4th NCSA Blue Waters Symposium,
Sunriver, Oregon, June 13-15, 2016

Multiphysics Simulations on Blue Waters for Steel Continuous Casting

Seong-Mook Cho[1] (Co-PI) and Brian G. Thomas[1,2] (PI and Presenter)

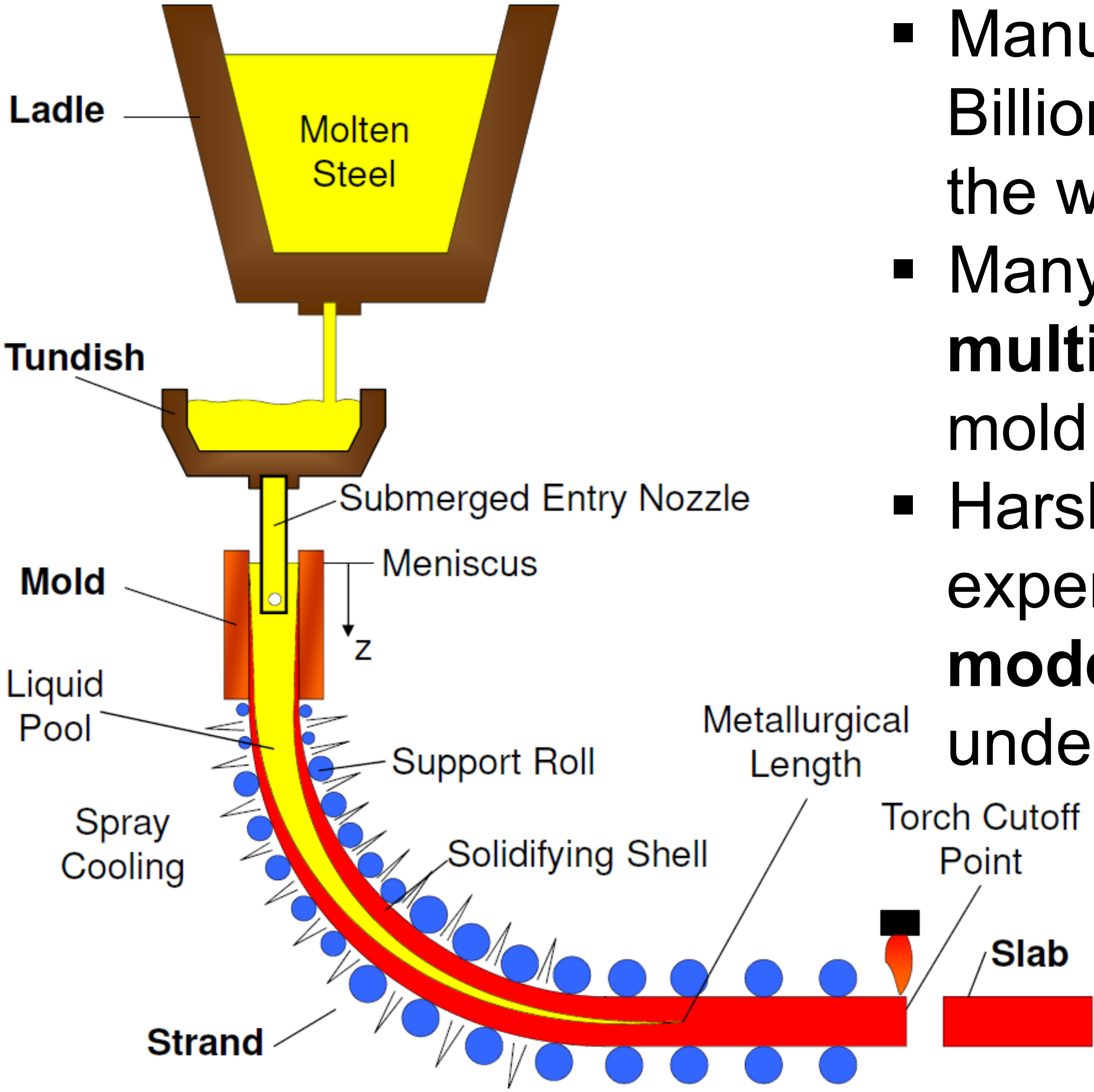
1. University of Illinois at Urbana-Champaign, Department of Mechanical Science and Engineering
2. Colorado School of Mines (CSM), Department of Mechanical Engineering

Acknowledgements

- Blue Waters / National Center for Supercomputing Applications (NCSA) at UIUC
- Co-PIs at U-Illinois: Kai Jin (Ph.D. Student), S.P. Vanka (Emeritus Professor of Mechanical Engineering), Hyunjin Yang (Ph.D. Student), Matthew Zappulla (M.S. Student), Xiaolu Yan (M.S. Student)
- Co-PIs at NCSA: Ahmed Taha (Senior Comp. Resource Coordinator), Seid Koric (Adjunct Associate Professor)
- ANSYS. Inc. for Fluent-HPC License Allocation
- Continuous Casting Consortium Members (ABB, AK Steel, ArcelorMittal, Baosteel, JFE Steel Corp., Magnesita Refractories, Nippon Steel and Sumitomo Metal Corp., Nucor Steel, Postech/Posco, SSAB, ANSYS/Fluent)

Introduction I:

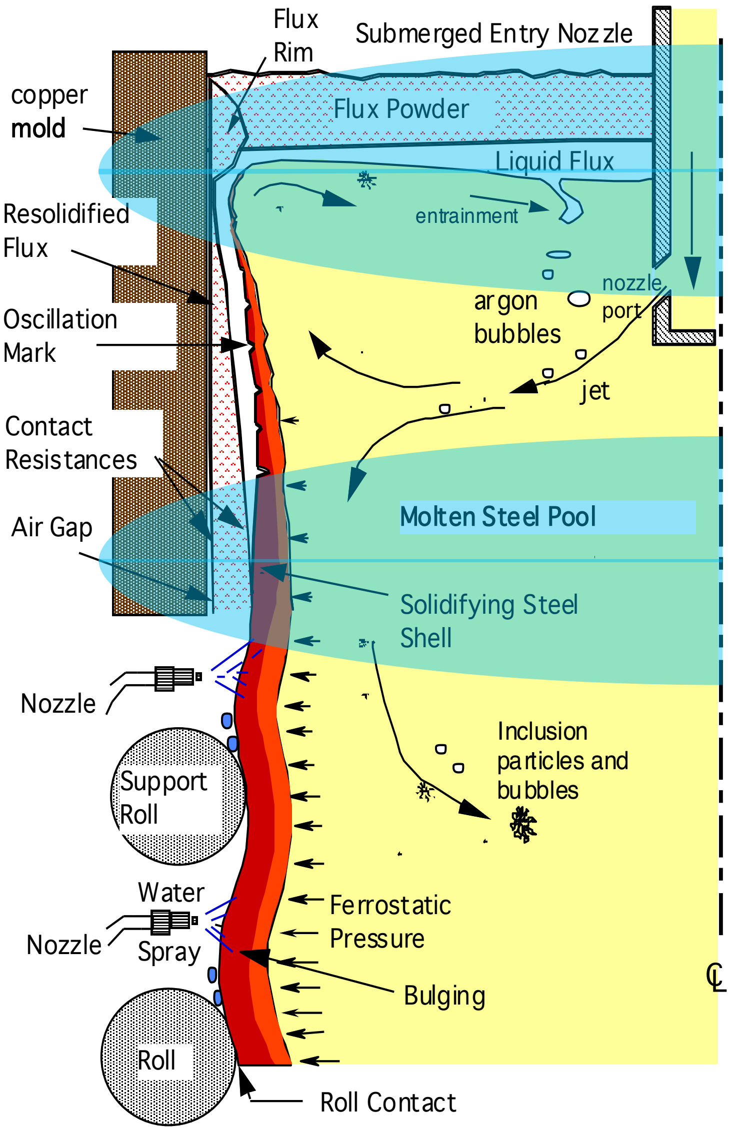
Continuous Casting of Steel



- Manufactures over 95% of 1.4 Billions tons of steel per year in the world[*1]
- Many defects related to **multiphysics phenomena** in mold
- Harsh environment makes experiments difficult; **computer models** allow process to be understood and improved

*1] Steel Statistical Yearbook 2014. (World Steel Association, Brussels, Belgium, 2014)

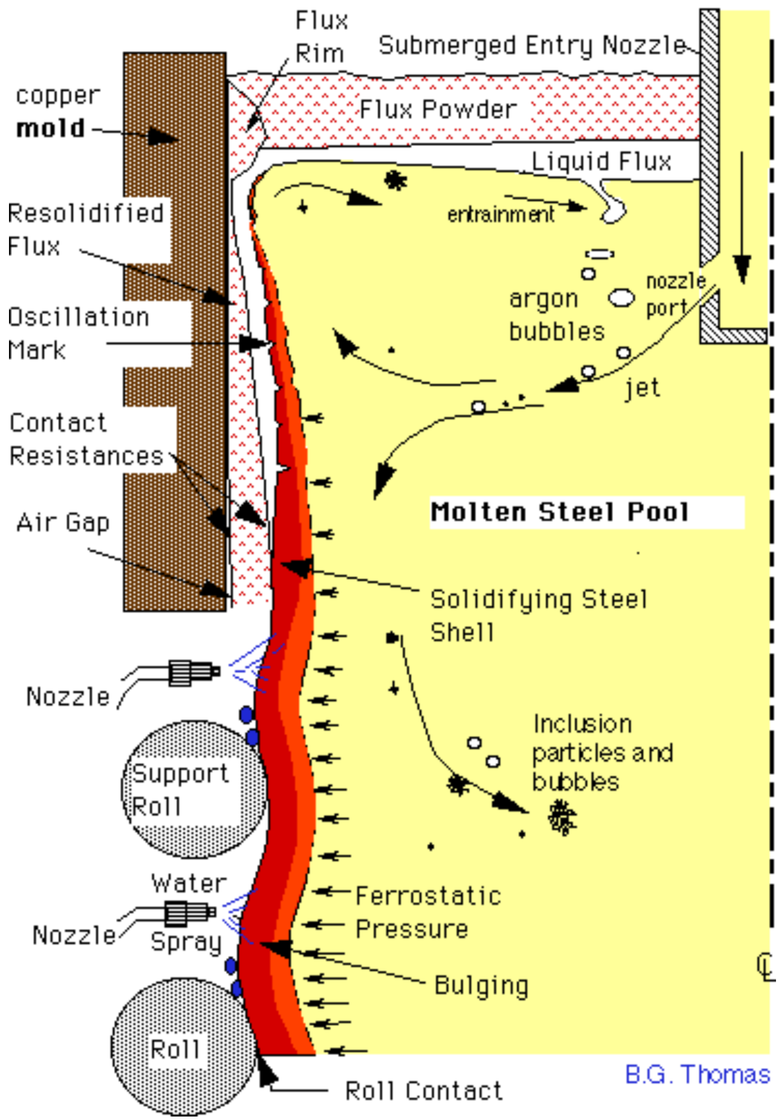
Introduction II: **Continuous Casting**
Phenomena are Complex



- **Turbulent multiphase flow**
- Heat transfer & solidification
- **Steel/slag interface & surface tension**
- Nucleation, collision, growth of steel crystals, **bubbles & inclusions**
- **Transport & removal of particles**
- Multiphase thermodynamics
- Mass transfer & segregation
- Deformation & stress
- Microstructure evolution
- Precipitate particles
- Embrittlement & cracks
- Multiple time & size scales

- **Electromagnetic fields (EMBr)**

Introduction III: **Multiphysics Phenomena Related to Defect Formation**



<Mold phenomena>

- **Instability of interface between molten steel and liquid mold flux**, can entrain liquid mold flux into molten steel pool, resulting in surface or internal defects.
- **Argon bubbles** make **mold flow more complex** and may be **entrapped by solidifying steel shell**, to create defects.
- Meniscus freezing and hook formation, affected by **fluid flow with superheat transport**, govern surface defects.

