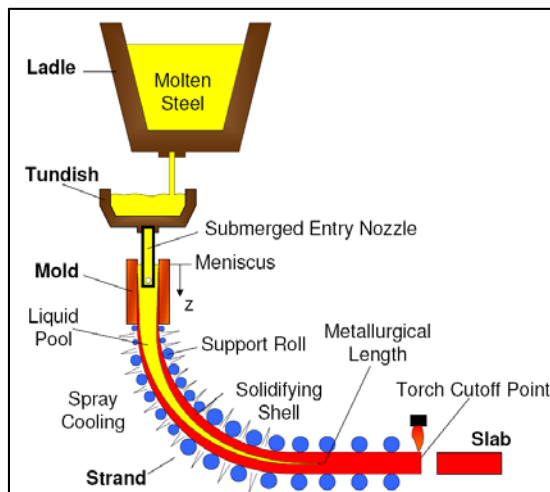


Fig. 1. Continuous Casting Process  
(Adapted from Lance C. Hibbeler [2])

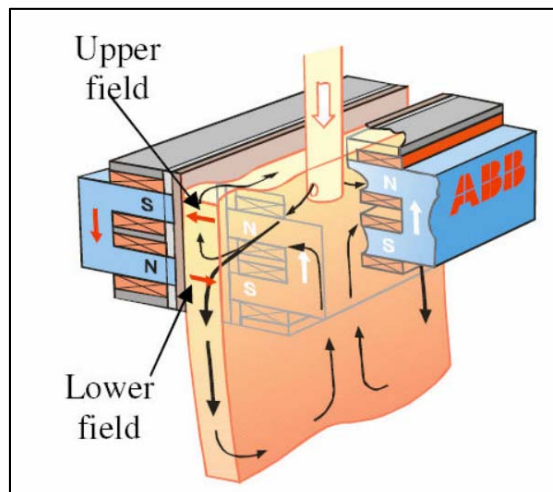


Fig. 2. Sketch of EMBR system  
(Adapted from Okazawa et al 2001[3])

### 4.3 *Why Blue Waters?*

To model the tremendously-complex, interrelated phenomena which govern the formation of defects in the continuous casting, several different computational codes are being applied. These are an in-house fluid-flow code CUFLOW, the commercial CFD package FLUENT (by ANSYS, Inc.), and the commercial code ABAQUS, for thermal stress analysis. The following 3 sections present a brief description of each model, followed by an evaluation of the performance of each code on Blue Waters.

#### **4.3.A.1 – In-house code CUFLOW for LES**

CUFLOW [10-12], was developed by UIUC Professor P. Vanka and coworkers to solve the governing equations for 3D MHD flow problem. The code employs Cartesian grids combined with the immersed boundary method to integrate the three-dimensional unsteady incompressible Navier-Stokes equations. The continuity and momentum equations are solved using the fractional step method and the pressure-poisson equation is solved by using a V-cycle multi-grid method, and red-black Gauss-Seidel SOR. Multi-GPU parallel computing was recently implemented in CUFLOW on Blue Waters (as part of our exploratory grant). The computational domain was first uniformly divided into several sub-domains, and then each sub-domain was assigned to one GPU. During the computation, the variables in the halo cells are first computed and then transferred during the computation of the inner part of the sub-domain. Data transfer between nodes was accomplished using Message Passing Interface (MPI), and the 3 steps involved in data transfer are illustrated in Fig. 4.3.A-1 below. During the computation, variables in the halo cells are first copied from the sender GPU memory to its system memory. Then, MPI calls are used to transfer appropriate data from sender system RAM to the receiver system RAM. Finally, the data in the receiver system RAM is copied into its own GPU memory.

The methodologies and code implementation of CUFLOW have been validated with both known solutions, and with experimental measurements in both laboratory and commercial-scale continuous casting machines. CUFLOW was implemented to run on Blue Waters, during our Exploratory Grant. Applied to test problems, it was found to scale very well with both multi-CPU

and multi-GPU configurations, with demonstrated 50X speedup, as documented in the next section. It is ready to use for practical simulations of flow in the real caster.

#### 4.3.A.2 Evaluation of CUFLOW performance on Blue Waters

In order to evaluate the performance of CUFLOW on Blue Waters, a 3D lid-driven cavity flow problem with 8.4 million cells was tested on our 4-GPU workstation and on Blue Waters. The number of cells in x, y and z direction was 128, 128 and 512, respectively. The computational domain was uniformly divided along z-direction and sub-domains were assigned to GPUs. Seven multi-grid levels were used in all calculations. The configurations of the two computer systems (4GPU desktop and BW) are shown in Fig. 4.3 A-1 and listed in Table 4.3.A-1.

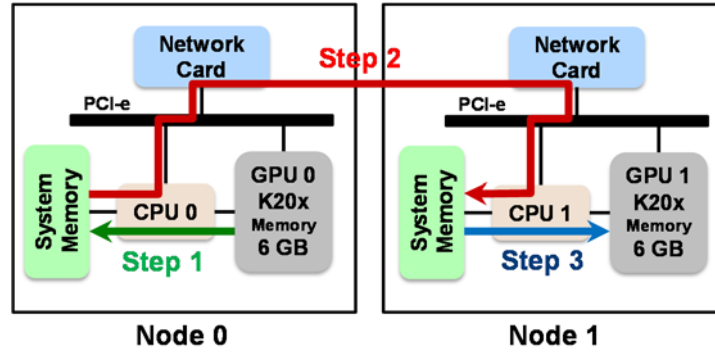


Fig. 4.3.A-1 Three steps of data transfer between different GPUs

Table 4.3.A-1. Configuration of 4-GPU Desktop and BW Supercomputer XK Node

	4-GPU Desktop	Blue Waters XK node
Number of Nodes	1	4224
GPU per node	4	1
GPU Specifications	Nvidia Tesla C2075 (5GB)	Nvidia Tesla K20x (6GB)
CPU Specifications	Xeon E5-2650v2, 2.60GHz, 8 Cores	AMD 6276, 2.3GHz, 16 cores

Both CPU and GPU versions of CUFLOW were developed and tested, and the computation time required for the lid-driven cavity flow problem (8.4 million cells for 500 iterations, extrapolated to 100s with time step 0.001s) is given in Fig. 4.3.A-2. The timing results in Fig. 4.3.A-2 show that on Blue Waters (BW), running CUFLOW on one GPU is ~42 times faster than running on 1 core. On the 4-GPU desktop, 2 GPU parallel execution is 1.8x faster than 1 GPU execution, while 4 GPU execution (ie 4 XK nodes) is 3.2x times faster than 1 GPU execution. On Blue Waters, although the scaling is slightly less than that on our 4-GPU desktop, the time needed to run the same simulations is less. The decrease in scaling is because 1) the Tesla K20x is more powerful



than Tesla C2075; and 2) when 4 GPU are used, the computation load on each GPU is light, so the time taken in communication is more important. In the proposed runs with ~23 million cells, it is expected that each GPU will have more computation load so scaling (speedup) on Blue Waters should be even better.

