COMPUTATIONAL STUDIES AND OPTIMIZATION OF PROCESSES IN A STEEL LADLE

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April 21, 2022

"Where Ideas Become Reality"

CENTER FOR INNOVATION THROUGH VISUALIZATION & SIMULATION

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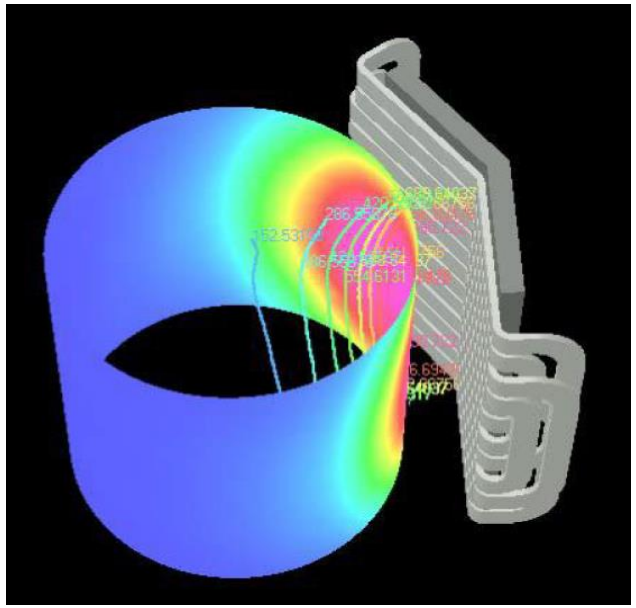
Presentation Outline

- Introduction
  - Objectives & Roadmap
  - Outcomes
  - Project Timeline
- Methodology and CFD Models
- 2022 Projects – Models and Applications
  - Hot Metal Desulfurization
  - Steel Desulfurization and Re-oxidation
  - Alloy Mixing Study – (NSF GOALI)
  - Smart Ladle
- Summary & Future Work

Motivation

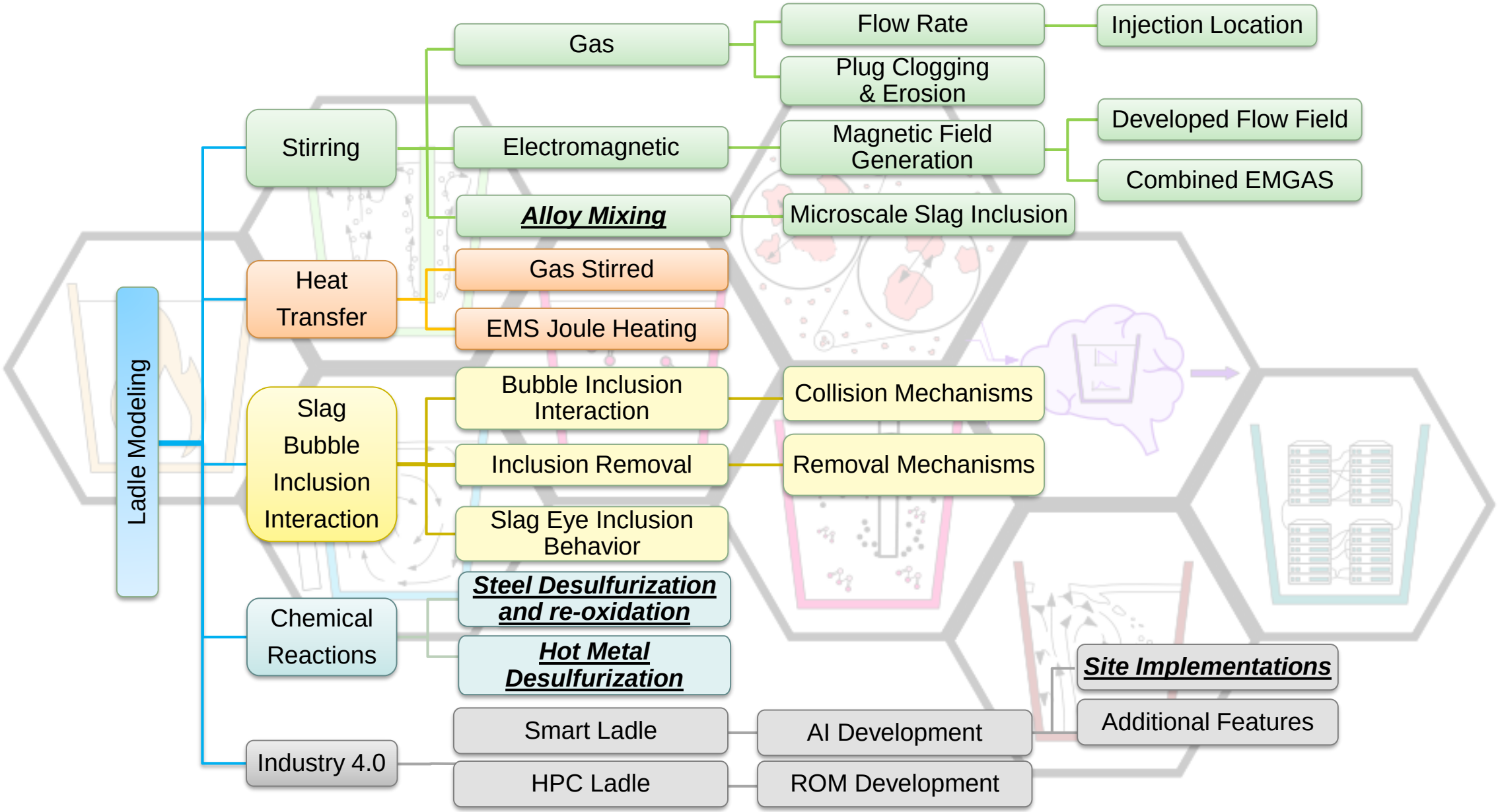
- Current Issues
  - Complex transport phenomena
  - Incomplete understanding the dynamics of multiphase flow, microscale inclusions evolution and chemical reactions
  - Incorporation of cutting-edge technologies such as machine learning and real-time process control
- Potential Impacts
  - Optimized flow condition and physical properties
  - Improved steel cleanliness
  - Reduce defects
  - Troubleshooting