Computational Models on Blue Waters

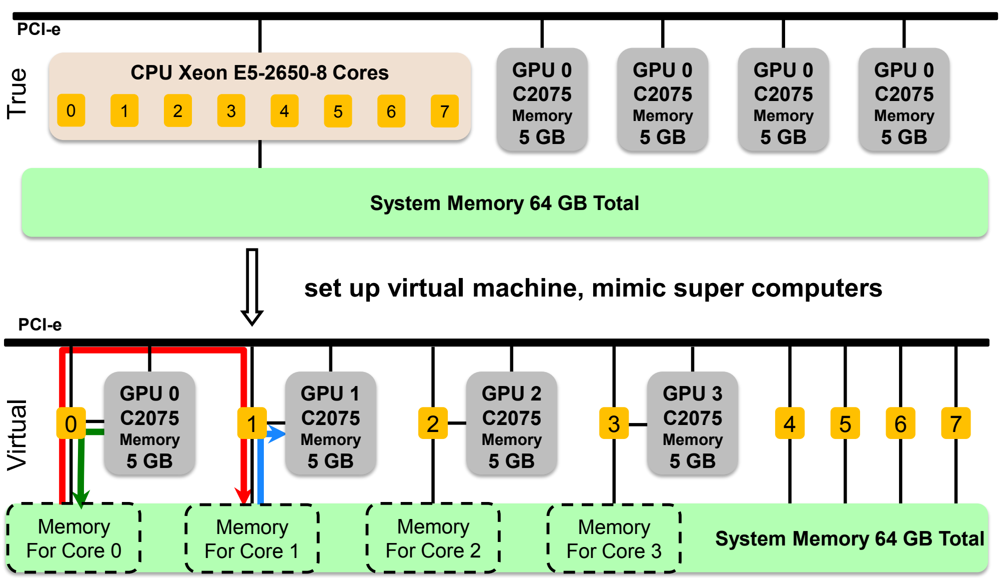
- **Why Blue Waters**
  - High-resolution prediction of multiphysics phenomena
  - Speed-up breakthrough on computing
- **Models: ANSYS FLUENT (commercial CFD package**
  CUFLOW (in-house multi-GPU based code)
  - Turbulent fluid flow models:
    - Large Eddy Simulation (LES),
    - Reynolds-Averaged Navier-Stokes (RANS, eg. k-ε)
  - Second-phase models:
    - Volume Of Fluid (VOF) for interface motion (phase fractions)
    - Discrete Phase Model (DPM) for particle motion
  - MagnetoHydroDynamics (MHD) model for magnetic field effect
  - Particle capture model
    - (based on local force balances on particles at solidification front)

CUFLOW: Configuration of nodes on BWs and Lab Workstations

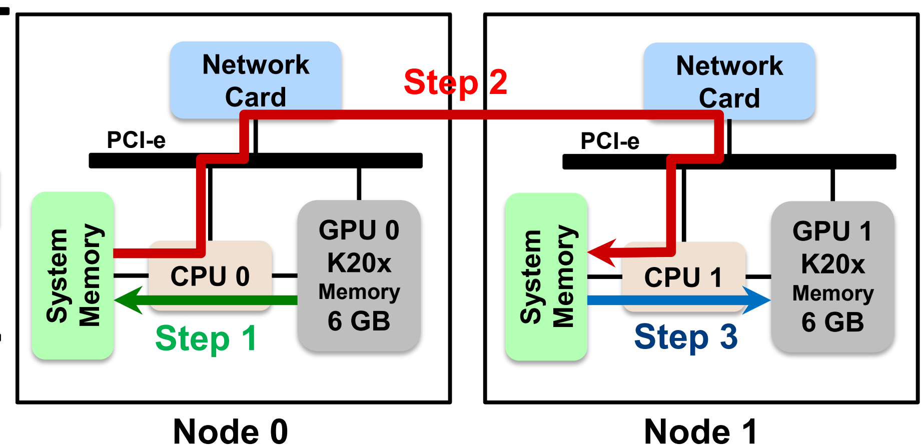
Currently, two versions of **CUFLOW**, CPU and GPU versions:

- CPU version, run on multi-CPU **PC** (data compunication through MPI)
- GPU version, run on multi-GPU **PC** and multi-CPU&GPU pair supercomputer (eg. **Blue Waters**)

	PC - 4GPU Workstation	**Blue Waters Supercomputer**
#of Nodes	1	4224
Node CPU	Xeon E5-2650v2 Ivy Bridge, 2.60 GHz, 8 cores	AMD 6276, 2.3 GHz, 16 cores
GPU/Node	**4** × Nvidia Tesla C2075, 4 × **5 GB**, 575 MHz	**1** × Nvidia Tesla K20x, 1 × **6 GB**, 732 MHz



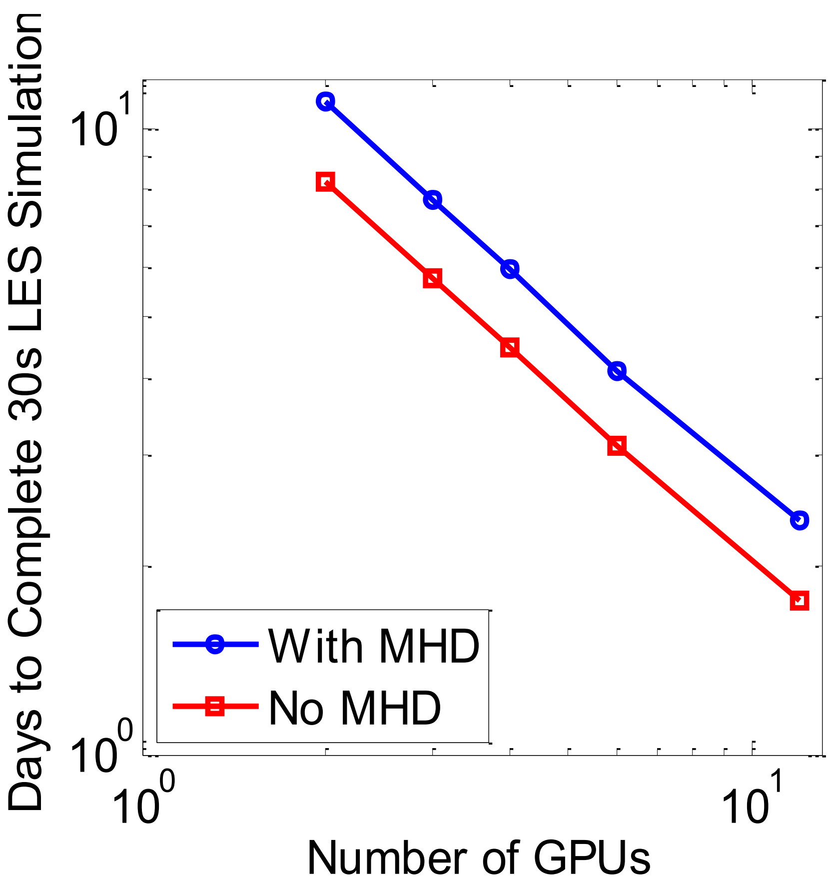
Configuration of 4GPU Workstation



Three Steps: cudaMemcpy(…), MPI_Send(…) and MPI_Recv(…), cudaMemcpy(…)

Configuration of BWs Nodes (showing 2 nodes)

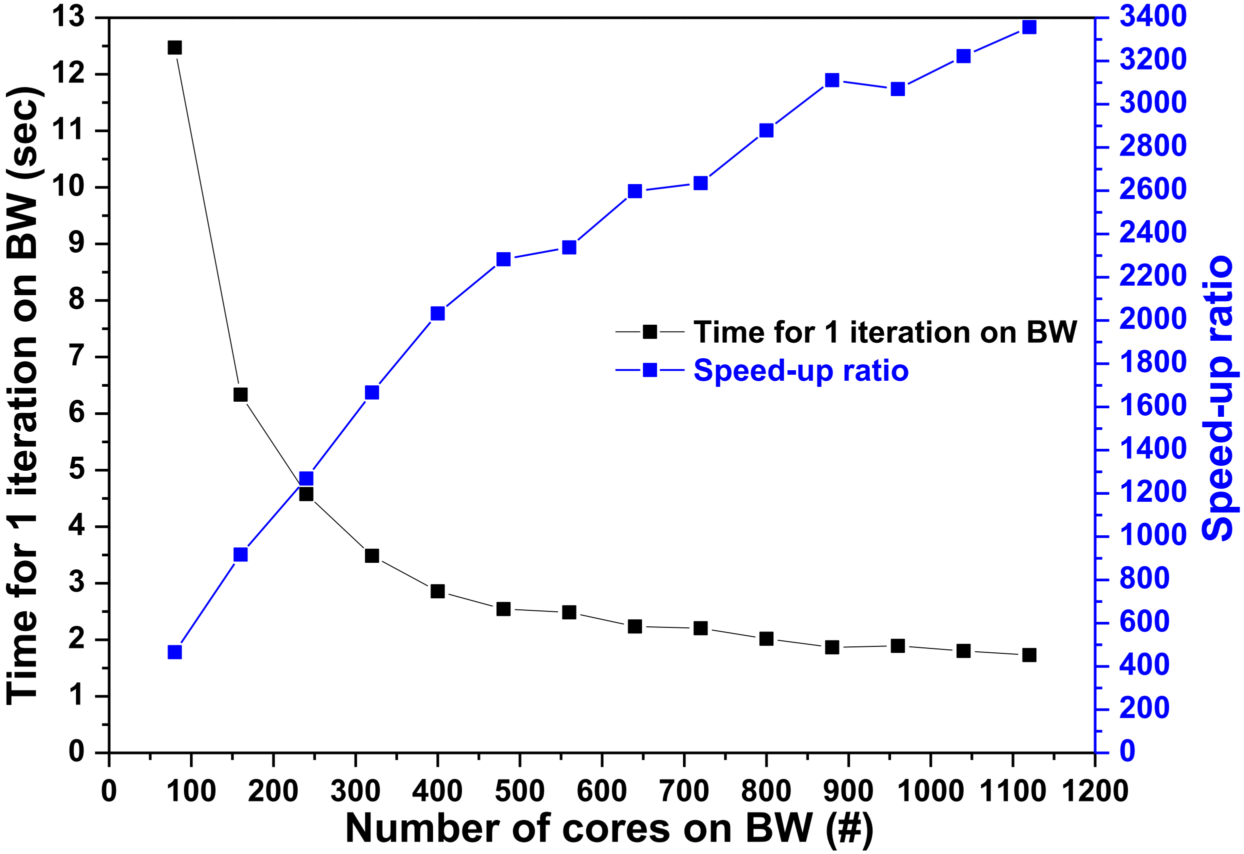
CUFLOW Speed-Up on Blue Waters



<Estimated time for 30s LES simulation of caster with 14.1 million cells[5]>

- 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.
- 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 Δt=0.0005s)

FLUENT Speed-Up on Blue Waters



- Lab Computer (LC) calculation: Dell T7600 (Intel ® Xeon ® CPU E5-2603 @ 1.80GHz, RAM 40.0 GB, using 6 cores

- **Speed-up ratio =** Computing time for 1 iteration on **LC /** Computing time for 1 iteration on **BW**

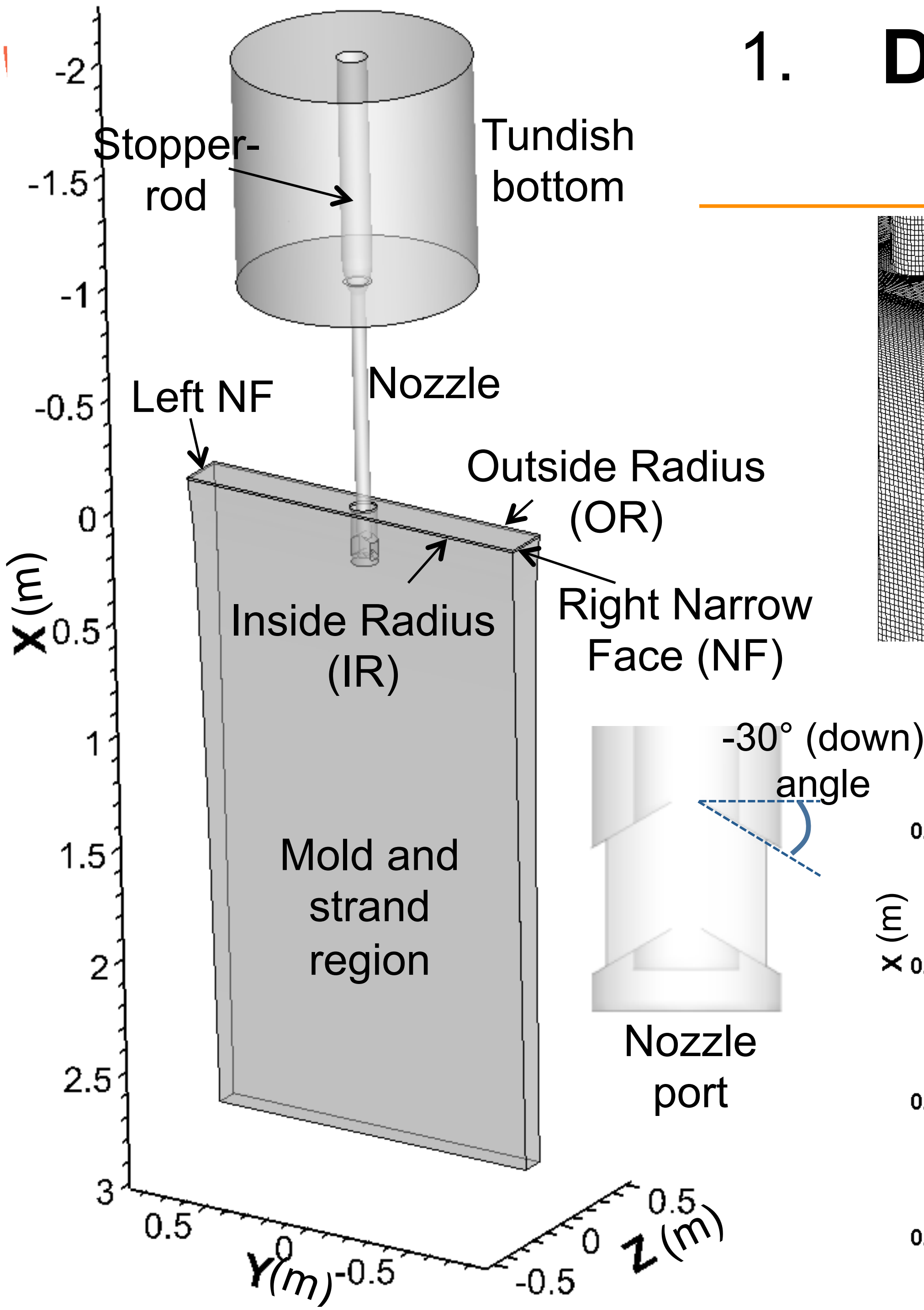
Speed-up test was performed for **L ES coupled with VOF** in domain o f **~22 million hexahedral cells**