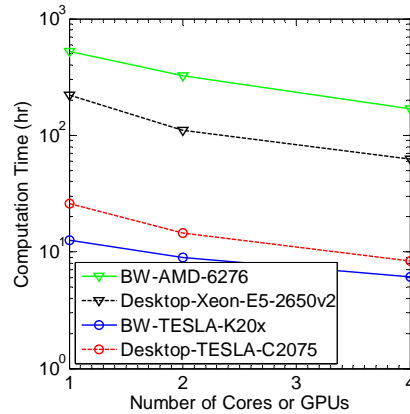


Fig. 4.3.A-2 Comparison of computation time

To investigate the effect of mesh size on the performance of CUFLOW, the Pressure-Poisson-Equation (PPE) solver was tested on a single Blue Waters XK7 node by solving a heat conduction problem in a 3 dimensional cube. The solver uses V-cycle multigrid technique and red/black successive over relaxation (SOR) method. Both CPU and GPU versions were developed and tested. Increasing grid size from 0.26 million to 0.56 billion cells increased speedup, to a maximum of 25X, as shown in Fig. 4.3.A-3. The model is being applied to predict the entrapment locations of inclusion particles in the solidified strand for conditions where measurements were obtained at an operating commercial caster [19].

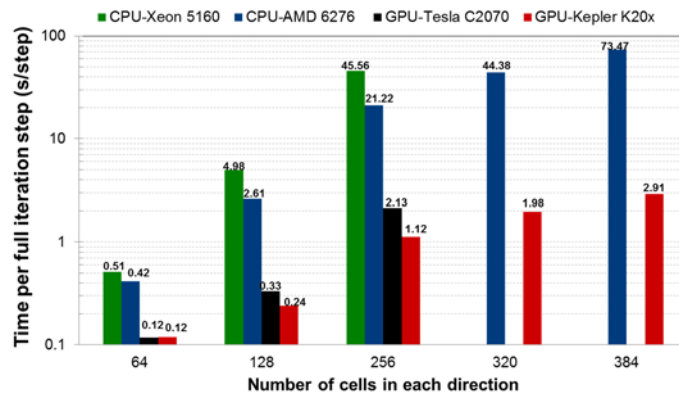


Fig. 4.3.A-3 PPE solver performance on Blue Waters CPU and GPU

Finally, CUFLOW was applied to perform a realistic caster LES simulation on Blue Waters with 4.5 million cells (cube with edge size 7.5mm) for 45s flow time with magnetic braking in a 6m-long domain with time steps of 0.0002s [19]. The run took ~48 hours to run on 6 GPUs (6 XK

nodes), which was 288 node hours, although load partitioning was non-optimal due to more cells assigned to the GPU in the mold region.

#### **4.3.B-1 – Commercial package ANSYS FLUENT for Multiphase Flow Modeling**

FLUENT is a widely used commercial software package from Ansys Inc. to solve fluid flow problems. It contains a very flexible finite-volume-based discretization of the continuity, momentum, and scalar transport equations which includes most standard FVM methods in the previous literature for solving turbulent flow problems. It includes the LES method, with several different subgrid-scale models, various other turbulence models, enhanced wall laws, the Euler-Eulerian, Euler-Lagrangian, and Volume-of-Fluid (VOF) methods for multiphase flow, and both structured and unstructured grid generation modules. FLUENT also features User Defined Functions (UDF) which enable easy implementation of further methodologies, such as we have developed for the current work: 1) mass and momentum sources to account for the solidifying steel, 2) a particle capture criterion function that includes a balance of more than 10 different forces on particles which contact the solidification front [19]. FLUENT model results on this problem have been validated with both test problems and experimental measurements (lab scale water model experiments and nail board dipping plant-tests) in previous work.

As part of our first year's grant, it was demonstrated that FLUENT can run efficiently on Blue Waters computer system at UIUC, including the UDFs. Several successful LES simulations have been performed, and excellent scaling was achieved, (over 100X speedup), as documented in the next section. FLUENT is now ready for realistic long-time transient LES simulations of multiphase flow.

#### **4.3.B-2 Evaluation of FLUENT performance on Blue Waters**

To evaluate the performance of FLUENT on Blue Waters, a real world problem of argon-steel two-phase turbulent flows in a continuous casting mold was run on several different computer systems. The test problem consists of 0.66 million hexahedral mapped computational cells and about ~8.4 million DOFs. The results show that 100 iterations on Blue Waters using 240 cores (15 XK nodes) require 11.15 second of wall clock time, or 0.111 second per RANS iteration. On a workstation (DELL Precision T7600 with Intel Xeon5650 2.67GHz CPU processor/node with 6

Cores) in the Metals Processing Simulation Laboratory (345 MEB), the same simulation (using 1 core) required 12 second of average wall-clock time per iteration. Thus, the speedup on Blue Waters is:  $12/0.111 = 108.1$  times. Further simulations on Blue Waters with different numbers of computer nodes show almost linear speedup with increasing nodes, as shown in Fig. 4.3.B-1. With 192 nodes, the simulations run  $\sim 100$  times faster than on our high-end PC workstations.

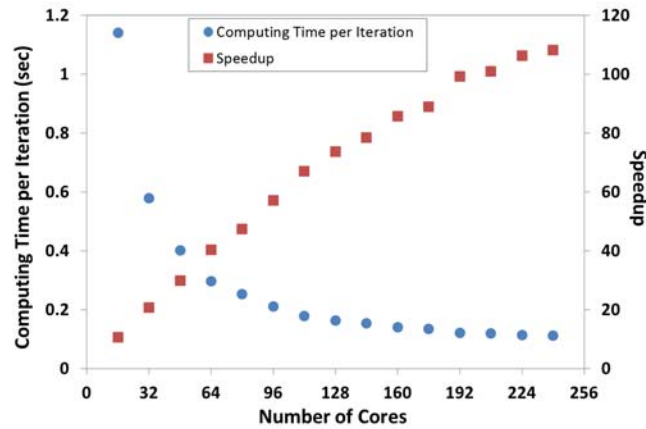


Fig. 4.3.B-1. FLUENT computational cost on Blue Waters, (per iteration of FLUENT) with speedup relative to a lab workstation.