Long Term Objectives

- To develop a validated comprehensive multiphase CFD model of a steel ladle using three stirring methods
  - Gas stirring
  - EMS stirring
  - Combined EM-Gas stirring
- To optimize ladle stirring conditions for
  - Steel cleanliness
  - Productivity
  - Equipment lifetime
  - Unexpected industrial problems
- To develop Industry 4.0 for ladle process control
  - AI, digital twin, and reduced order models

Model Development Roadmap



2022 Application Roadmap

Project 12: Shipping Temperature and Superheat Control

Associated Models:
- *Smart Ladle*

Site Companies:
- *Site A: Steel Dynamics, Inc.*
- *Site B: Nucor Steel*
- *Site C: Tata Steel*
- *…*

Project 16: Microscale Inclusions and Alloy Mixing (NSF GOALI)

Associated Models:
- *Gas and EMS Stirring Models*
- *Inclusion model*
- *…*

Site Companies and Partner Institution:
- *Nucor steel*
- *SSAB*
- *CMU*

01/2022 – 12/2022

01/2022 – 12/2022

06/2022 – 12/2022

01/2022 – 08/2022

06/2022 – 05/2023

Project 10: Hot Metal Desulfurization

Associated Models :
- *Gas and EMS Stirring Models*

Companies interested:
- ***Cleveland-Cliffs (Site company)***
- *ArcelorMittal Global R&D*

Project 15: Minimization of Ladle Erosion and Wear

Associated Models:
- *Gas and EMS Stirring Models*

Companies interested:
- ***Charter Steel (Site company)***
- *ArcelorMittal Global R&D*

Project 17: Reduced Order Modeling and Performance Prediction

Associated Models:
- *HPC Ladle, Inclusion Model, …*

Companies interested:
- *Several sites*

Major Outcomes - Models & Applications

Projects (2016 – 2022): Completed: 5, Ongoing: 6

- *Project #1:* Isothermal Gas-stirred Ladle Flow Model
  - Reduced time for homogenization by changing plug distance ratio and separation angle
- *Project #2:* Effect of Heat Transfer in Gas-stirred Ladle
  - Compared temperature loss rate with different wall temperatures
- *Project #3:* Gas-Stirred Inclusion Growth-Removal Model
  - Developed inclusion growth-removal model based on Eulerian-Lagrangian multiphase approach
  - Improved inclusion removal efficiency by changing plug separation angle
- *Project #4:* EMS Isothermal Ladle – AM Generic Ladle
  - Identified effects of EMS flow on wall shear stress, bulk velocity and slag-eye size
- *Project #5:* Inclusion Removal Enhancement & Validation
  - Validated CFD model against measurement data (avg. 12.1% error in inclusion number density)
  - Higher inclusion removal rate by changing plug separation angle
- *Project #6:* Plug Clogging and Erosion Study
  - 37% growth in time for mixing by doubling flow rate, but with increased wall shear stresses (98% increase in peak stress)
- *Project #7:* Combined EMS-Gas Model– AM Generic Ladle
  - 98% increase in time for mixing and 30% growth in wall shear stress using EMS-Gas stirring method compared to EMS method
- *Project #8:* Steel Desulfurization & Re-oxidation
  - **Model validation (difference: S<5%, Al < 7%, Mn<8%, Si<6%)**
  - **Desulfur. efficiency increase from 32.84% to 43.25% when the flow rate changes from 5 SCFM to 20 SCFM**
  - **Increased oxide mass by 51.53% in 180° 20-20 SCFM compared to 90° 5-5 SCFM**
- *Project #9:* Smart Ladle
  - Prediction model of tundish midpoint temperature and slope using industry data by machine learning method
  - 1.4°F mean absolute error with a standard deviation of 2°F
  - Smart Ladle Web Tool on SMSVC member's page
  - **Implemented SL software at SDI, Nucor is in progress**
- *Project #10:* Hot metal desulfurization
  - **Validated CFD model in CaC_2/CaO injection desulfurization against exp. from literature (6.3% difference)**
- *Project #16:* Alloy Mixing (NSF GOALI)
  - **Developed single phase alloy addition with ferromanganese as the alloying element**