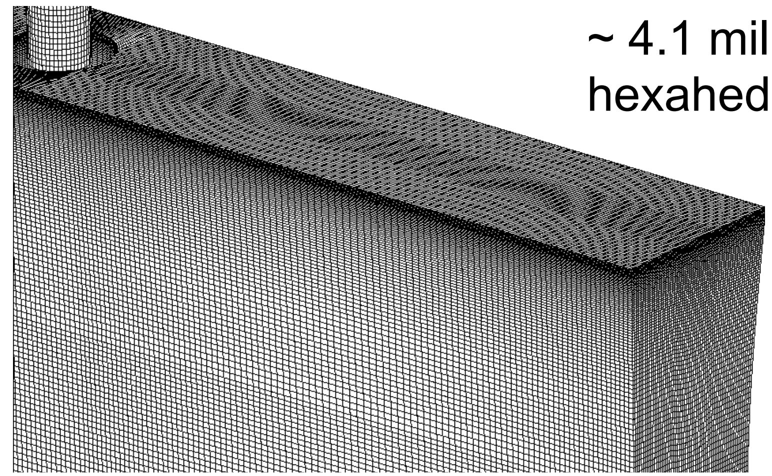
- With **1120 cores (70XE nodes),** the simulation on BW runs **~ 3357 times faster than on our LC**: one iteration on BW using 1120 cores (70 XE nodes) requires **~1.7 seconds** of wall clock time. one the other hand, on the LC, the same simulation requires **~ 5808 seconds** of wall-clock time for 1 iteration.
- For this case, Fluent-14.5 HPC on BW shows **speed-up breakthrough** with 1120 cores (70 XE nodes); **getting much more efficiency for much finer mesh domain**

Recent Research with Blue Waters

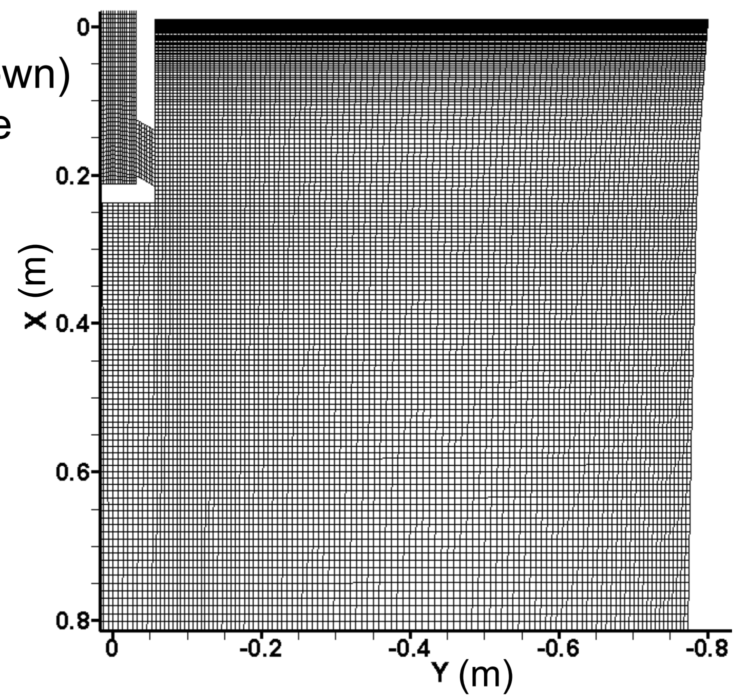
- **Topic I[1]: Transient** liquid slag/molten steel **interfacial motion** at mold surface
- **Topic II[2]: Nozzle swirl and mold-surface variation** of molten steel-argon bubble flow with and without double-ruler Electro-Magnetic Braking (EMBr)
- **Topic III[3]: Argon bubble capture** into solidifying steel shell in mold
- **Topic IV[4]: Parametric studies**: eg. Effect of double-ruler EMBr strength on mold flow pattern

1. **Domain** and **Mesh**

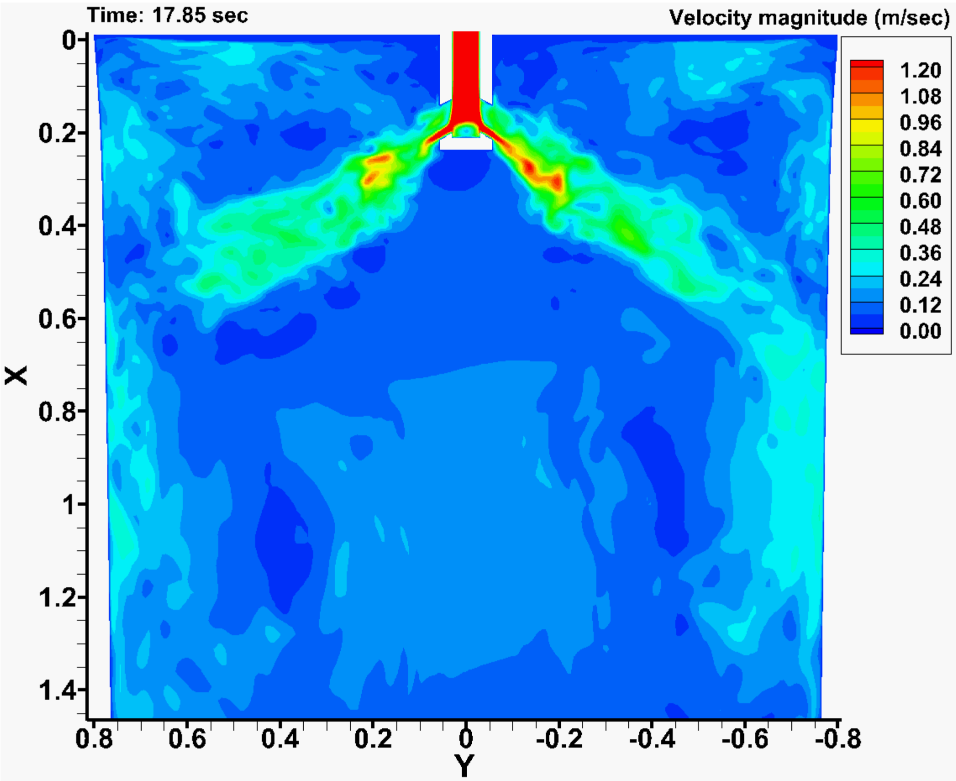




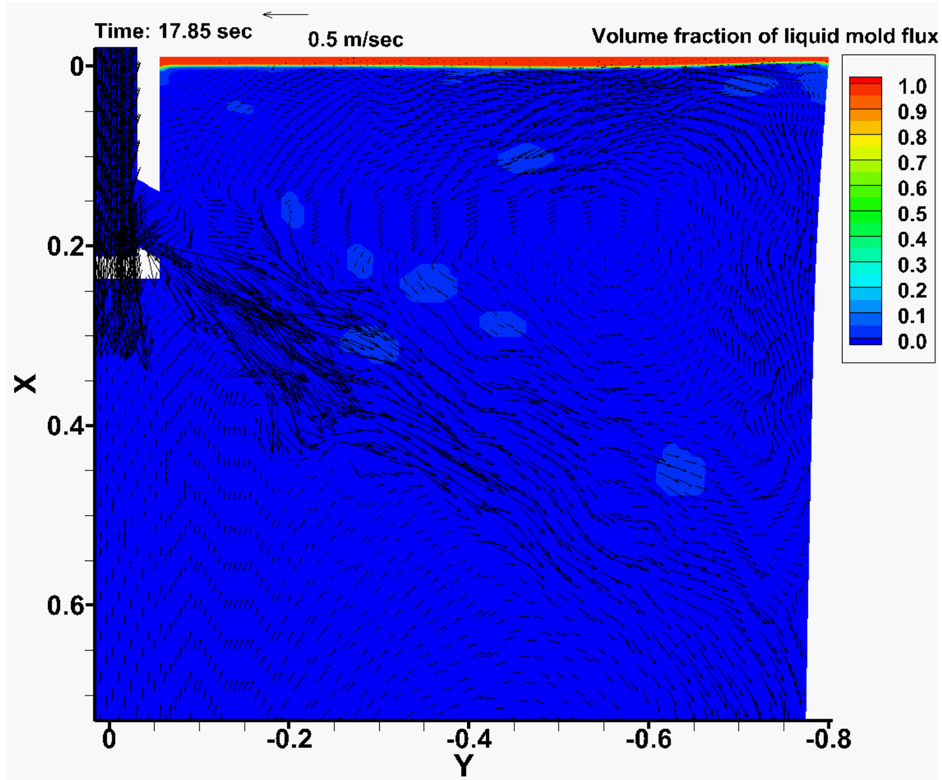
~ 4.1 million hexahedral cells



Transient Mold-Flow Pattern: LES-VOF



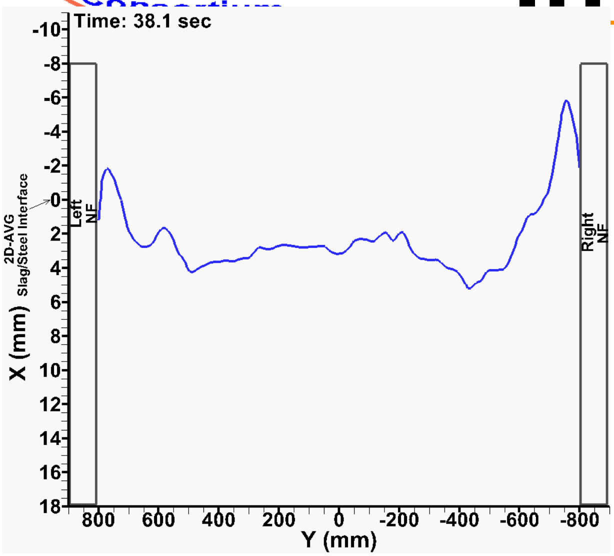
Steel Velocity Magnitude



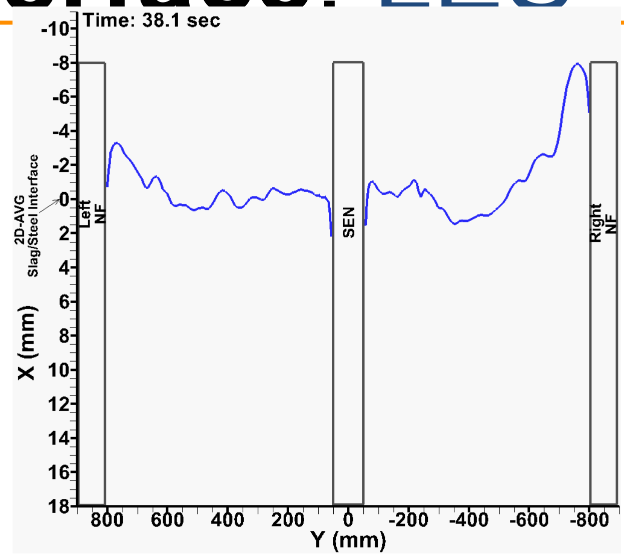
Velocity-vectors and slag volume fraction