#### 4.3.C-1 – Commercial package ABAQUS for Thermal-Stress Analysis

For the thermal-stress analysis, the commercial package, ABAQUS/Explicit will be used to conduct the thermal-mechanical multi-scale simulations of mechanical behavior the solidifying steel shell. The governing dynamic tensor differential equations comprising the force-stress, stress-strain, and strain-displacement are solved using the finite-element method, with hexahedral elements [13, 14]. We have developed elastic-viscoplastic constitutive equations that include the effects of thermal strain, inelastic creep/plasticity for the multiple phases of steel (liquid, delta-ferrite, and austenite) and fluid-flow strain [13]. We have developed specialized numerical methods (implemented via user subroutines) to incorporate the effects of fluid flow [15], and superheat [16] and to use a highly-scalable explicit solver for this complex highly-coupled thermal-mechanical problem with solidification [17].

As part of our Exploratory Grant, both implicit and explicit ABAQUS performance was investigated briefly. Although significant speedup was found with implicit ABAQUS, the scaling was not optimal. ABAQUS Explicit shows excellent promise, so will be the focus of future work on the stress analysis part of the project.

#### **4.3.C-2 Evaluation of ABAQUS performance on Blue Waters**

For the stress analysis, several runs with a mesh of 375,200 elements, 754,554 nodes and 2,263,662 DOF were completed on Blue Waters with implicit ABAQUS, which allows input and use of the phase field. The CPU time for one Newton iteration, consisting of 0.57 Tflop, is presented in Table 4.3.C-1 for different numbers of threads. The optimum number of threads is  $\sim 64$ . The efficiency is not considered acceptable and appears to be limited by the FEM assembly process, coupling between DOFs during solving, or by communication across processors. Results with this model show how temperature and shape of the distorted mold evolve during a caster startup, and match with plant inclinometer measurements on the cold-face exterior [20].

Table 4.3.C-1. ABQUS runs on BW -- CPU time required for different threads number

Threads Number	CPU Time (s)	CPU time per thread (s)	Wall Clock Time Required for 1 sec simulation (Day)
32	15	0.47	6.80
64	9	0.14	5.25
128	6	0.05	5.50
256	4	0.02	5.50

Preliminary work with ABAQUS Explicit on a small test problem has shown that a dual-core, 2.2 GHz Intel Core2 progresses at about  $5e-5$  seconds of casting simulation per wall clock second for the 1.2-million DOF model. The simulation of  $\sim 10$  seconds of casting time, requires about 560 hours with 2 cores for the test problem.

#### **4.2, 4.3 References**

[1] Singh, Ramnik. "High Fidelity Numerical Investigations of Tailored Magnetic Fields for Defect Reduction in Continuous Casting of Steel." MS Thesis, University of Illinois at Urbana-Champaign, IL, (2013).

[2] <https://wiki.engr.illinois.edu/display/cs519sp11/Lance+C.+Hibbeler+Project+Page>

- [3] Okazawa, K., T. Takehito, J. Fukuda, T. Kawase, and M. Toki, "Fluid Flow in a Continuous Casting Mold Driven by Linear Induction Motors," *ISIJ International*, 2001, Vol. 41, No. 8, pp. 851-858.
- [4] Singh, R., B.G. Thomas, and P. Vanka, "Effects of a Magnetic Field on Turbulent Flow in the Mold Region of a Steel Caster," *Metallurgical and Materials Transactions B*, 44: 5, pp. 1201-1221, 2013.
- [5] X. Miao, K. Timmel, D. Lucas, S. Ren, Z. Eckert, and G. Gerbeth: *Metall. Mater. Trans. B*, 2012, vol. 43B, pp. 954–72.
- [6] Thomas, B. G., X. Huang, and R. C. Sussman, "Simulation of Argon Gas Flow Effects in a Continuous Slab Caster," *Metallurgical and Materials Transactions B*, 25B:4, 527-547, 1994.
- [7] Cho, Seong-Mook, Kim, Seon-Hyo, and Brian G. Thomas, "Transient Fluid Flow during Steady Continuous Casting of Steel Slabs, Part I: Measurements and Modeling of Two-phase Flow, *ISIJ International*, Vol. 54, No. 4, (April), 2014, pp. 845-854.
- [8] Cho, Seong-Mook, Kim, Seon-Hyo, and Brian G. Thomas, "Transient Fluid Flow during Steady Continuous Casting of Steel Slabs, Part II: Effect of Double-Ruler Electro-Magnetic Braking (EMBr)", *ISIJ International*, , Vol. 54, No. 4, (April), 2014, pp. 855-864.
- [9] Murali, Aravind, "Thermal-stress analysis of columnar microstructures and intergranular crack formation", *CCC Annual Meeting*, University of Illinois, 2014.
- [10] Vanka, S. P., Shinn, A. F., and Sahu, K. C., "Computational Fluid Dynamics Using Graphics Processing Units: Challenges and Opportunities," In *Proceedings of the ASME 2011 IMECE Conference*, Denver, CO, 2011.
- [11] Shinn, A. F., "Large Eddy Simulations of Turbulent Flows on Graphics Processing Units: Application to Film-Cooling Flows," *Ph.D Thesis*, University of Illinois at Urbana-Champaign, IL, 2011.
- [12] Chaudhary, R., "Studies of Turbulent Flows in Continuous Casting of Steel with and without Magnetic Field," *Ph. D. Thesis*, University of Illinois at Urbana-Champaign, IL, 2011.