Major Accomplishments since November 2021

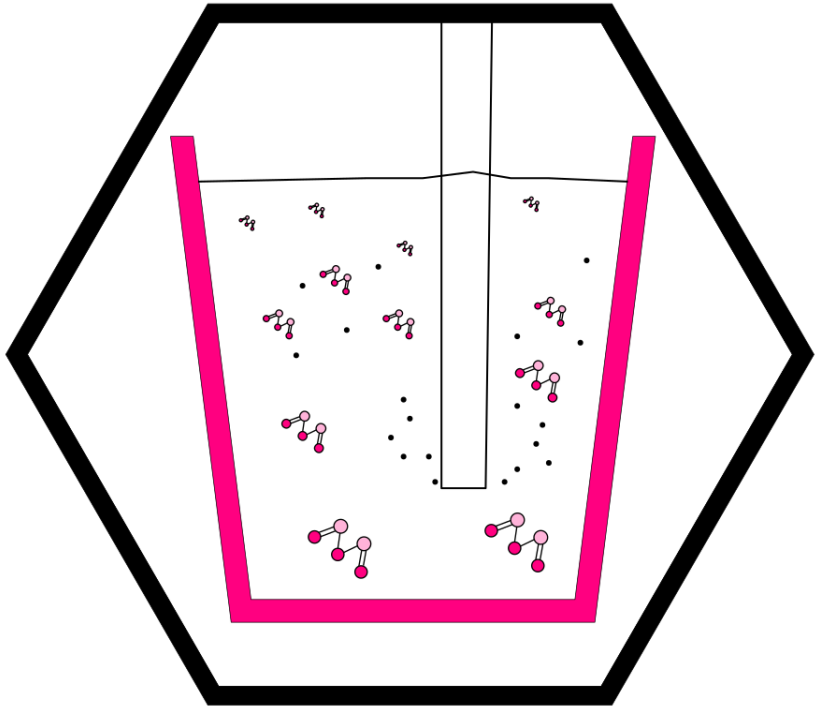
- **<u>Project #8</u>: Steel Desulfurization & Re-oxidation**
  - Validated re-oxidation model for Al and Mn and Si against measurement (max. 7.34% difference)
  - Compared desulfurization effectiveness under different flow rate and plug separation angle (max. 35.23% improvement)
- **<u>Project #9</u>: Smart Ladle**
  - Implemented Smart Ladle at SDI Butler Division
  - Data training and early model development for Nucor Berkeley
- **<u>Project #10</u>: Hot Metal Desulfurization**
  - Developed and validated model by CaC_2/CaO injection against experiment measurements (~6.3% difference)
  - Developed hot metal desulfurization model by Mg gas injection
- **<u>Project #16</u>: Microscale Inclusions and Alloy Mixing (NSF GOALI)**
  - Developed single phase alloy addition with ferromanganese as the alloying element
  - Developed flow field using both methods on frozen flow and normal flow

2022 Objectives

- **<u>Project #7:</u> Combined Gas-Stirring and EMS**
  - To investigate inclusion generation and removal in gas-stirred & EMS ladle
- **<u>Project #8:</u> Desulfurization and Re-oxidation**
  - To develop validated model for chemical reactions in the ladle furnace
- **<u>Project #10:</u> Hot Metal Desulfurization**
  - To build and validate hot metal desulfurization model
- **<u>Project #12:</u> Shipping Temperature and Superheat Control**
  - To complete implementation and testing of Smart Ladle and expand to other sites
- **<u>Project #16:</u> Microscale Inclusions and Alloy Mixing (NSF GOALI)**
  - To build a validated model for alloy-based mixing studies
  - To develop a slag microscale inclusion generation model
  - To perform experimental work on surface behavior
- **<u>Project #17:</u> Reduced Order Modeling and Performance Prediction (HPC Ladle)**
  - To identify target variables for Reduced Order Model creation

2022 Timeline

	Task	Jan	Feb	Mar	Apr	May	Jun	Jul	Aug	Sep	Oct	Nov	Dec
Project 6 Plug Clogging and Erosion	Literature search												
	Ladle erosion and wear model												
Project 7 Combined Gas-Stirring and EMS	EM-Gas flow field												
Project 8 Steel Desulfurization and Re-oxidation in Ladle	Literature search												
	Re-oxidation												
	Desulfurization couples with Re-oxidation												
Project 10 Hot Metal Desulfurization	Literature search												
	Model development and validation												
	Model application												
Project 12 Shipping Temperature and Superheat Control	Data collection												
	Model development and implement												
Project 16 Microscale Inclusions and Alloy Mixing (NSF GOALI)	Literature search												
	Model development and validation												
	Experimental work												
Project 17 Reduced Order Modeling and Performance Prediction (HPC Ladle)	Literature search												
	Target variable selection and baseline simulation												



Project 10:

Hot Metal Desulfurization Model Development and Validation

Site: Cleveland-Cliffs
Start: October 2021

Overview

- Motivation:
  - Hot metal desulfurization serves as the main unit process for removing sulfur in blast-furnace-based steelmaking
  - The model can be used to predict sulfur removal rate in the hot metal
- Objective:
  - To develop an comprehensive 3D CFD model to predict the sulfur removal rate in the ladle
- Potential Impacts:
  - Improvement in the efficiency of desulphurization by:
    - Decrease in reagent consumption
    - Increase in productivity.

CFD Methodology

Multiphase Flow Model

- Iron/gas/solid multiphase
  - Flow velocity and turbulence

liquid flow field

- Species transport model
  - Local element content distribution in iron

velocity
turbulence

species
mass fraction

species
source term

Chemical Reaction Model

- Reaction rate calculation
  - Calculation of parameters based on multiphase flow field by user-defined function
  - Source terms of the element in the bath

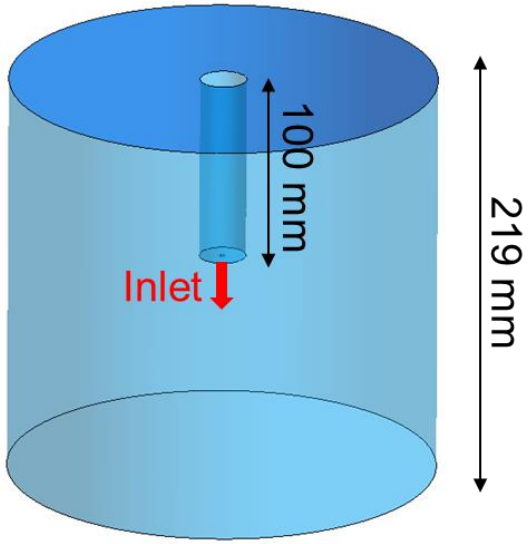
Desulfurization Mechanism

- Desulfurization reagents: $CaO/CaC_2(s)$, Mg(s), or both
- Sulfur and $CaO/CaC_2(s)$ react at particle surface
- High temperature of hot metal, Magnesium powder vaporize quickly. ~80% of vaporized Mg dissolve into iron
- Desulfurization at slag-iron interface