- Classic **double-roll flow pattern** in mold
  (center middle plane between wide faces)

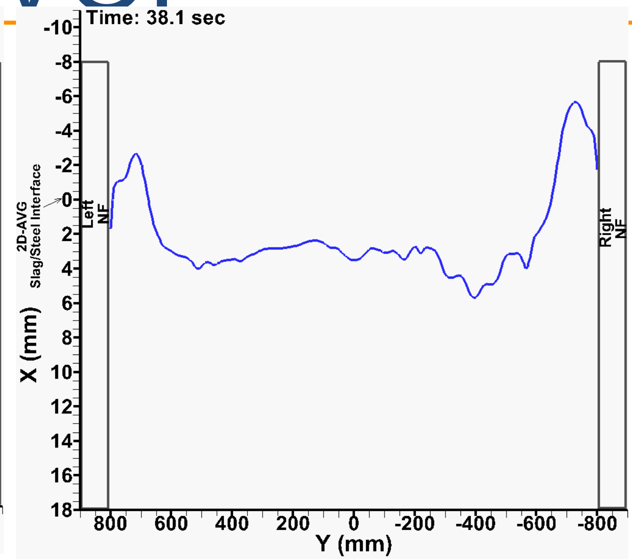
Transient Slag/Steel Interface: LES-VOF



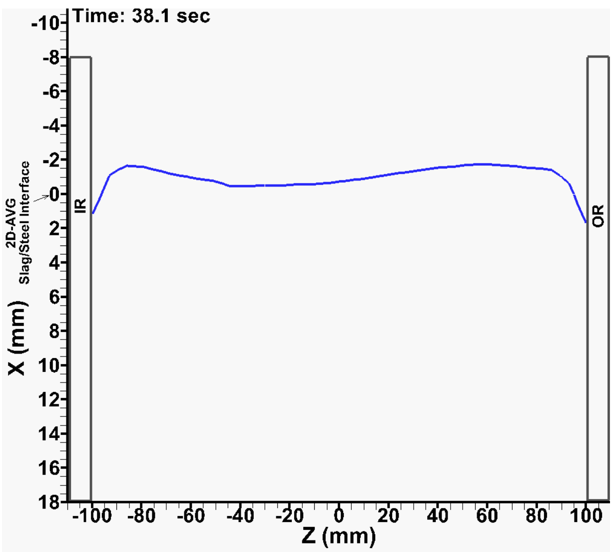
IR



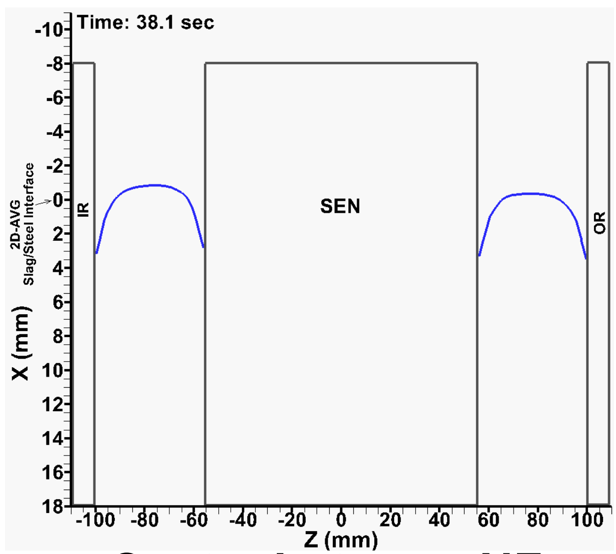
Center-plane between IR and OR



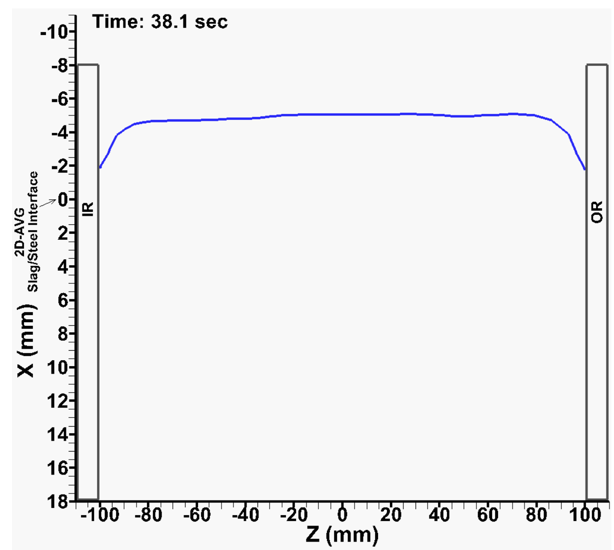
OR



Left NF



Center between NFs



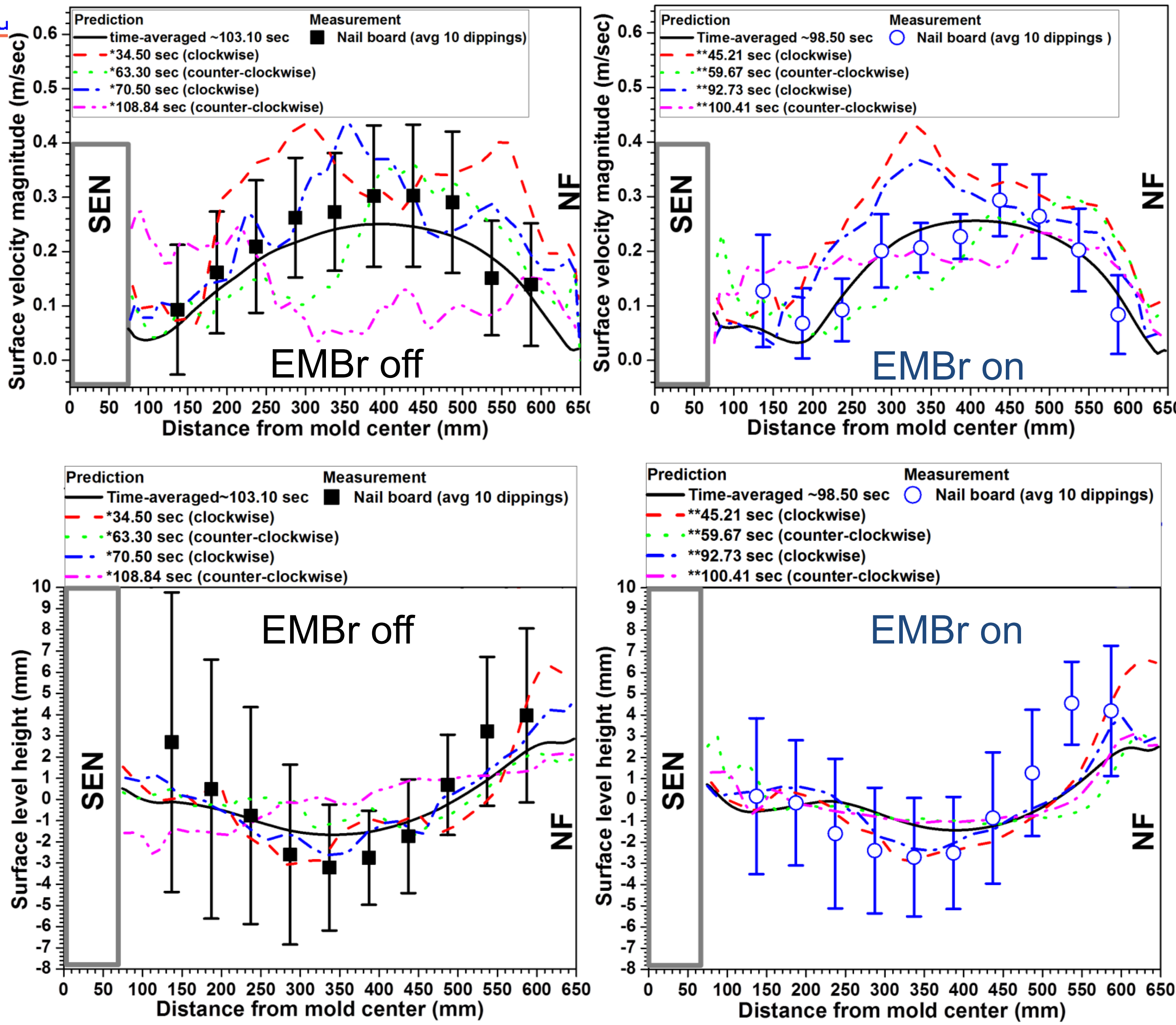
Right NF

Validation with Plant Measurements

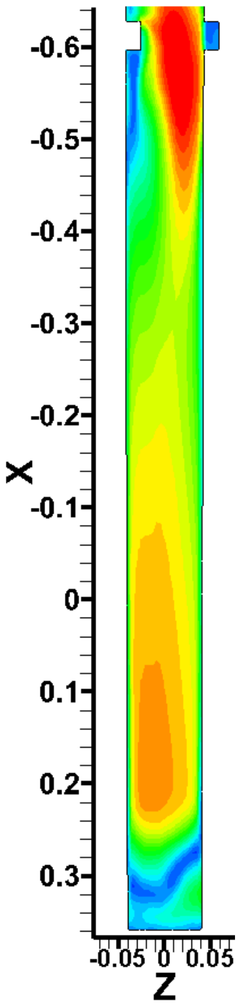
LES-DPM-MHD calculations vs. Nail-Board tests