- [13] Li, C. and B. G. Thomas, “Thermo-Mechanical Finite-Element Model of Shell Behavior in Continuous Casting of Steel,” *Metallurgical and Materials Transactions B*, 35B:6, 1151-1172, 2004.
- [14] S. KORIC, B. G. THOMAS Efficient thermo-mechanical model for solidification processes, *International Journal for Numerical Methods in Engineering*, 2006:66 pp. 1955-1989
- [15] S. KORIC, L. C. HIBBELER, R. LIU, and B. G. THOMAS, Multiphysics Modeling of Metal Solidification on the Continuum Level, *Numerical Heat Transfer B*, 2010:58 pp. 371-392
- [16] S.Koric, B. G. Thomas, V. R. Voller, “Enhanced Latent Heat Method to Incorporate Superheat Effects Into Fixed-Grid Multiphysics Simulations,” *Numerical Heat Transfer B*, 2010:57 pp. 396-413.
- [17] S. Koric, L. C. Hibbeler, and B. G. Thomas, “Explicit coupled thermo-mechanical finite element model of steel solidification.” *International Journal for Numerical Methods in Engineering*, vol 73 (2009), pg 1—31.
- [18] Standard Performance Evaluation Corporation for Xeon5650:  
<http://www.spec.org/cpu2006/results/res2011q3/cpu2006-20110829-18521.html>
- [19] K. Jin, “Effect of EMBr on Flow and Particle Capture and Parametric Studies of Transient Flow with LES on GPU”, CCC Annual Meeting, University of Illinois, 2014.
- [20] L. C. Hibbeler, B. G. Thomas, R. C. Schimmel, and H. H. Visser, “Simulation and Online Measurement of Narrow Face Mold Distortion in Thin-Slab Casting.” *Proceedings of the 8th European Continuous Casting Conference*, 2014, in press.
- [21] <http://otp.investis.com/clients/us/ansys/usn/usnewsstory.aspx?cid=806&newsid=30561>
- [22] <http://www.prnewswire.com/news-releases/ansys-and-cray-smash-supercomputing-records-300139525.html>

## *4.4. Accomplishments*

Significant progress has been made in 2015 on several aspects of this multifaceted project. This brief report summarizes some new results accomplished this year on two different aspects.

### **4.4 Accomplishments A-1**

#### **Dynamics of argon bubbles in steel continuous casting with a magnetic field**

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#### **Executive Summary**

This project aims to mathematically model multiphase flow in the steel continuous casting in order to gain increased understanding and practical insights to improve this important commercial process. Specifically, Large Eddy Simulations of turbulent fluid flow are conducted to investigate the dynamic motion of argon bubbles in the caster with different casting conditions such as electro-magnetic braking (EMBr), in order to minimize inclusion entrapment. The present work quantifies how the oscillations of the shape and velocity of the rising bubbles can be damped with the application of a static external magnetic field.

#### **Introduction**

Continuous Casting (CC) is used to produce more than 95% of steel in the world [1] so even small improvements can have a large impact. In this process, Fig. A-1-1 shows how molten steel flows into the mold, to solidify a thin shell against the walls that is withdrawn downward at the casting speed to support the liquid pool below the mold. Most defects arise in the mold region, due to the entrapment of inclusion particles into the solidifying shell, and crack formation in the newly-solidified steel shell. To improve steel products requires understanding the mechanisms of defect formation, and to find windows of safe operation. The harsh environment makes experiments difficult, so computer simulations are an important tool. Argon gas is often injected and affects defect formation in several ways, including the attachment of inclusions to the surface of rising argon gas bubbles, so it is important to understand the complex motion and dynamics of the bubbles. The shape and motion of the bubbles are modified by applying external magnetic fields. To simulate the complex motion of argon gas bubbles rising in turbulent molten steel and their interaction with inclusion particles and external magnetic fields requires advanced computational models and computing capabilities.

#### **Methods**

To better understand the behavior of argon bubbles and their interaction with inclusion particles during steel continuous casting, the motion of a single argon gas bubble rising in quiescent liquid steel under an

external magnetic field is studied numerically using a Volume-of-Fluid (VOF) method implemented into the finite-difference fluid-flow program CUFLOW [2]. To mitigate the spurious velocities generated in numerical simulation of multiphase flows with large density differences, an improved algorithm for surface tension modeling, originally proposed by Wang and Tong [3] is applied.

The in-house multi-GPU code CUFLOW has been developed and tested on Blue Waters XK node, which has Nvidia K20x GPU as co-processors, and good speed up has been obtained. Fig. A-1-2 shows that less than 2 days are required for a 30s-LES simulation of flow in a caster domain with 14.1 million cells (based on 100 time step test run with average time step size  $\Delta t = 0.0005s$ ). Preliminary results show that ANSYS FLUENT also has good scaling on Blue Waters for this problem. To resolve turbulent flow in the real caster complete with thousands of bubbles is only feasible with petascale computing, such as Blue Waters.

As shown in Fig. A-1-3(a) the computational domain of  $6d \times 6d$  (section)  $\times 16d$  (long) contains  $192 \times 192 \times 512$  (about 19 million) cells. A spherical argon bubble of diameter  $d$  was initially centered at the center of the container bottom. A uniform magnetic field was applied in  $x$ . The dimensionless shape and velocity are tracked with dimensionless time  $t^* = t\sqrt{g/d}$ .

## Results

Fig. A-1-3 shows that rise velocity is smooth and non-oscillatory at early stages ( $t^* < 0.5$ ), especially with small bubbles. Without a magnetic field, velocity increases to 2.5 and then decreases slightly, due to the inclined motion of the 3mm bubble. Applying a transverse magnetic field of  $B = 0.2$  T, lowers the rise velocities by 4%. Increasing the field strength to 0.5 T, decreases the rise velocities by 24% to 1.83. For a 7 mm bubble, without no magnetic field, the rise velocity becomes oscillatory after  $t^* > 1.0$ , due to the varying drag force, as the bubble shape expands and contracts along different axes. With a magnetic field of 0.2 T, the oscillations eventually are dampened. Increasing the field to 0.5 T completely damps the oscillations, resulting in a steady rise velocity, that is reduced by  $\sim 25\%$ , relative to no field.

Fig. A-1-4 shows isosurfaces of  $z$  vorticity  $\omega_z^* = \pm 1$  at  $t^* = 9$  for the 7 mm bubble. The alternating patterns are more complex than those behind a 3 mm bubble. With a 0.2 T field, the isosurfaces elongate in the magnetic field ( $x$ ) direction because the  $y$  and  $z$  velocities in the surrounding fluid are reduced, so the flow perpendicular to the magnetic field is dampened. The magnetic-field damping effect was studied previously [5] in a driven cavity. Increasing the field strength to 0.5 T makes complex wake structure almost disappear. The front isosurface is wider (in  $x$ ) near the bubble, and bundled below, where the wake spreads (in  $y$ ).

In related work, Large Eddy Simulations were applied to investigate the flow in a commercial caster. Fig. A-1-5(a) and (c) show instantaneous velocity magnitude in top views of the caster (casting speed 1.5 m/min). Applying an EMBr field greatly lowers the velocity near the top surface, which can lead to problems of meniscus freezing, where the steel around the 3-phase perimeter solidifies into detrimental hook structures which capture inclusions and bubbles. Fig. A-1-5(b) and (d) show velocity in side views. Applying EMBr deflects the jets upward, but the flow in the top region is reduced by the dampening effect of the field. The steel plant that was experiencing this problem lowered the field strength towards the top of the mold and increased the casting speed, which has improved quality.



