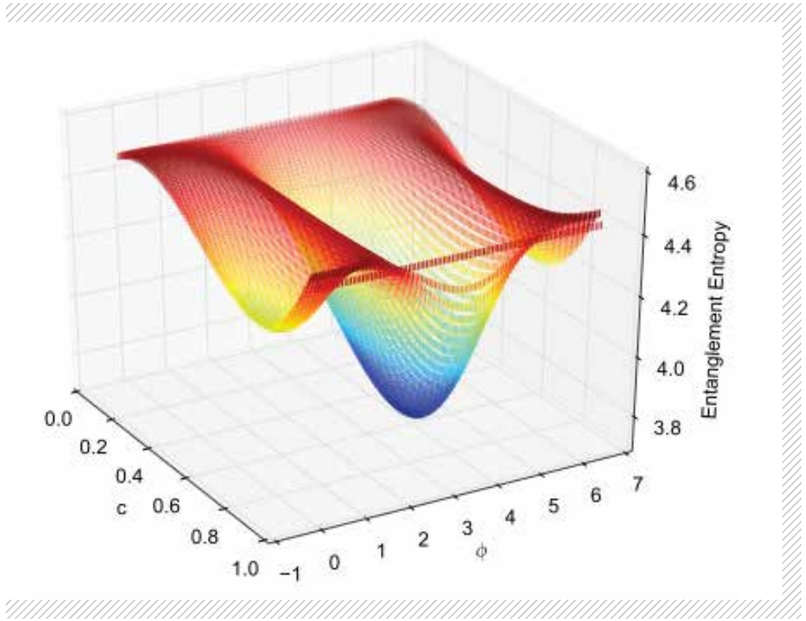

FIGURE 2: Renyi entanglement entropy for the 42b cluster as a function of c, φ obtained from the reduced density matrix along two topologically non-trivial cuts. The linear combinations corresponding to local minima of the entanglement suggesting the existence of a topological phase.

compute all properties of the topological phase, but computing the entire set of twists required over 100,000 node hours.

Many-Body Localization

Blue Waters was essential to this project because of the multiple layers of computation needed. Many-body localized phenomena involve disordered systems. Therefore, any computation requires an average of over thousands of disordered realization. For each of these disordered realizations, a sweep over multiple target energies lambda is required. Finally, each (lambda, disordered configuration) point requires tens of applications of the SIMPS algorithms to converge to the excitation.

NEXT GENERATION WORK

Frustrated Magnetism

We discovered a chiral spin liquid in our system at a single phase point. We would like to discover whole regions that have spin liquid behavior because that will give us the best chance of finding realizations in nature of these exotic phenomena. Unfortunately, each point in this region requires an entire calculation comparable to the one we have done for the chiral spin liquid. It is only with Track-1 systems that this will become possible.

Many-Body Localization

Our SIMPS methodology currently allows us to access states within the many-body localized region, but fails at the critical point, and understanding the nature of this critical point is key to understanding many-body localization. We are developing new tensor network methodologies which may be able to access this point, but the computational complexity of running them will require the next-generation machines to achieve the system sizes necessary.

PUBLICATIONS AND DATA SETS

Chen, X., et al., Many-body localization transition in Rokhsar-Kivelson-type wave functions. *Phys. Rev. B*, 92:21 (2015), p. 214204.

Yu, X., D. Pekker, and B.K. Clark, Finding matrix product state representations of highly-excited eigenstates of many-body localized Hamiltonians. *arXiv* preprint arXiv:1509.01244 (2015).

Yu, X., D.J. Luitz, and B.K. Clark, Bimodal entanglement entropy distribution in the many-body localization transition, *arXiv* preprint arXiv:1606.01260 (2016).