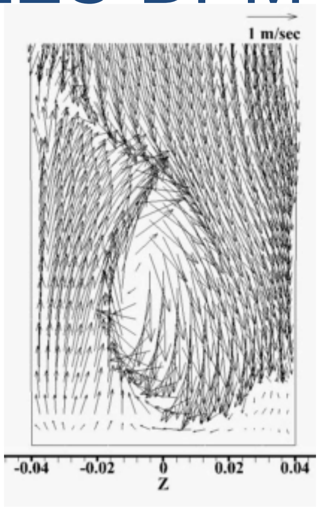
Surface velocity

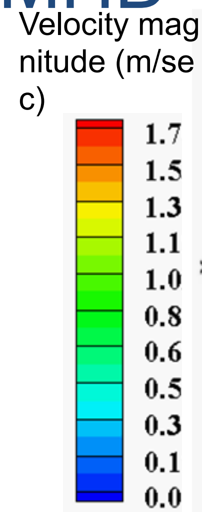
Surface level

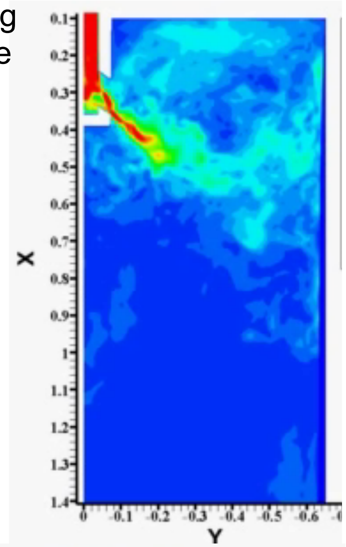


Mechanism of Surface Velocity Variations of Molten Steel-Argon Flow: LES-DPM-MHD

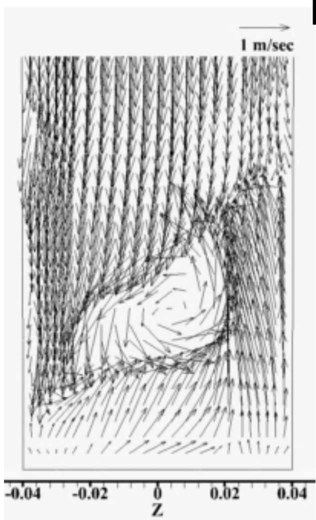


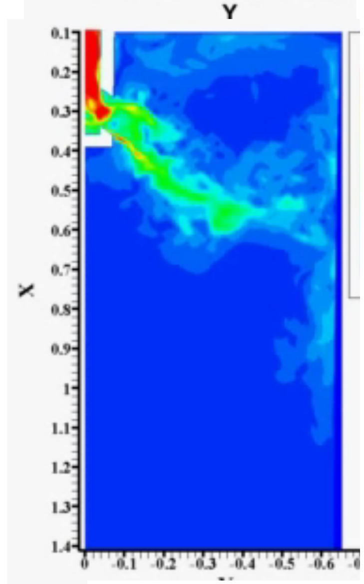






EMB off

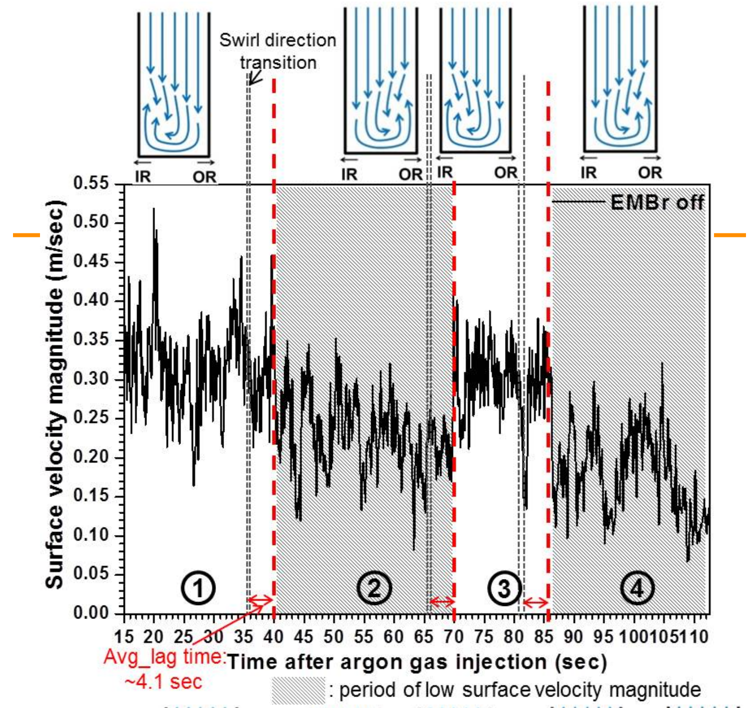


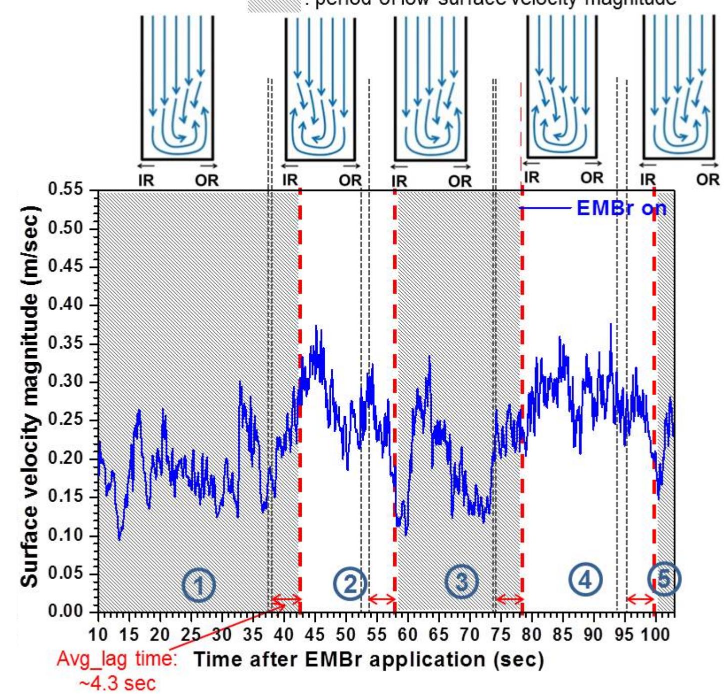


EMB on

Nozzle swirl

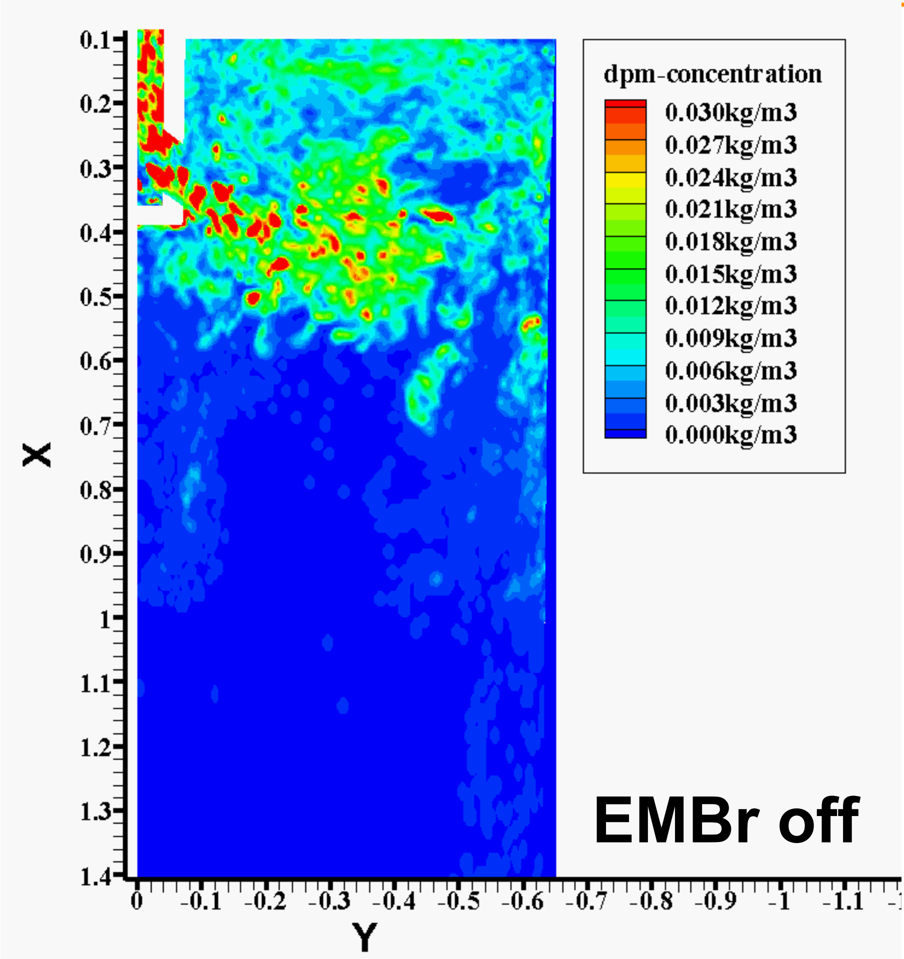
Mold flow

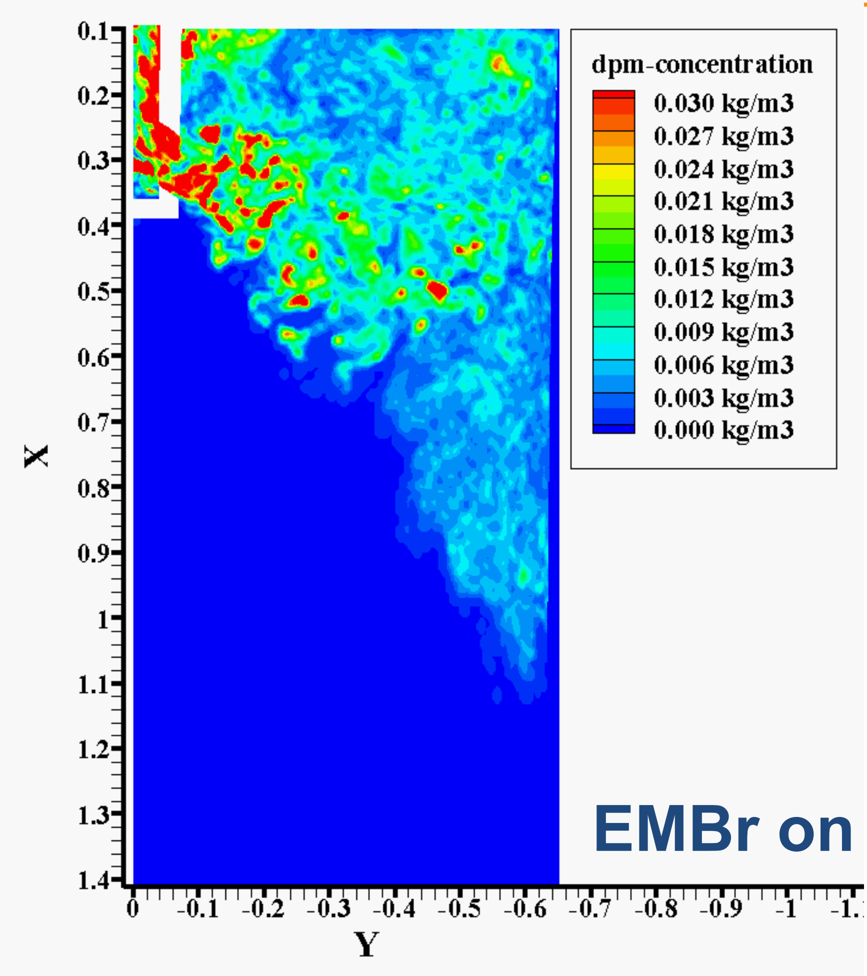




Surface velocity variations

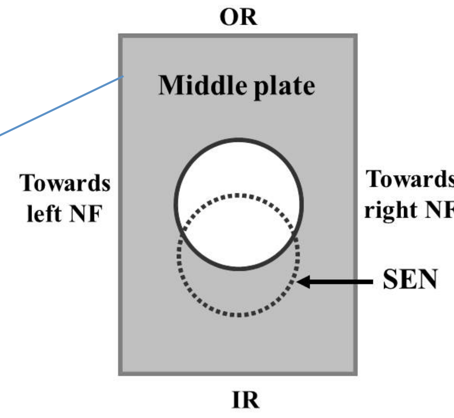
Argon Bubble Distribution in Mold: LES-DPM-MHD

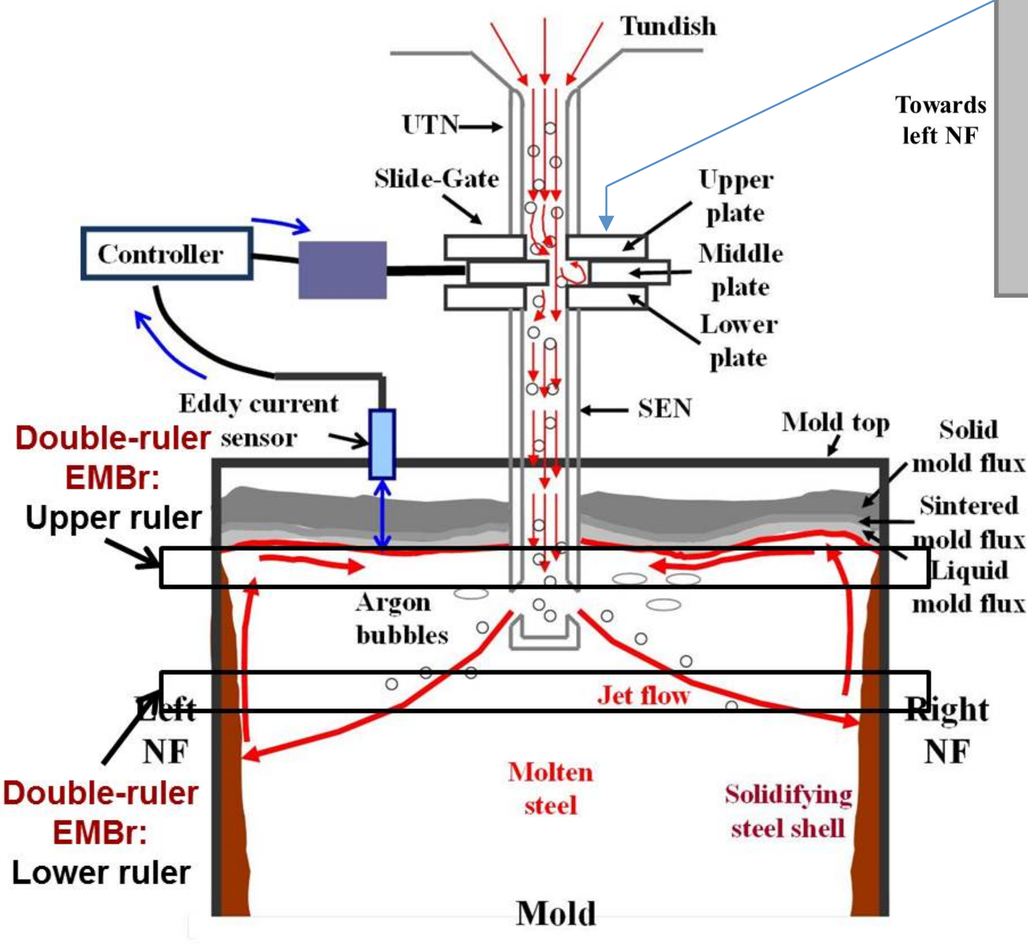




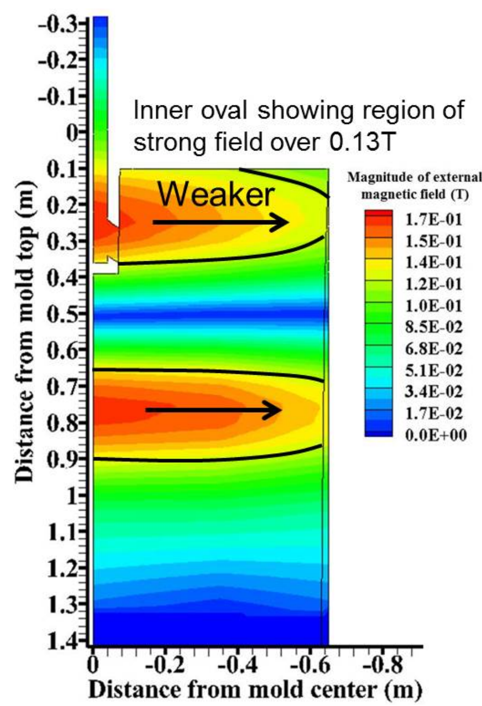
- Transient jet wobbling affects variations of argon gas distribution in mold