## References

- [1] Steel Statistical Yearbook 2014, Worldsteel Assoc., Brussels, (2014)
- [2] Chaudhary, R., B.G. Thomas, and S.P. Vanka, "Effect of Electromagnetic Ruler Braking (EMBr) on Transient Turbulent Flow in Continuous Slab Casting using Large Eddy Simulations," *Metallurgical and Materials Transactions B*, 43B: 3, 532-553, 2012.
- [3] Wang, Z. Y. and A. Y. Tong, "Deformation and oscillations of a single gas bubble rising in a narrow vertical tube," *ASME 4th International Conference on Nanochannels, Microchannels, and Minichannels*, (Limerick, Ireland, June 19–21, 2006), pp. 1195-1202.
- [4] Jin K., P. Kumar, S. P. Vanka and B.G. Thomas, "Rise of an argon bubble in liquid steel in the presence of a transverse magnetic field," *Physics of Fluids*, paper submitted and under review.
- [5] Jin K., S. P. Vanka, and B. G. Thomas, "Three-dimensional flow in a driven cavity subjected to an external magnetic field," *Journal of Fluids Engineering*, 137 (2015), 071104.

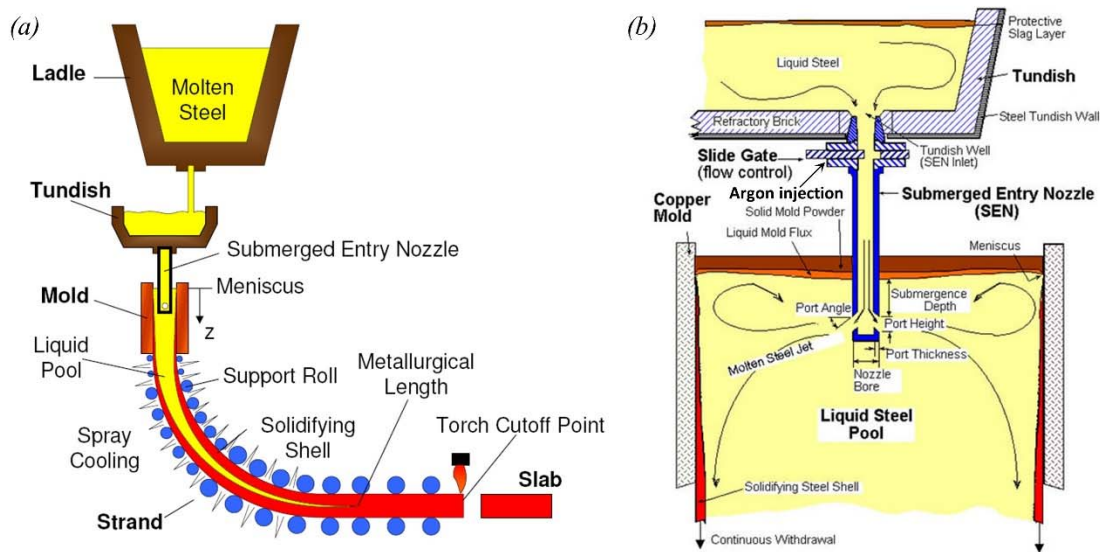


Fig. A-1-1. (a) Schematic of the continuous casting process and (b) Closeup view into the mold region of the caster. Argon gas is injected near the slide gate

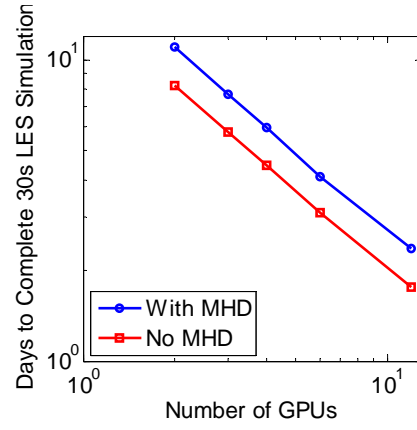


Fig. A-1-2. Estimated time for 30s LES simulation of caster with 14.1 million cells

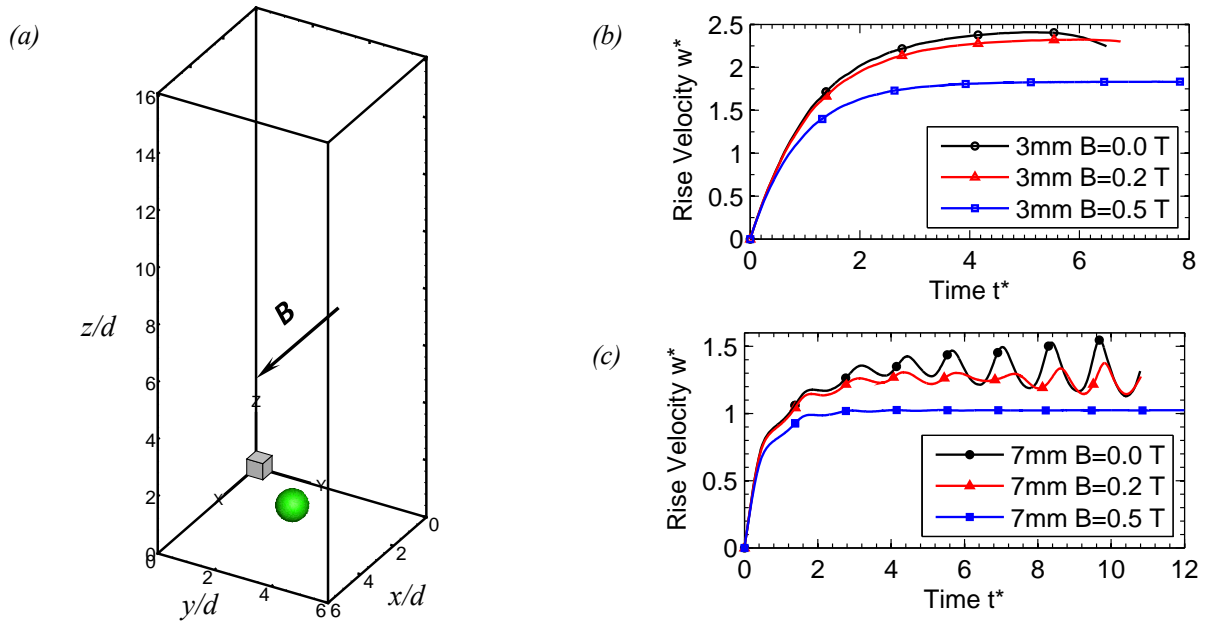


Fig. A-1-3. (a) Computational domain and initial bubble location (b) Rise velocity of 3 mm argon bubble and (c) Rise velocity of 7 mm argon bubble [4]