TRANSIENT TWO-PHASE FLOW AND ELECTRO-MAGNETIC FIELD EFFECT IN STEEL CONTINUOUS CASTING

Allocation: Illinois/200 Knh
PI: Brian G. Thomas[1,2]
Co-PIs: Seong-Mook Cho[1], Kai Jin[1], S.P. Vanka[1], Hyunjin Yang[1], Matthew Zappulla[1], Xiaolu Yan[1], Ahmed Taha[1], and Seid Koric[1]

[1]University of Illinois at Urbana-Champaign
[2]Colorado School of Mines

EXECUTIVE SUMMARY

This project aims to advance current state-of-the-art, computationally-intensive models of multiphase phenomena including turbulent fluid flow, particle transport, and MagnetoHydroDynamics (MHD) in the continuous casting of steel. Also, the project applies these current models to gain practical insights into the transient flow phenomena related to defect formations and to improve this important commercial process. In this study, a transient, two-phase Large-Eddy-Simulation model of molten steel-argon gas flow was applied to investigate anisotropic (directionally dependent) turbulent flow in the caster, with and without a double-ruler electro-magnetic field. The model calculations have been validated with plant measurements and applied to understand the mechanism of the flow variations, which is important to surface defect formation in the final product. Also, the effects of the magnetic field on the flow stability in the caster has been quantified with different process parameters.

INTRODUCTION

Continuous casting is used to manufacture more than 95% of steel in the world [1]. Molten steel flows from a tundish container, through a slide gate control valve, and down a vertically bifurcated nozzle into the mold (Fig. 1). Once in the mold, molten steel solidifies against the water-cooled, copper mold walls to form a solid shell. Transient fluid-flow phenomena in the mold are very important to quality and defects in the final product. Abnormal surface flow aggravates level fluctuations, shear instability of the molten slag/steel interface, and vortex formation near the submerged entry nozzle (SEN), which leads to mold slag entrainment. These detrimental flow phenomena in the mold become more complex with argon gas, which is injected into the nozzle to prevent clogging. Furthermore, the argon gas bubbles may become entrapped into the solidifying steel shell, forming other defects. To stabilize and optimize the transient fluid flow in the mold, electro-magnetic fields are often applied, especially at high casting speed [2-4].

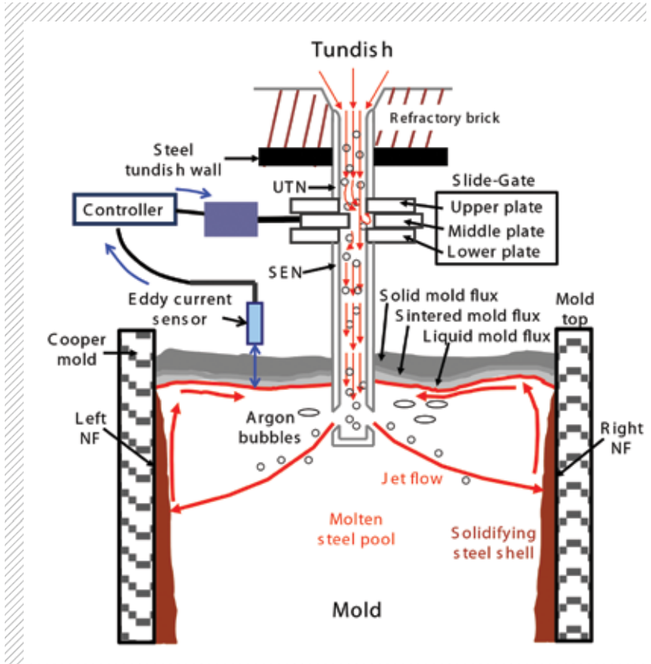

FIGURE 1: Schematic of the continuous steel slab-casting process.