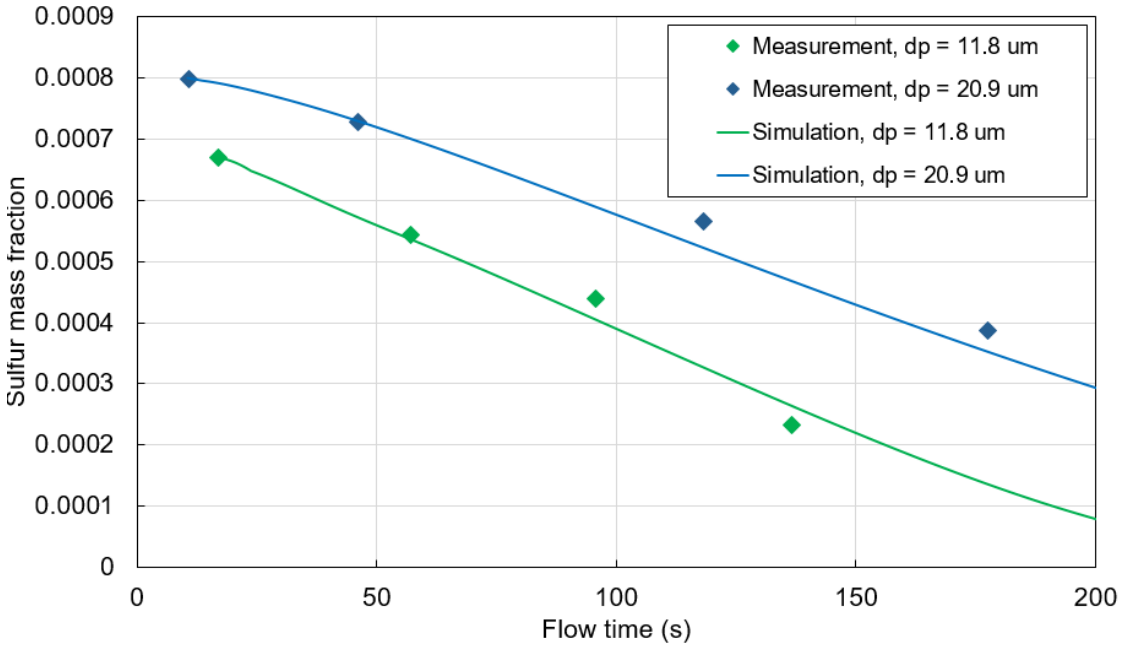
Reaction number	Chemical formulas	Reaction site
Reaction 1	S+ CaO = CaS + O	CaO particle
Reaction 2	S + Mg(l) = MgS(s)	MgS particle
Reaction 3	S + Mg(g) = MgS(s)	Gas bubble
Reaction 4	-	Slag-Iron interface

Validation of CaC_2 Desulfurization

- Experimental[1] data from Coudure at al, 1992
- Penetration ratio is calculated[2] and applied at a rate of 23.74%
- The average difference between measurements and CFD simulation are **6.8%** (case 1, 11.8 um) and **5.8%** (case 2, 20.9 um)



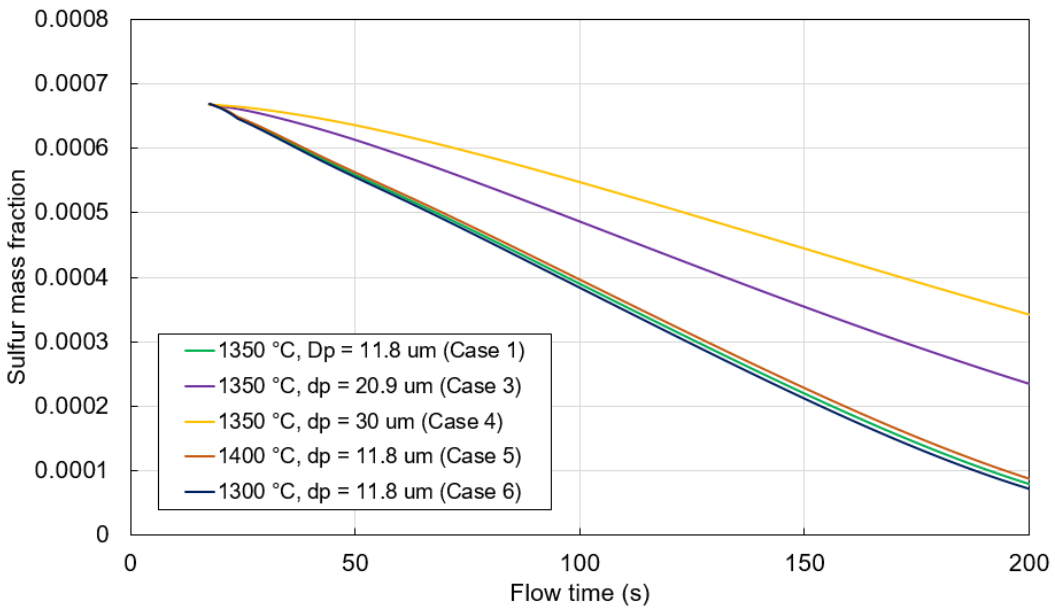
Carrier gas	N_2
Gas flow rate	13 SLPM
CaC_2 flow rate	200 g/min
Particle diameter	**11.8 um (Case 1)** **20.9 um (Case 2)**
Initial sulfur content	**670 ppm (Case 1)** **800 ppm (Case 2)**