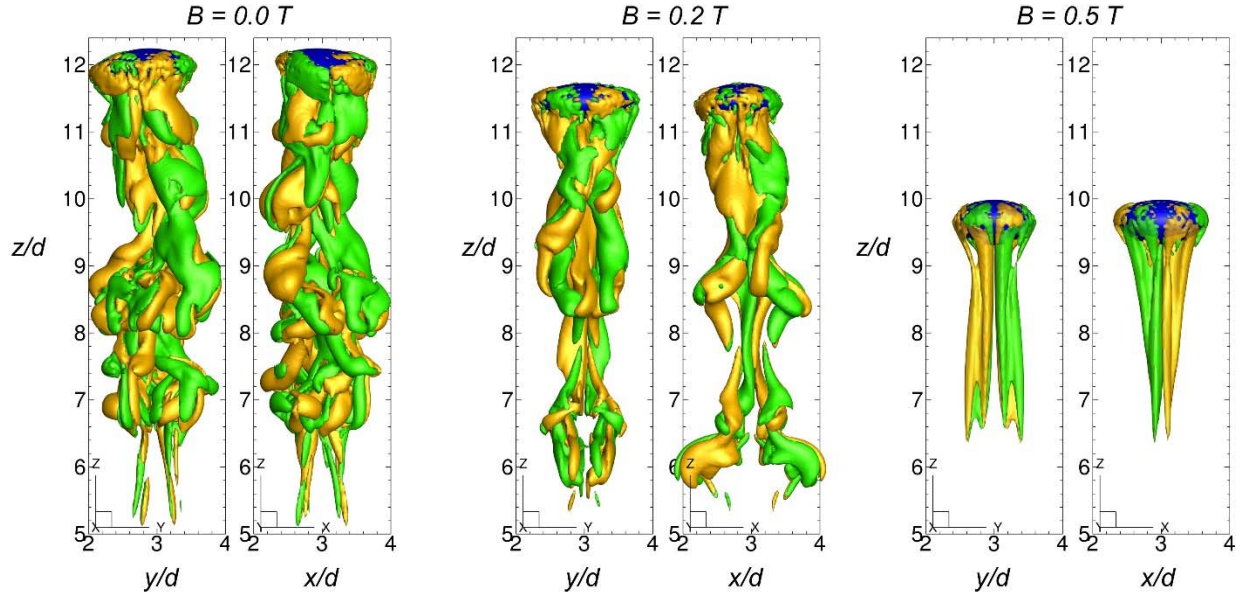


Fig. A-1-4. Front and side views of the bubble (blue), isosurfaces of  $\omega_z^* = 1$  (yellow) and  $\omega_z^* = -1$  (green) at  $t^* = 9$  for 7 mm bubble [4]

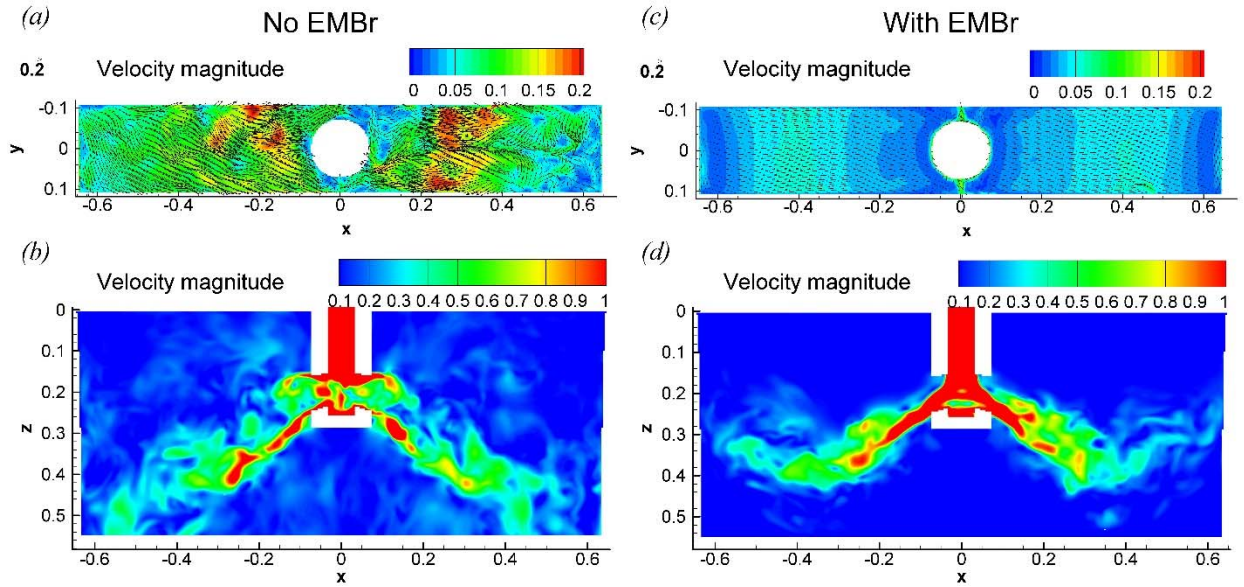


Fig. A-1-5. Predicted velocity in horizontal plane near top surface (top) and in the middle vertical plane of the caster mold (bottom) for cases without (left) and with (right) an external magnetic field

## **4.4 Accomplishments – A-2**

### **Effect of Nozzle Port Angle on Jet Wobbling and Surface Flow Instability in a Mold of Steel Slab Casting**

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#### **Executive Summary**

This project focus on developing transient fluid flow model to get insights of surface flow instability related to surface defect formation, which can be detrimental to final product quality produced by the steel slab casting process. Both LES model and Reynolds Averaged Navier-Stokes (RANS) model with standard k- $\epsilon$  model are applied to predict time-averaged and –dependent flows in nozzle and mold. The computational results shows reasonable match with the measurements using lab scale water model. The results from this project can suggest the optimal nozzle port angle to reduce surface instability defect in the considered casting condition.