2. **Slide-gate** and **Double-Ruler EMBr** in Continuous Slab Casting





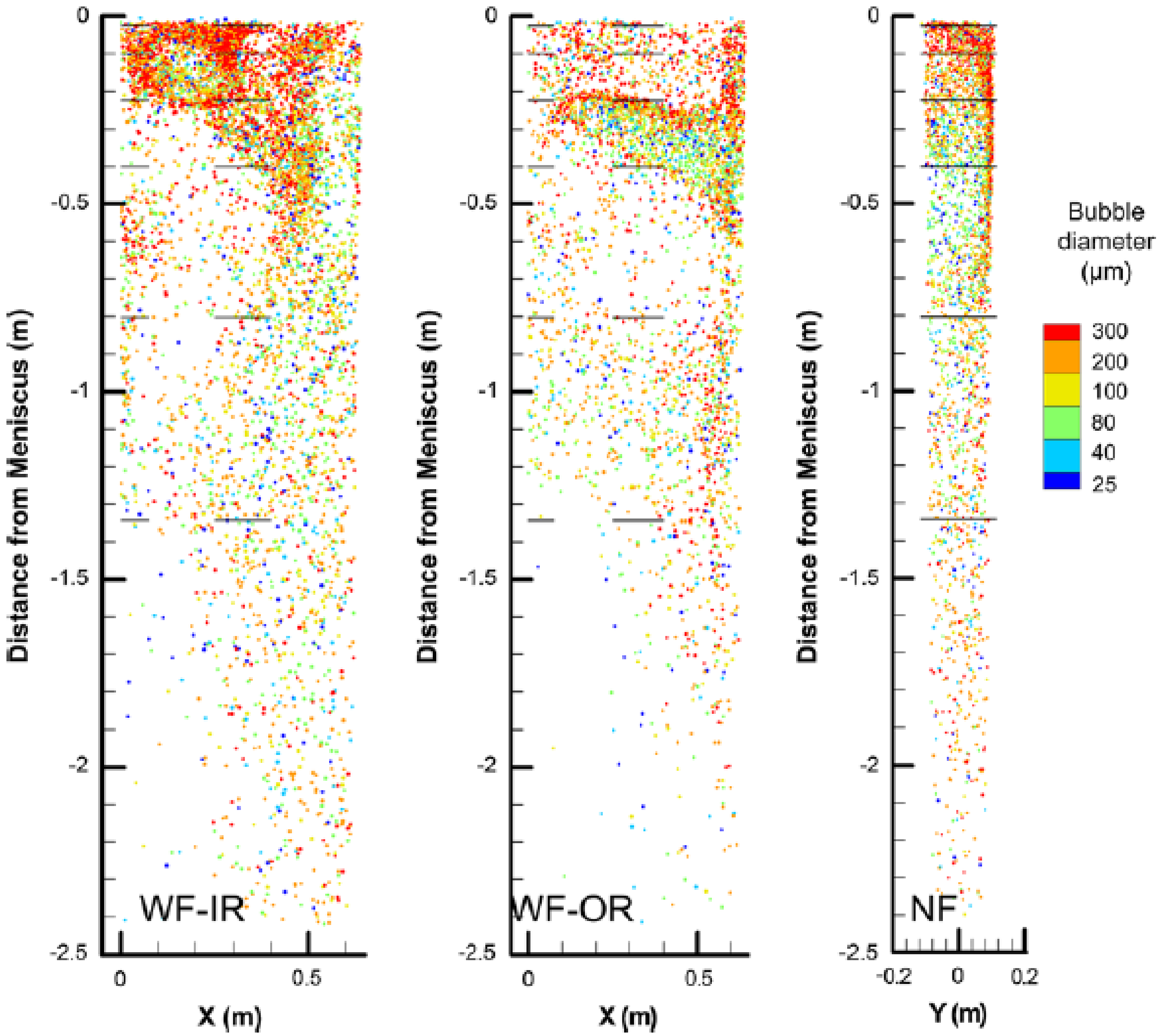
- Slide-gate produces asymmetric open area for flowing molten steel



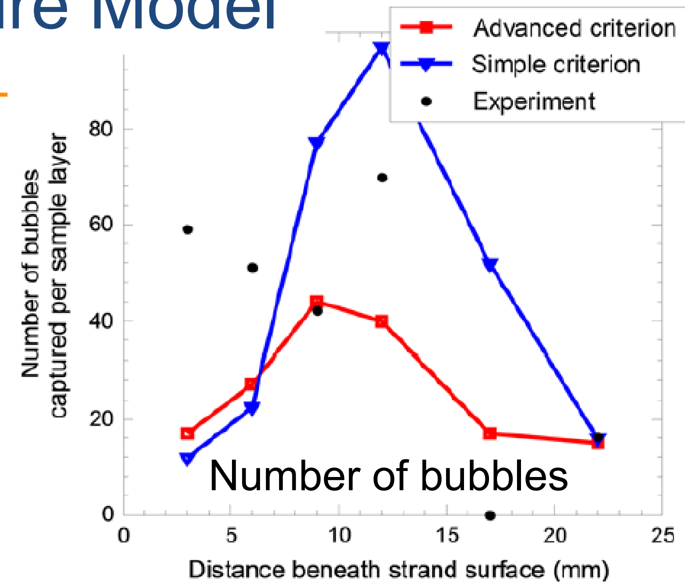
- Double-ruler EMBr has 2 ruler-shaped magnet fields: 1) just above the port 2) below nozzle port

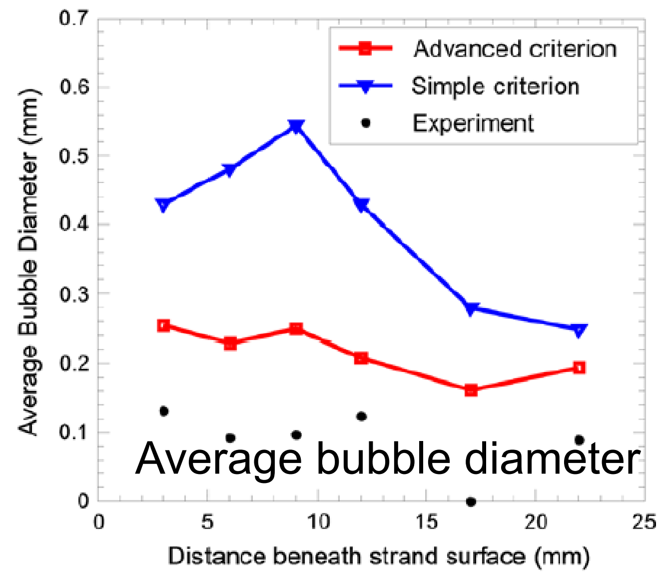
<Double-ruler EMBr Field>

3. Argon Bubble Entrapment into Steel Shell: RANS with Particle Capture Model



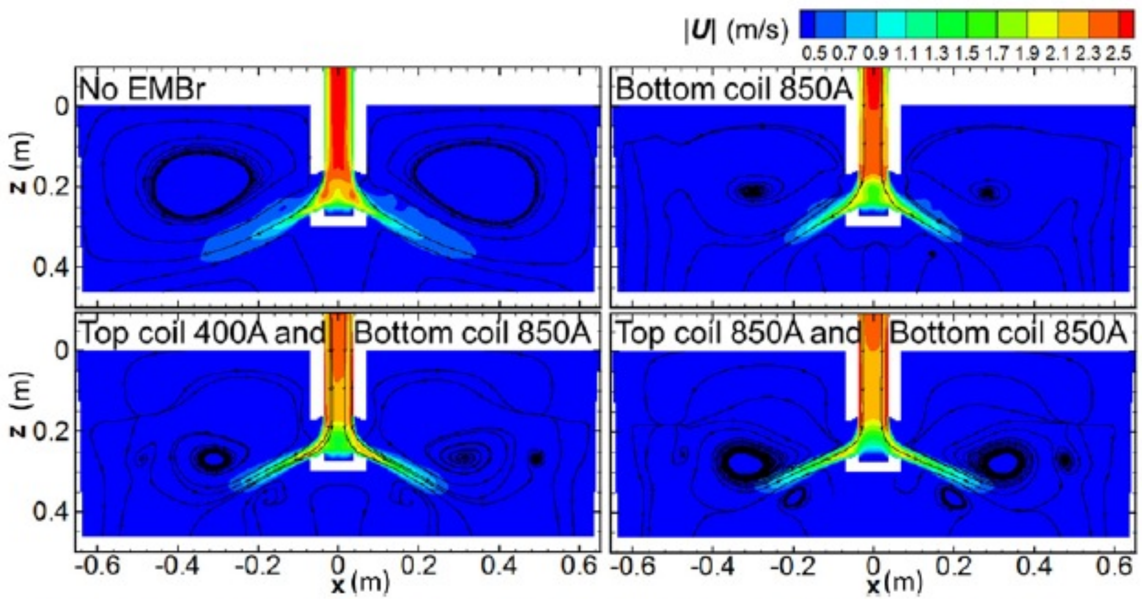
<Captured bubble distributions>



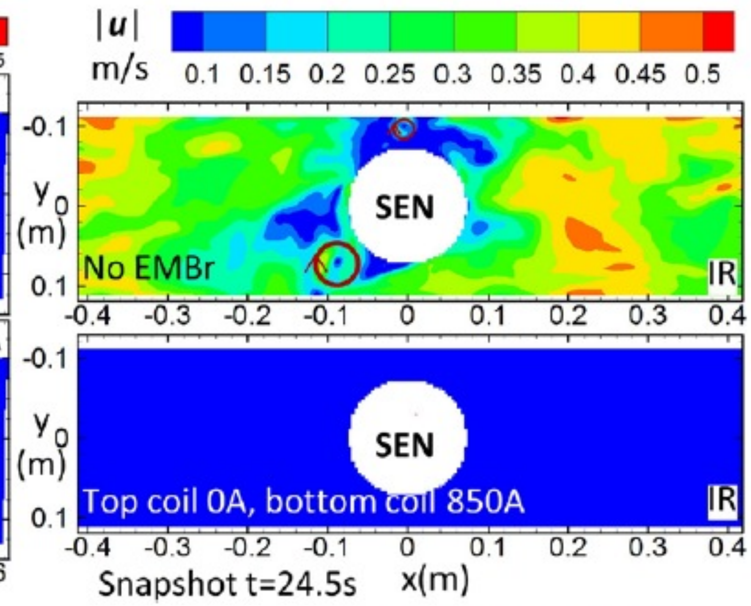


<Model validation: captured bubbles on each NF-sample layer>

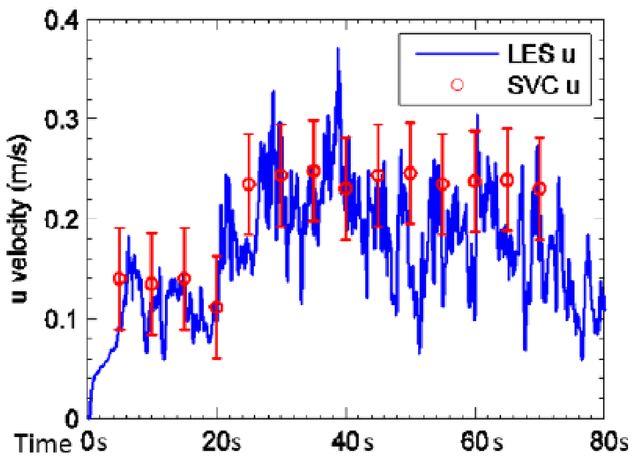
4. **Effect of Double-Ruler EMBr strength**: LES-MHD: CUFLOW



<Velocity magnitude and stream traces in mold>



<Flow near top surface>



<Model validation>

- Good agreement between computational model and SVC sensor measurements
- Optimization of magnetic field strength is important to control surface velocity

Summary

- **Blue Waters (BW)** supercomputing resource augments modeling capability for **Continuous Casting (CC) research**.
  - **ANSYS Fluent HPC on BW XE nodes** shows speed-up breakthrough: multiphase flow simulation runs ~ 3357 times faster than on lab workstation.
  - In-house multi-GPU code, **CUFLOW** also shows good efficiency on **BW XK nodes**
  - **Turbulence models (LES and RANS) coupled with VOF, DPM, MHD**, and **particle capture model (user subroutine) on BW** can produce high-resolution results showing good agreement with measurements, to predict transient **multiphysics phenomena** (slag/steel interface motion, molten steel-argon bubble flow, particle entrapment, EMBr effect) in CC

Recent Publications (with Blue Waters)

[1] CCC Annual Meeting, University of Illinois, August, 2016, pending

[2] 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. *Metallurgical and Materials Transactions B*, 2016, accepted.