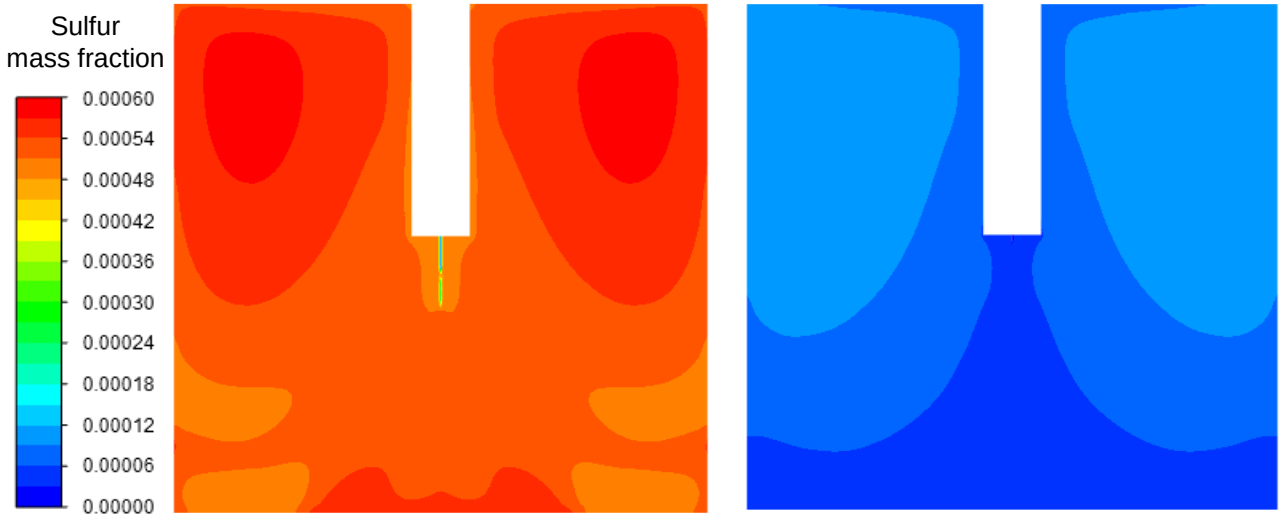


[1] JM, Coudure, and Irons GA. "The Effect of Calcium Carbide Particle Size Distribution on the Kinetics of Hot Metal Desulphurization." *ISIJ international* 34.2 (1994): 155-163.
[2] Wang, N., L. B. Zhang, and Z. S. Zou. "Three basic parameters determining desulphurization efficiency of hot metal by powder injection." *J. Iron. Steel Res* 12.9 (2000): 10-15.

Effect of Particle Size and Temperature on Desulfurization

- The smaller particle size, higher temperature, the better desulfurization rate
- Particle size is more dominant to desulfurization compare to temperature
- Sulfur content higher at dead zone
- Clean iron move to bottom of ladle