#### **Introduction**

Many defects in continuous slab casting of steel are related to transient fluid flow in the mold region. Thus, small improvements to understanding transient flow phenomena and its effect on steel product quality can lead to large savings. Surface instability are well known as the most important transient flow phenomena to be related to surface defect formation during operating the process. Severe fluctuations of velocity and level <sup>[1-4]</sup> and abnormal high surface velocity <sup>[5]</sup> at the mold surface can entrap slag into the molten steel. To control the surface level and velocity to avoid defects in the process, many efforts have been made to optimize nozzle geometry and caster operating conditions. Nozzle port angle is the most important process factor to control mold flow pattern and surface flow. Thus, this study performed both transient LES modeling and standard k-  $\epsilon$  modeling for several nozzle port angles to understand nozzle port angle effect on surface flow, and to find optimal angle for reducing surface defects.

#### **Methods**

LES model is applied to calculate transient nozzle and mold flow field for +15° (up) angle and -15° (down) angle cases. The model domains include tundish bottom region, nozzle, mold cavity and consist of ~3 million hexahedral cells. Time step size is ~0.005 sec to capture transient flow in both nozzle and mold. During the calculations, transient velocity histories and transient flow field snapshots are recorded to understand relation between flow field value and flow pattern in the nozzle and mold. The RANS model calculated time-averaged velocity field and turbulent kinetic energy field with quarter domain consisting of ~0.15 million hexahedral cells. The model results are validated with measured mold flow patterns and surface velocity from 1/3 scale water model experiments as shown in Fig. A-2-1. Furthermore, the predicted surface velocity and its fluctuation profiles are compared with the measured one from plant tests using nail dipping method.

## Results

Fig. A-2-2 shows transient mold flow patterns for two cases (+15° (up) and -15° (down) angle). From both measurements and predictions, the case of +15° (up) angle nozzle shows more variations of jet flow. In other words, jet flow from the nozzle port with 15° (up) angle, induces more severe jet wobbling. The more jet wobbling produces higher surface velocity fluctuations even though it has lower surface velocity, as shown in Fig. A-2-3. This means that higher surface velocity fluctuations are not always caused by faster surface flow, but surface instability depends on casting conditions. Up-angled nozzle port produces more severe jet wobbling for the conditions simulated, resulting in lower velocity and higher velocity fluctuations at the surface. This problem could increase surface cracks, powder entrapment, associated defect formation.

To extrapolate this results to real steel caster case, surface velocity and its fluctuation profiles are compared for plant measurements, 1/3 scale water model experiments, and computational model as shown in Fig. A-2-4. There is limitation to understand surface flow in real mold caster from water model measurement and computational modeling of water model. Thus, computational modeling for real caster case including steel shell and liquid mold flux layer is needed to understand relation between surface flow variations and surface defect formation.

## Acknowledgements

This work is supported by NSF Grant CMMI-11-30882, and by the Continuous Casting Consortium at the University of Illinois. This research is part of the Blue Waters sustained-petascale computing project, which is supported by the National Science Foundation (awards OCI-0725070 and ACI-1238993) and the state of Illinois. Blue Waters is a joint effort of the University of Illinois at Urbana-Champaign and its National Center for Supercomputing Applications

## References

- [1] C. Ojeda, B. G. Thomas, J. Barco, and J. L. Arana, Proc. Of AISTech 2007, Assoc. Iron Steel Technology, Warrendale, PA, USA (2007), pp. 269
- [2] J. Sengupta, C. Ojeda, and B. G. Thomas, Int. J. Cast Metal. Res., Vol. 22 (2009), pp. 8
- [3] M. Iguchi, J. Yoshida, T. Shimizu, and Y. Mizuno, ISIJ Int., Vol. 40 (2000), pp. 685
- [4] R. Hagemann, R. Schwarze, H. P. Heller, and P. R. Scheller, Metall. Mater. Trans. B, Vol. 44B (2013), pp. 80
- [5] Seong-Mook Cho, Brian G. Thomas, Seon-Hyo Kim, Hyoung-Jun Lee, Ho-Jung Shin, Wung-Yuel Choi, Joo Choi, "Investigate of Flow Pattern, Surface Behavior, and Mold Slag Entrainment using and Oil-Water Model, CFD model, and Plant Test", CCC Annual Report 2015