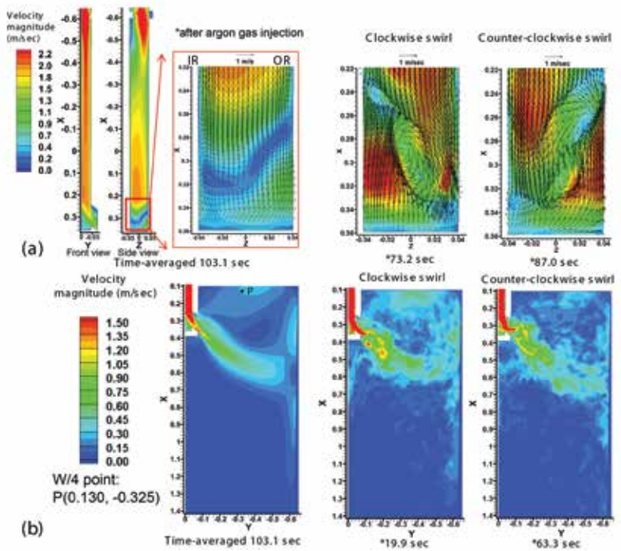

FIGURE 2: Time-averaged and instantaneous flow patterns in (a) nozzle and (b) mold.

In the present work, Large Eddy Simulations (LES) of multiphase flow are performed to quantify the transient behavior of molten steel-argon gas flow in the nozzle and mold during nominally-steady continuous casting of steel slabs. The model has been validated with plant measurements and applied to investigate the mechanism of multiphase flow stability, argon-bubble entrapment into the steel shell and effects of double-ruler Electro-Magnetic Braking (EMBr) on the transient flow variations for different process conditions.

METHODS & RESULTS

To calculate transient flow of molten steel and argon gas in the nozzle and mold, a three-dimensional finite-volume LES model coupled with Discrete Phase Model (DPM) for particle tracking has been developed to consider the interaction between the molten steel flow and argon bubble motion. This model was implemented into a special multi-license version of ANSYS Fluent software on Blue Waters.

Time-averaged and instantaneous flow patterns in the nozzle and mold are shown in Figure 2 [3]. The asymmetrically-positioned slide gate middle plate, with its open area near the Outside Radius (OR) side, produces swirl flows in the nozzle well bottom, alternating chaotically between clockwise and counter-clockwise rotation. Instantaneous mold flow patterns show up-and-down wobbling of the jet in the mold, which produces different impingement points on the narrow face. When the nozzle flow from the slide gate flips sides down the nozzle (Fig. 2a), it produces counter-clockwise swirl exiting the ports, impinges downwards on the narrow faces, and results in slow surface flow in the mold. When the nozzle flow goes straight down to produce clockwise swirl exiting the port, the accompanying faster jet bends upwards, impinges the narrow face horizontally, and produces 50% faster surface flow (Fig. 3a).

Time-averaged and instantaneous profiles of surface velocity magnitude predicted by the LES model are compared with nail board measurements in Figure 3b. Each line shows surface velocity magnitude profiles across the mold width at the center-plane 10mm below the interface between the molten steel and liquid mold flux layers. Symbols with error bars present time averages and standard deviations of 10 nail-dipping tests at each measurement location [4]. The model predictions of the average velocity profile, and its time and spatial variations, all agree with the measurements. This confirms that the LES-DPM model on Blue Waters is an accurate tool to predict complex mold-flow phenomena including multiphase effects.

Related work coupling turbulent flow with DPM to model bubble transport and capture, based on local force balances on argon-gas bubbles at the solidification front, has revealed that biased flow across the mold surface can aggravate bubble capture [5].

The effect of double-ruler EMBr was added to the LES-DPM model by implementing the magnetic induction MHD equations. The EMBr in the current work has one peak centered across the mold above the port and the other centered below the nozzle port. With EMBr, swirl direction flipping occurs more frequently, flow asymmetries are reduced, turbulence from jet wobbling is reduced, and thus, surface velocity fluctuations are smaller [3]. Furthermore, an efficient multi-GPU based code, CUFLOW, was used to perform LES to investigate the effects of several SEN depths and double-ruler EMBr strengths [6], to suggest the best choice of operating conditions to control surface flow.