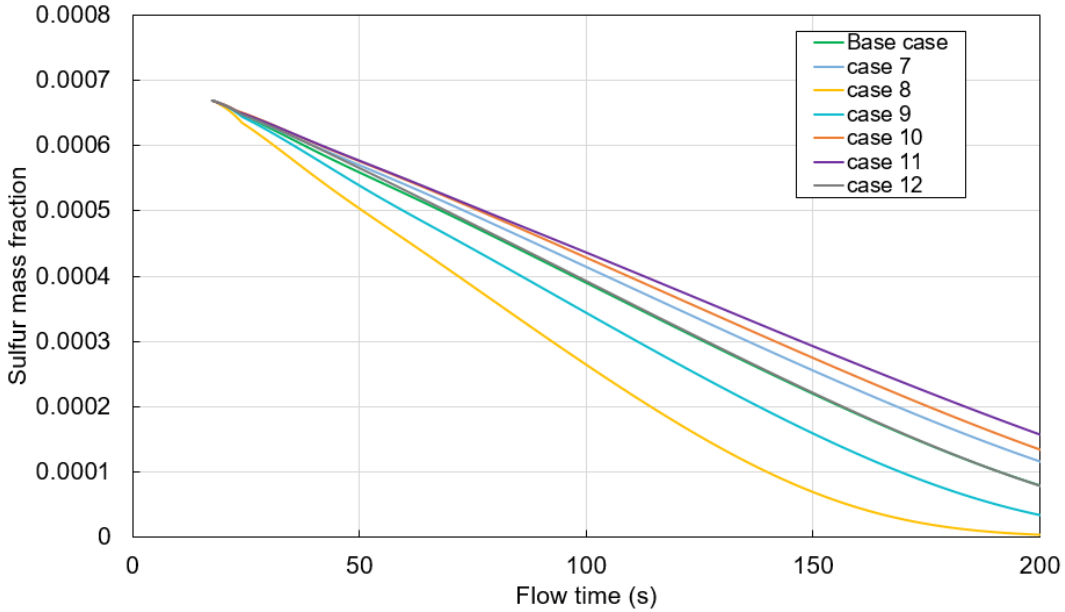


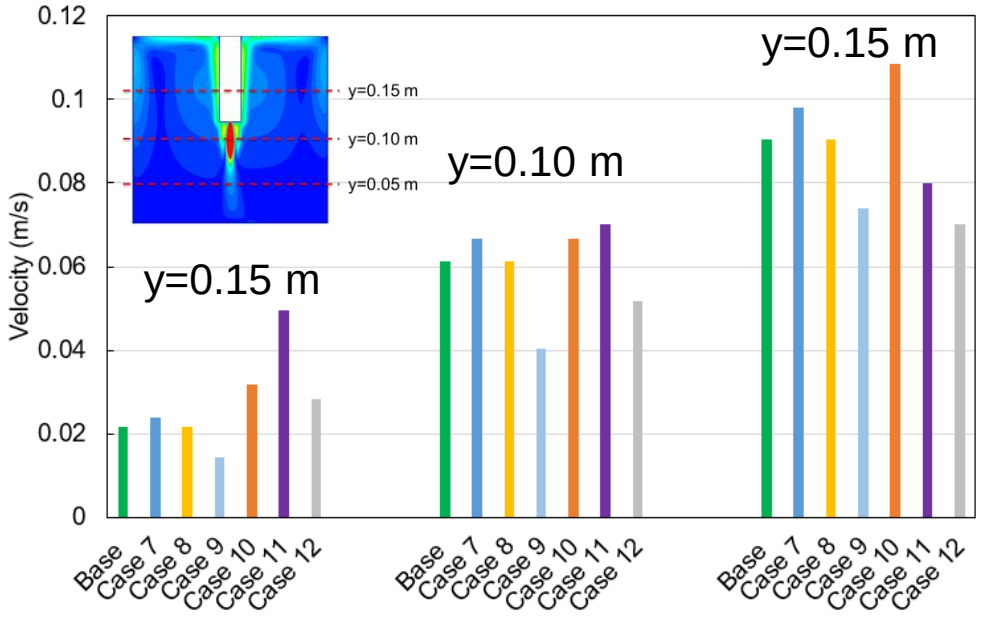
50 s 200 s

	Particle size	HM temp.
Base Case	11.8 um	1350 °C
Case 3	**20.9 um**	1350 °C
Case 4	**30.0 um**	1350 °C
Case 5	11.8 um	**1400 °C**
Case 6	11.8 um	**1300 °C**

Effect of Flow rate and Lance Location on Desulfurization

	N_2 flow rate	CaC_2 flow rate	Lance depth	Lance location	Desulf. Rate (at 200s)
Base Case	13 SLPM	200 g/min	100 mm	Center	88.18%
Case 7	**15 SLPM**	200 g/min	100 mm	Center	82.68%
Case 8	13 SLPM	**300 g/min**	100 mm	Center	99.47%
Case 9	13 SLPM	200 g/min	**60 mm**	Center	94.96%
Case 10	13 SLPM	200 g/min	**140 mm**	Center	79.96%
Case 11	13 SLPM	200 g/min	100 mm	**1/3R off center**	76.52%
Case 12	13 SLPM	200 g/min	100 mm	**1/3R duo lance**	88.26%





- 7 cases relate to carrier gas flow rate, reagent flow rate, lance location are studied
- Effect of flow rate: CaC_2 - 300 g/min > base case > N_2 – 15 SLPM
- Effect of lance depth: 60 mm > 100 mm > 140 mm
- Effect of lance location: duo lance > single lance > 1/3R single lance
- Residence time of particle is inversely proportional to flow velocity

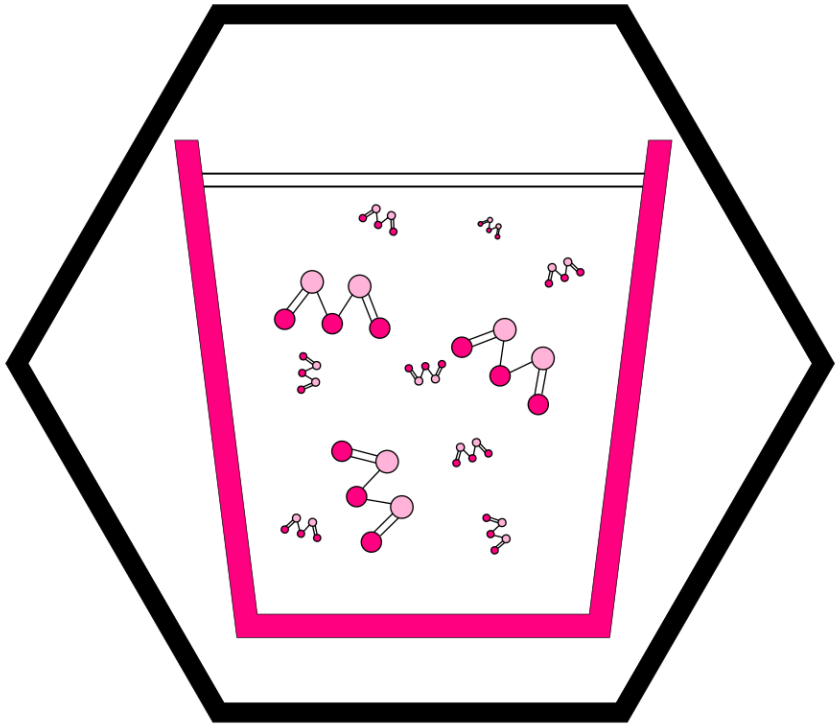
Model Applications

Simulation Capability

- The sulfur mass fraction in different scenarios
  - Plug arrangement
  - Lance depth and location
  - Carrier gas flow rate
  - Reagent usage

Industry Implementation

- Sulfur control
  - Sulfur content prediction
- Ladle design optimization
  - Layout improvement for more efficient desulfurization
- Cost reduction
  - Treatment time estimation



Project 8:

Steel Desulfurization and Re-oxidation Model Development and Validation

Site: Generic
Start: March 2020

Overview

- **Motivation**
  - Sulfur and alloying oxides in steel lead to surface defects and fatigue cracks, impairing the steel strength and resistance
  - The content of sulfur and alloying oxides can be controlled by chemical reactions between steel and slag
- **Objective**
  - To develop a model for the desulfurization and re-oxidation process
  - To validate the model with industry sampling
  - To apply the model to the practical ladles and optimize the operating conditions to control sulfur content as well as alloying oxides
- **Potential Impact**
  - Improved product quality and castability