[3] Jin, K., B.G. Thomas, and X. Ruan, Modeling and Measurements of Multiphase Flow and Bubble Entrapment in Steel Continuous Casting. *Metallurgical and Materials Transactions B*, Vol. 47B, No. 1 (2016), pp. 548-565. DOI: 10.1007/s11663-015-0525-5

[4] Jin, Kai, Surya P. Vanka, Brian G. Thomas, and Xiaoming 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.

[5] Thomas, B. G., Kai Jin, Pratap Vanka, Hyunjin Yang, Matthew Zappulla, Seid Koric, A hmed Taha, Dynamics of argon bubbles in steel continuous casting with a magnetic fi eld, Blue Waters Annual Report 2015

Two-Phase Flow Equations (argon gas & steel)

- Continuity Equation

$$\frac{\partial u_i}{\partial x_i} = S_{\text{mass sink}}$$

- Steel momentum equation

$$\frac{\partial u_i}{\partial t} + u_j \frac{\partial u_i}{\partial x_j} = -\frac{1}{\rho}\frac{\partial p}{\partial x_i} + \nu \frac{\partial u_i}{\partial x_j x_j} + F_i + S_{i\ \text{momentum sink}}$$

- Steady-State RANS Turbulence Model (*k*-*ε*)

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_k}\right)\frac{\partial k}{\partial x_j}\right] - \rho\overline{u'_i u'_j}\frac{\partial u_j}{\partial x_i} - \rho\varepsilon \qquad \mu_t = \rho C_\mu \frac{k^2}{\varepsilon}$$

$$\frac{\partial}{\partial t}(\rho\varepsilon) + \frac{\partial}{\partial x_i}(\rho\varepsilon u_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{\sigma_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right] + C_{1\varepsilon}\frac{\varepsilon}{k}\left(\rho\overline{u'_i u'_j}\frac{\partial u_j}{\partial x_i}\right) - C_{2\varepsilon}\rho\frac{\varepsilon^2}{k}$$

$$C_{1\varepsilon} = 1.44; \qquad C_{2\varepsilon} = 1.92; \qquad C_\mu = 0.09; \qquad \sigma_k = 1.0\,; \qquad \sigma_\varepsilon = 1.3$$

$$\rho\overline{u'_i u'_j}\frac{\partial u_j}{\partial x_i} = \mu_t\left(\nabla\vec{u} + \left(\nabla\vec{u}\right)^T\right) : \nabla\vec{u}$$

$\vec{u}$ Steel velocity

$\vec{g}$ Gravity

ρ Steel density

$\vec{F}$ Source terms (gas &EMBr)

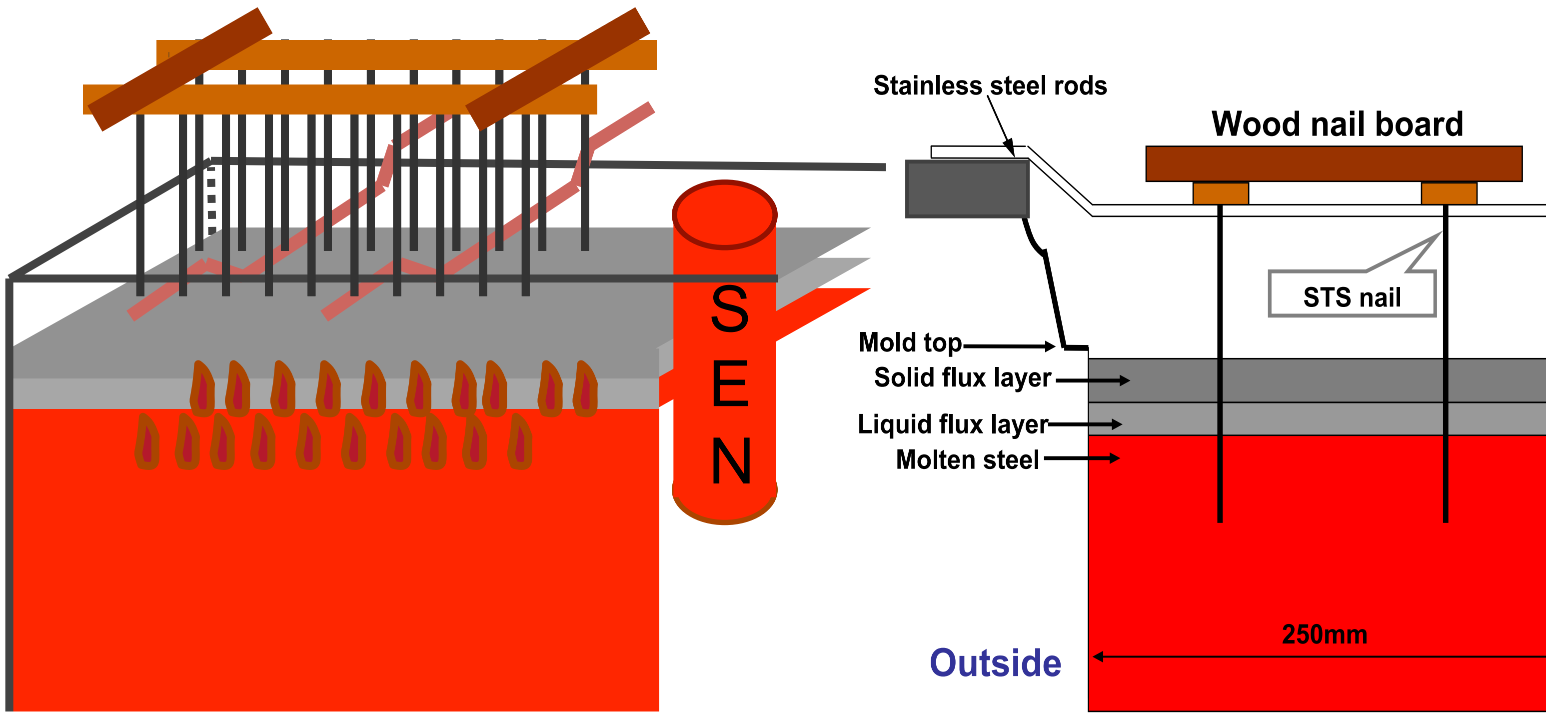
μ Steel dynamic viscosity

k Turbulent kinetic energy

ε Turbulent dissipation rate

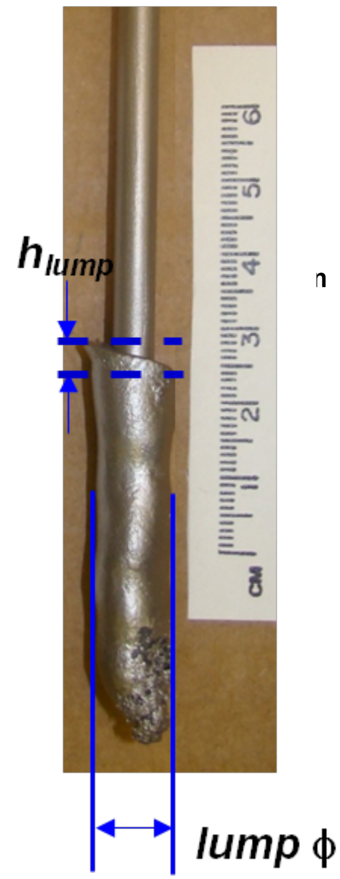
Nail Board Measurements: Surface Velocity (Baosteel Caster #4)

Flux La
Surf



< WF View >

< NF View >

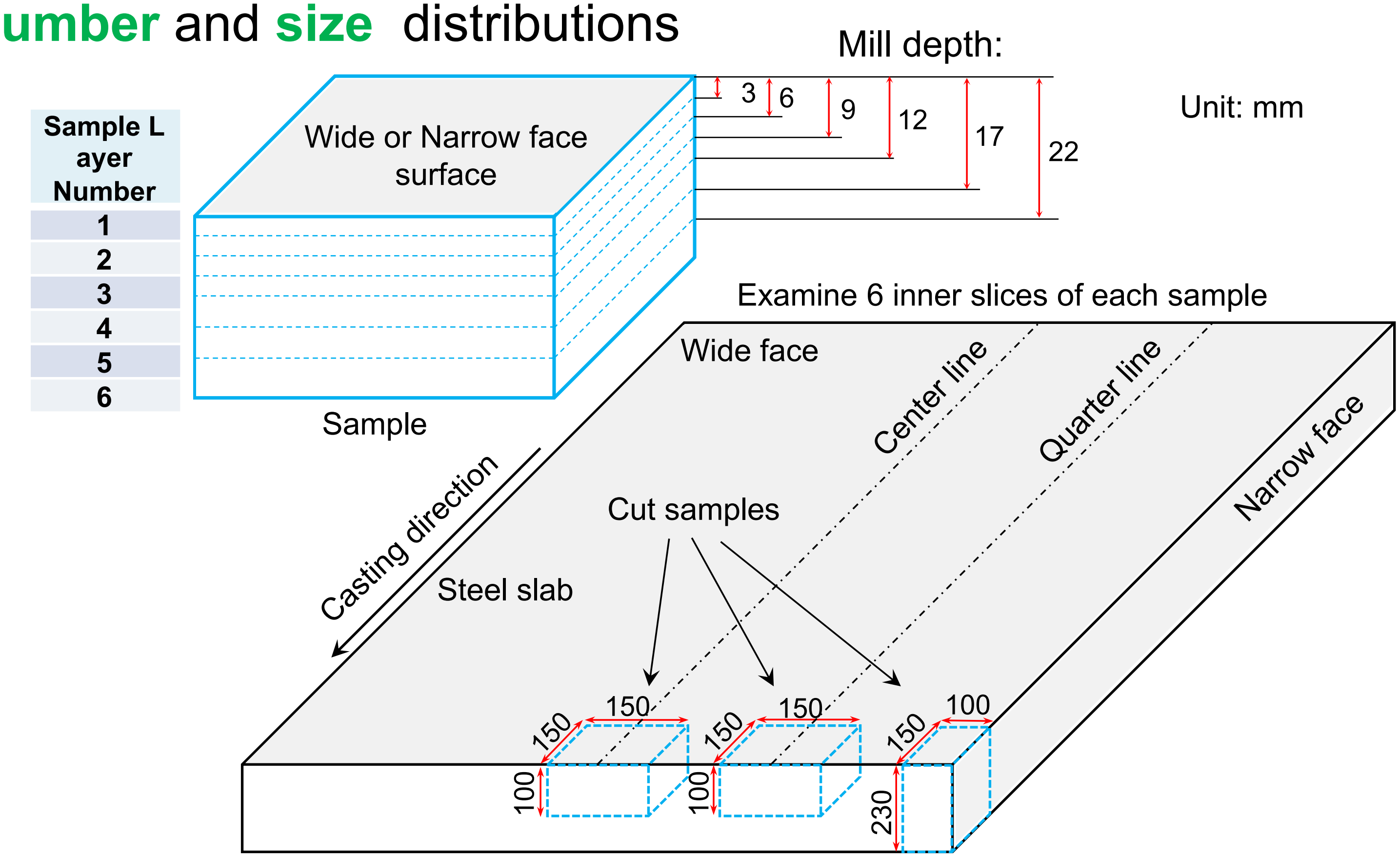


Positioning Nail Board in the Mold

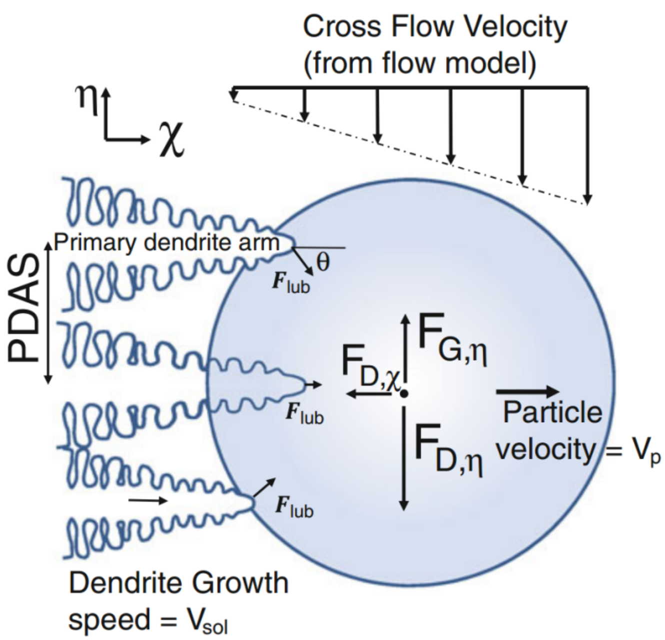
Dauby et al, LTV Steel, 1985; SM-Cho et al, TMS, 2011