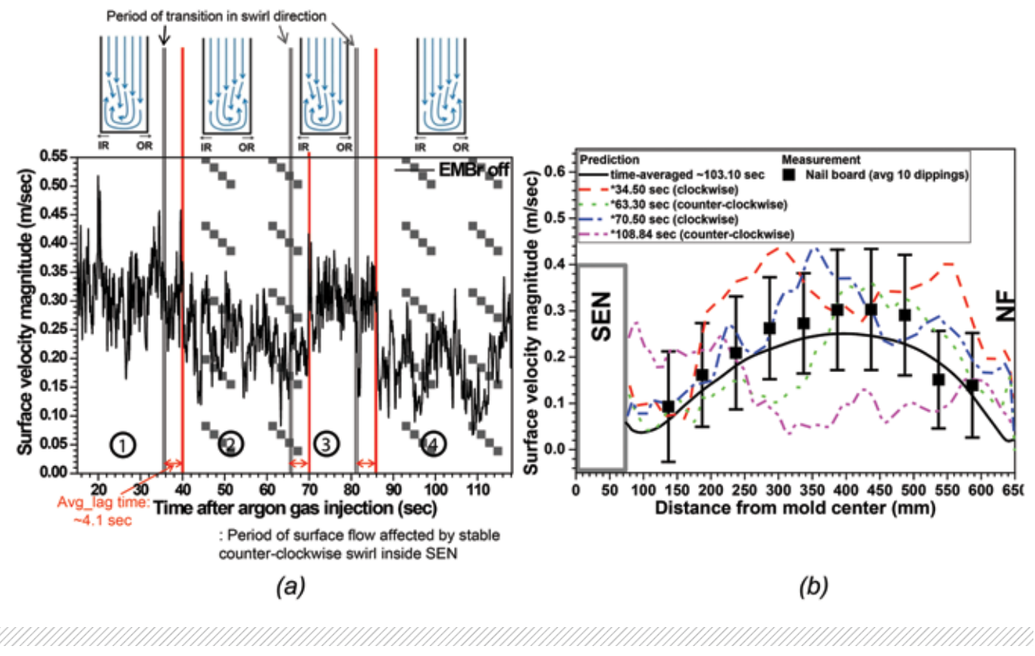

FIGURE 3: (a) Instantaneous surface velocity magnitude at W/4 point and (b) comparison of predicted surface velocity profiles with plant nail-board measurements

WHY BLUE WATERS

Multiphase flow simulations in the continuous caster are enabled by Blue Waters, including the large domain volume (e.g. 0.2 m X 1.6m X 4.6m) and fine mesh (e.g. ~22 million cells) needed to properly capture and resolve the turbulent flow in the casting process. Specifically, the Fluent-14.5 HPC software on Blue Waters ran 3,357 times faster than on an ordinary work station PC (Dell T7600: Intel® Xeon® CPU E5-2603 @ 1.80GHz, RAM 40.0 GB, using 6 cores) with 1,120 floating cores (70 XE nodes).

NEXT GENERATION WORK

A validated two-dimensional thermal-fluid model of solidification phenomena at the slag/molten steel interface near the meniscus region [7], will be extended into the full 3-dimensional LES mold discussed here, to investigate how anisotropic multiphase flow variations affect initial solidification, with and without magnetic fields.

PUBLICATIONS AND DATA SETS

Jin, K., B.G. Thomas, and X. Ruan, Modeling and Measurements of Multiphase Flow and Bubble Entrapment in Steel Continuous Casting., *Metall. Mater. Trans. B*, 47B:1 (2016), pp. 548-565. DOI: 10.1007/s11663-015-0525-5

Cho, S-M., B G. Thomas, and S-H. Kim, Transient two-phase flow in slide-gate nozzle and mold of continuous steel slab casting with and without double-ruler electro-magnetic braking. *Metall. Mater. Trans. B*, (2016) pp. 1-19.

Jin, K., S. P. Vanka, B.G. Thomas, and X. Ruan, Large eddy simulations of the effects of double-ruler electromagnetic braking and nozzle submergence depth on molten steel flow in a commercial continuous casting mold. *TMS Annual Meeting, CFD Modeling and Simulation in Materials Processing Symposium*, Nashville, TN, Mar. 14-18, 2016, TMS, Warrendale, PA, 2016, pp. 159-166.