CFD Methodology

Multiphase Flow Model

- Steel/argon multiphase
  - Flow velocity and turbulence

liquid flow field

- Species transport model
  - Local element content distribution in steel

velocity
turbulence

species
mass fraction

species
source term

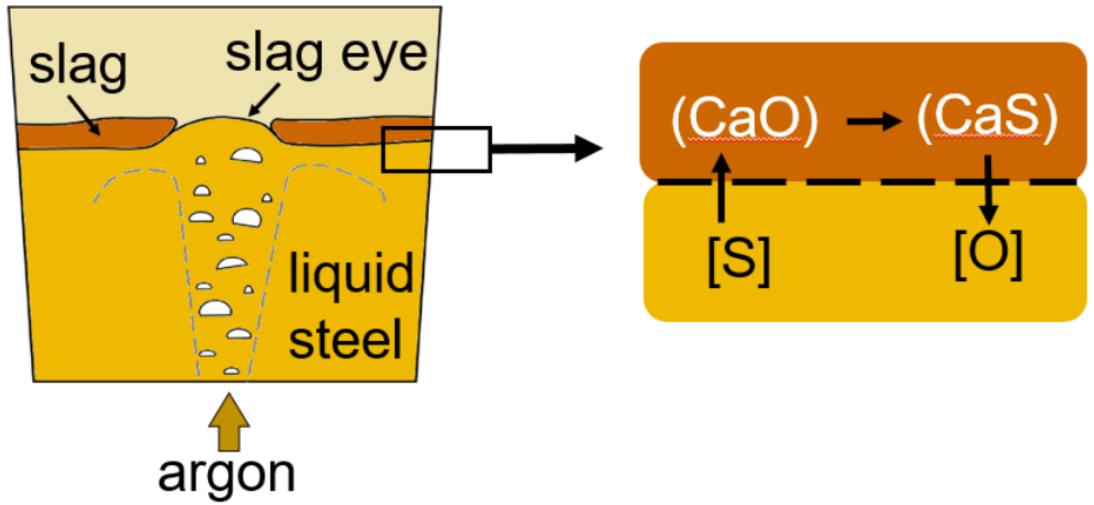
Chemical Reaction Model

- Reaction rate calculation
  - Calculation of parameters based on multiphase flow field by user-defined function
  - Source terms of the element at the slag-steel interface

Desulfurization and Re-oxidation Mechanism

- **Desulfurization** occurs at the slag-steel interface where sulfur reacts with CaO in slag phase, forming CaS and releasing oxygen element into steel

$$[S]+(O^{2-})=(S^{2-})+[O]$$

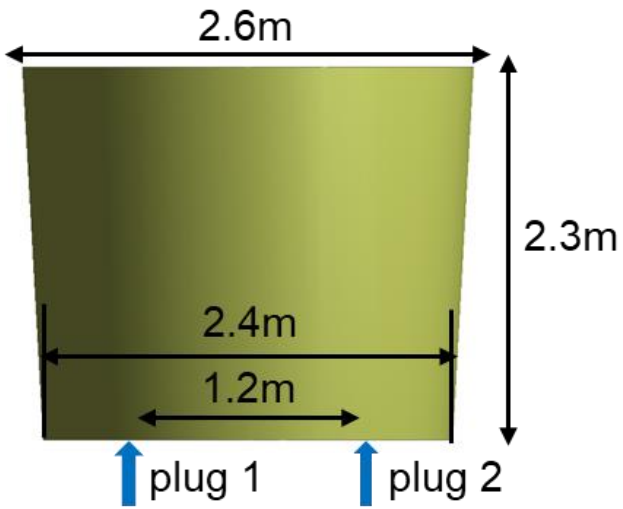


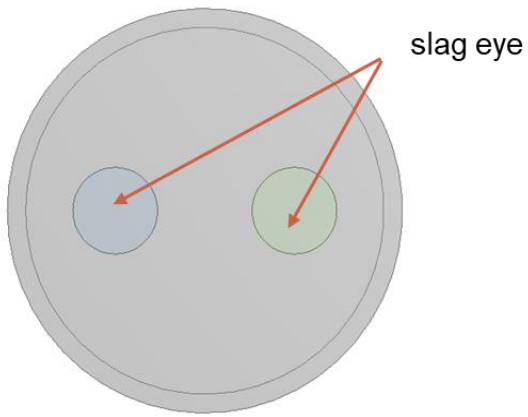
- **Re-oxidation** occurs when the oxygen element is released at the interface due to desulfurization, and oxygen absorption at the slag eye can be expressed as:

$$[Al]+1.5[O]=(AlO_{1.5})$$
$$[Si]+2[O]=(SiO_2)$$
$$[Mn]+[O]=(MnO)$$

Validation Conditions

- 80-ton ladle with two plugs, slag eye calculated from equation[1]
- 3 scenarios are validated, the initial species compositions listed in table



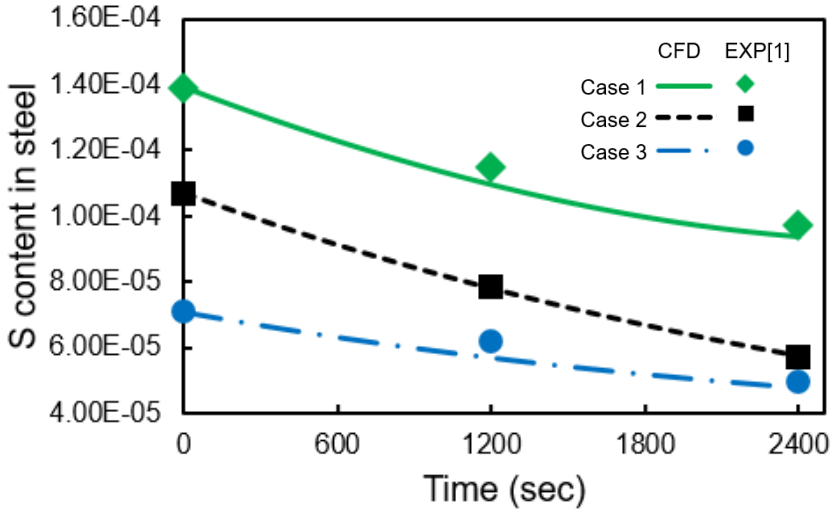


	Composition in steel (mass %)[1]					Composition in slag (mass %)[1]							Temp.[1] (K)
Case	[Al]	[Si]	[Mn]	[C]	[S]	(Al_2O_3)	(SiO_2)	(CaO)	(MnO)	(S)	(FeO)	(MgO)	
NO.1	0.056	0.181	0.662	0.352	0.0107	21.32	5.84	57.79	0.24	0.07	0.95	6.02	1855
NO.2	0.06	0.201	0.62	0.403	0.0139	28.52	9.05	52.82	0.21	0.26	1.02	5.33	1866
NO.3	0.009	0.191	0.241	0.382	0.0071	25.41	12.35	53.13	0.23	0.13	1.25	6.31	1842

[1] Lou, Wentao, and Miaoyong Zhu. "Numerical simulation of desulfurization behavior in gas-stirred systems based on computation fluid dynamics–simultaneous reaction model (CFD–SRM) coupled model." *Metallurgical and Materials Transactions B* 45.5 (2014): 1706-1722.