Inclusion Measurements (Baosteel Caster #4)

- Cut samples from as-cast slab: WF center, WF quarter, and NF;
- Mill away steel layer by layer.
- Examine bubbles with 35x optical microscope
- Record **number** and **size** distributions



Forces Acting on Particle at Dendritic Interface
(Needed for Bubble Capture Criterion)



Buoyancy / gravity force: F_G
Drag force: $F_{D\chi}$ and $F_{D\eta}$
Lift force: F_L

(Press gradient, str ess gradient, added mass, and Basset forces can be neglected.)

Lubrication force acts on the particle along particle's radius towards dendrite tip

$$F_{\text{lub}} = 6\pi\mu V_{sol} \frac{R_p^{\,2}}{h_o}\left(\frac{r_d}{r_d + R_p}\right)^2$$

Van der Waals force pushes particle away fr om dendrite tip

$$F_I = 2\pi\Delta\sigma_o \frac{r_d R_p}{r_d + R_p}\frac{a_o^{\,2}}{h_o^{\,2}} \qquad \Delta\sigma_o = \sigma_{sp} - \sigma_{sl} - \sigma_{pl}$$

Interfacial concentration gradient force push es particle toward solidification front

$$F_{Grad} = -\frac{m\beta\pi R_p}{\xi^2}\left\{\frac{\xi^2 - R_p^{\,2}}{\beta}\ln\frac{(\xi + R_p)\left[\alpha(\xi - R_p)+\beta\right]}{(\xi - R_p)\left[\alpha(\xi + R_p)+\beta\right]} + \frac{2R_p}{\alpha} - \frac{\beta}{\alpha^2}\ln\frac{\alpha(\xi - R_p)+\beta}{\alpha(\xi + R_p)+\beta}\right\}$$

$$\alpha = 1 + nC_o \qquad \beta = nr_d\left(C^* - C_o\right)$$

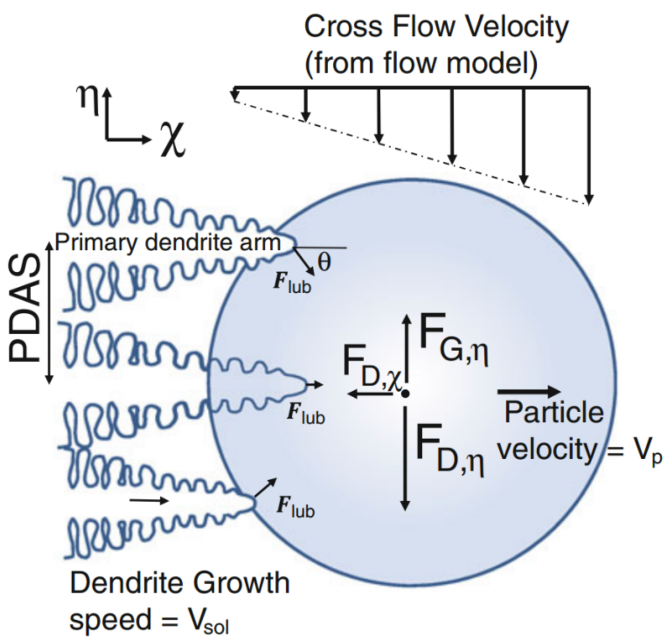
$$\xi = R_p + r_d + h_o \qquad \frac{r_d V_{sol}}{2D_s} = \frac{C^* - C_o}{C^*(1-k)}$$

R_p	particle radius
V_{sol}	solidification velocity
r_d	dendrite tip radius
h_o	distance between dendrite tip and particle
a_o	atomic diameter of the liquid
C_o	sulfur content of steel
D_s	diffusion coefficient of sulfur in steel
k	distribution coefficient

Bubble capture criteria

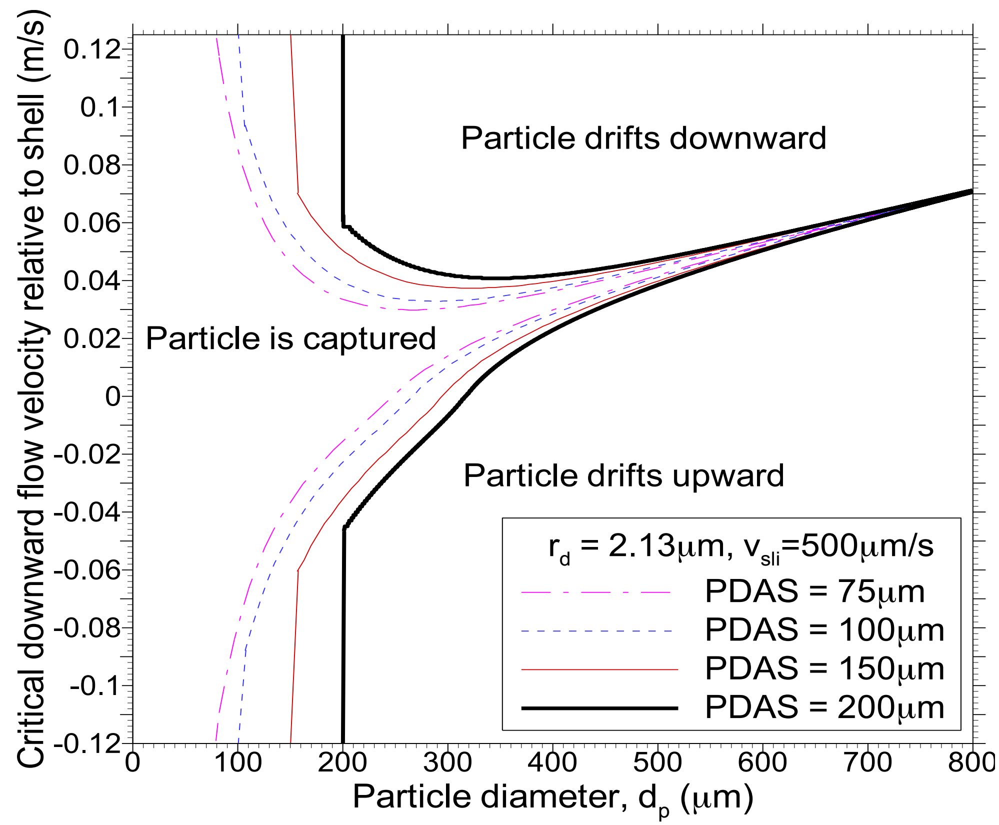
"**Simple**": touch boundary = captured

"**Advanced**":



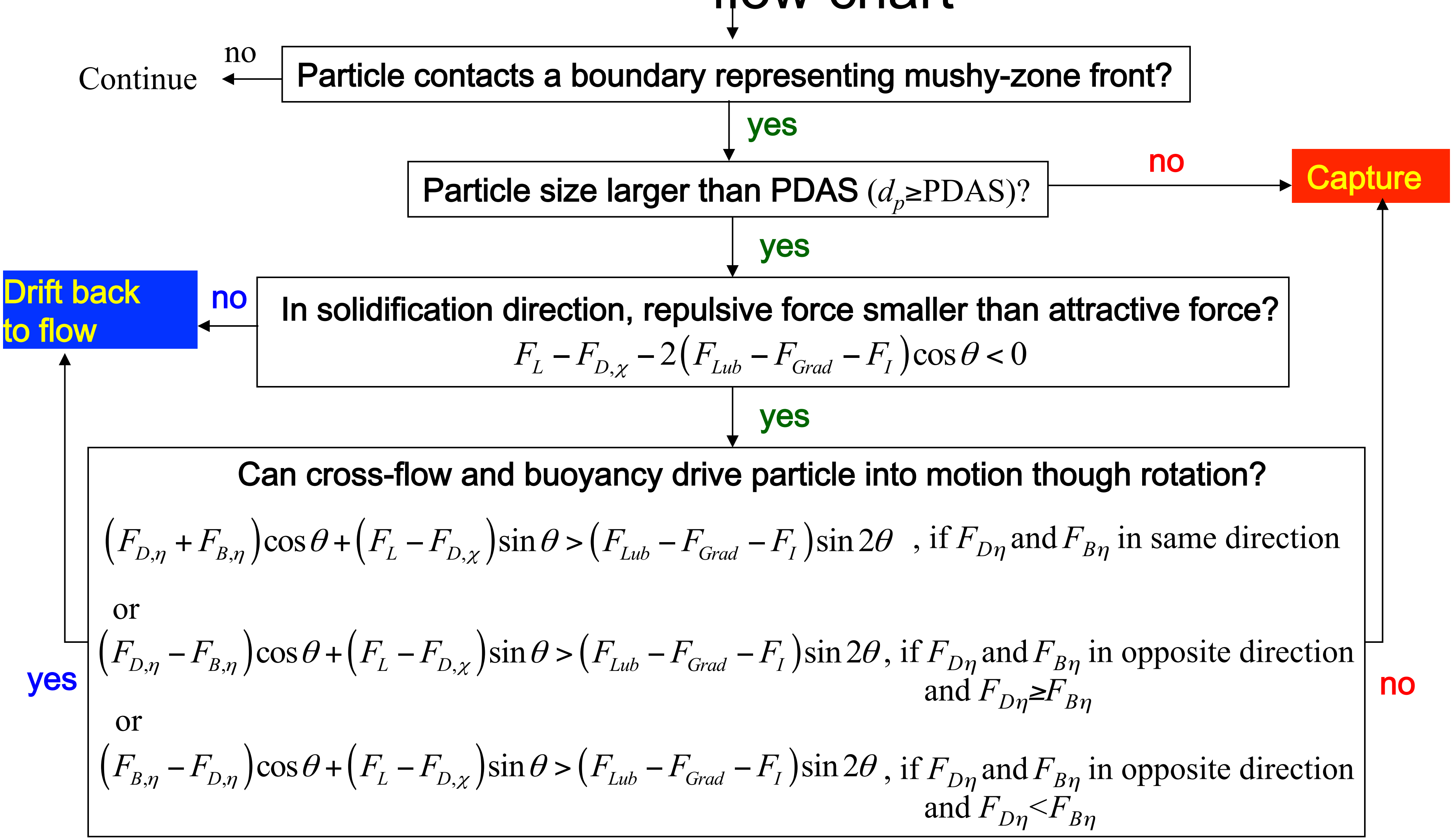
A Bubble/Particle Touching 3 Dendrite Tips
(Fig from Thomas, BG., et al [5])

Example Critical Cross-flow velocity maps



- Q. Yuan, PhD, 2004 [4]; S. Mahmood MS, 2006; BG Thomas et al, MMTB, 2014 [2]
- Yuan Q., and B.G. Thomas, 3rd ICSTS, AISTech, Charlotte, NC, May 9-11, 2005

"Advanced" Bubble Capture Criterion – flow chart



Quan Yuan, Ph.D. thesis, 2004

Figure from Sana Mahmood, Master thesis, 2006