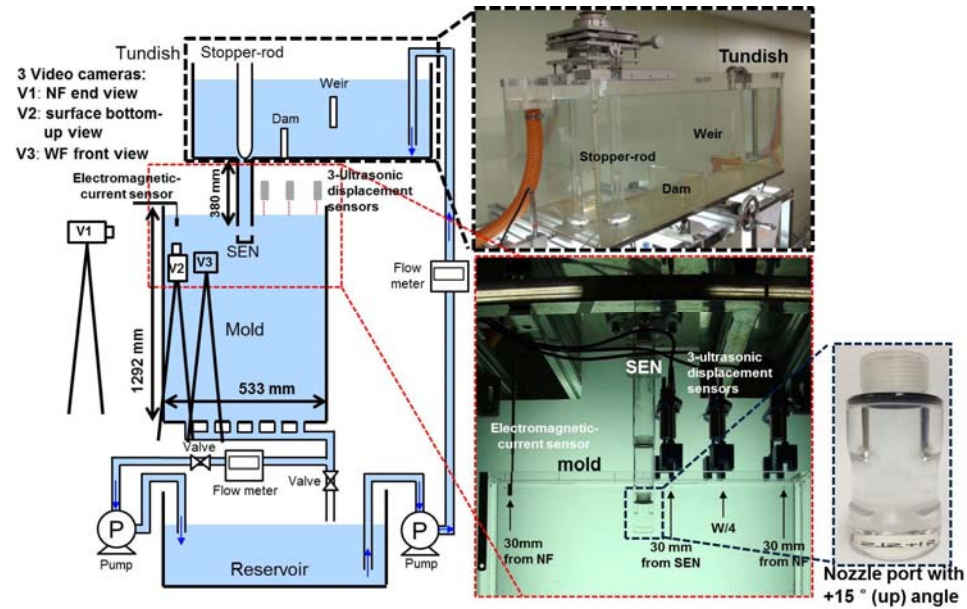


Fig. A-2-1. Schematic and photos of a 1/3 scale water model

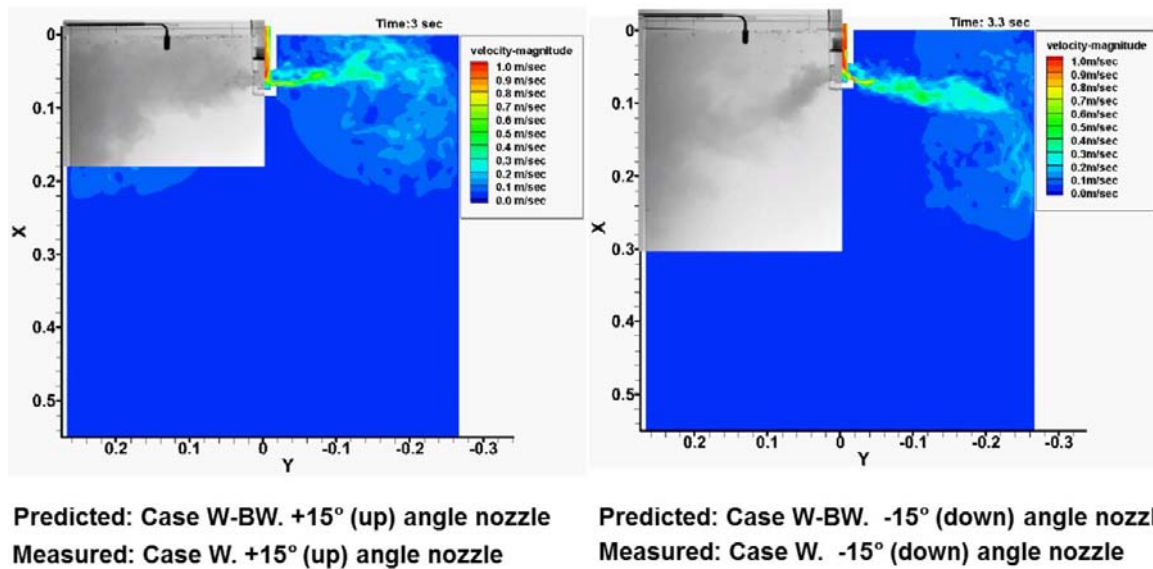


Fig. A-2-2. Comparison of instantaneous mold flow patterns predicted with LES on Blue Waters and measurements in water model, demonstrating good agreement, and effect of port angle



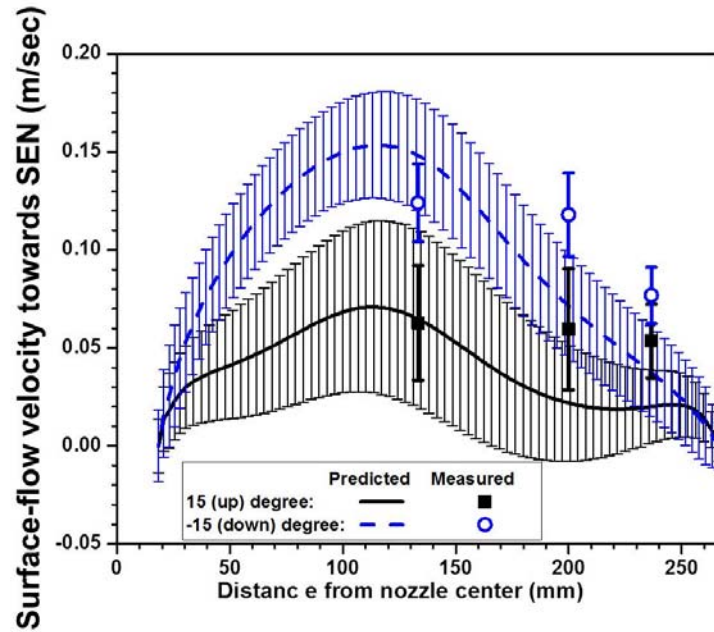


Fig. A-2-3. Surface velocity and its fluctuation profiles

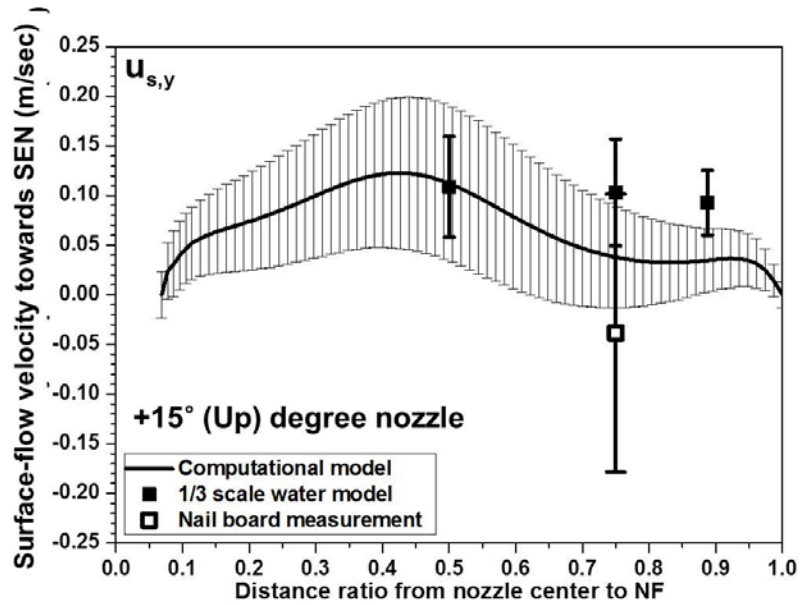


Fig. A-2-4. Comparison of plant measurements, 1/3 scale water model measurements, computational model

## 5. List of Publications associated with this work

- [1] Jin K., S. P. Vanka, and B. G. Thomas, Three-dimensional flow in a driven cavity subjected to an external magnetic field. *Journal of Fluids Engineering*, 137 (2015), 071104.
- [2] Jin K., P. Kumar , S. P. Vanka and B.G. Thomas, Rise of an argon bubble in liquid steel in the presence of a transverse magnetic field, *Physics of Fluids*, submitted and is under review.
- [3] Jin K., S. P. Vanka, R. K. Agarwal and B.G., GPU Accelerated Simulations of Three-Dimensional Flow of Power-law Fluids in a Driven Cube, *Journal of Fluids Engineering*, submitted and is under review
- [4] Seong-Mook Cho, Brian G. Thomas, Hyoungh-Jun Lee, and Seon-Hyo Kim, “Effect of Nozzle Port Angle on Mold Surface Flow in Steel Slab Casting”, AlSTech 2016, abstract accepted. Journal papers are in preparation as well.

In addition to the above, several presentations on research performed using Blue Waters was presented at the Annual Meeting of the Continuous Casting Consortium at UIUC (Aug. 19, 2015, 2005 MEL).

And, several more publications based on simulations using Blue Waters are in preparation, with publication expected in 2016.