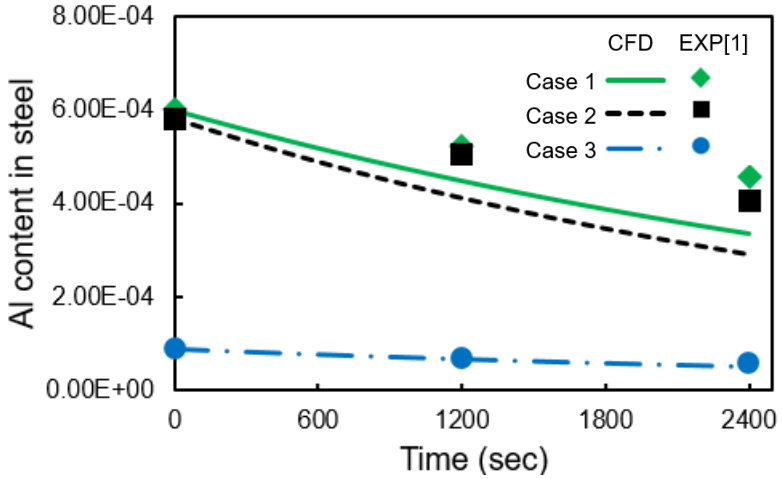
Model Validation

- Mass content of S, Al, Mn and Si in steel



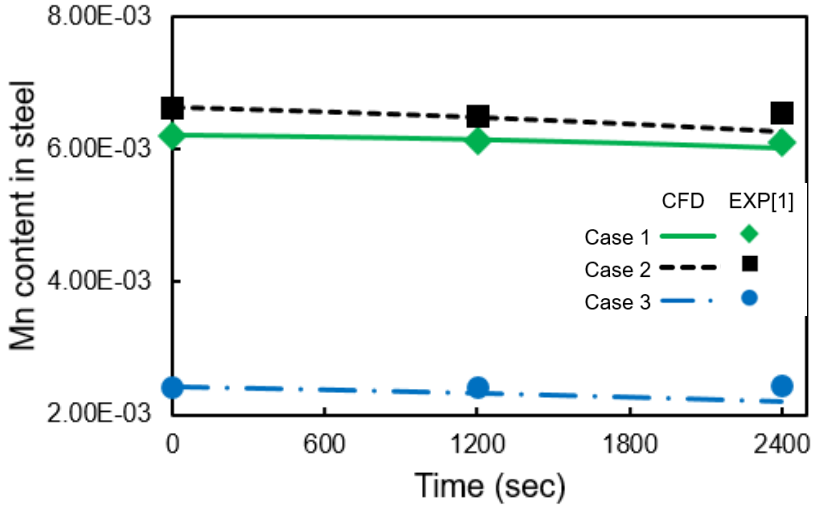
Difference

- Case 1: **3.85%**
- Case 2: **1.02%**
- Case 3: **4.15%**



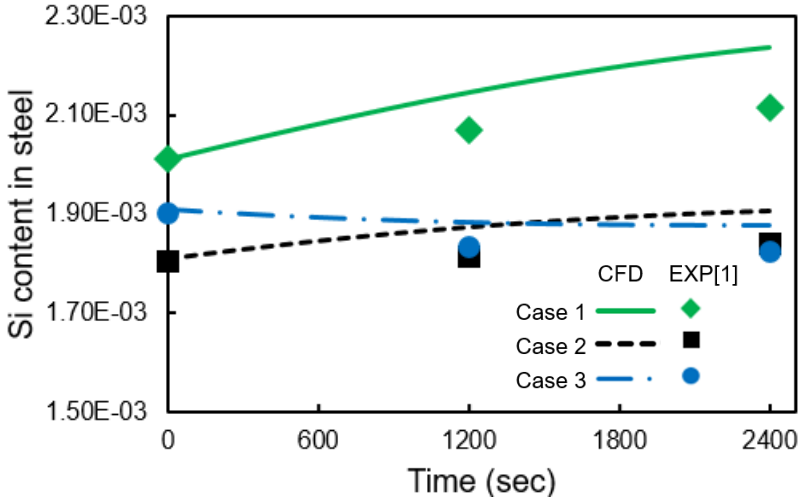
Difference

- Case 1: **6.33%**
- Case 2: **4.68%**
- Case 3: **4.81%**



Difference

- Case 1: **1.33%**
- Case 2: **4.43%**
- Case 3: **7.79%**



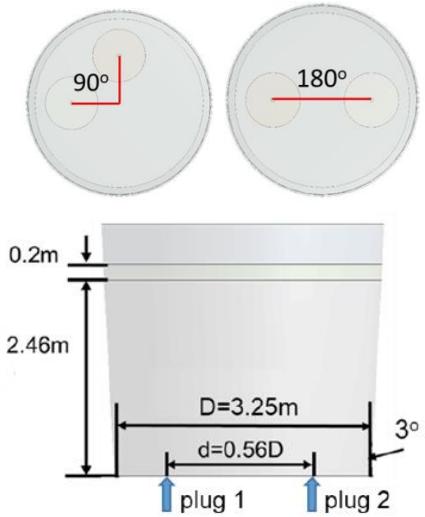
Difference

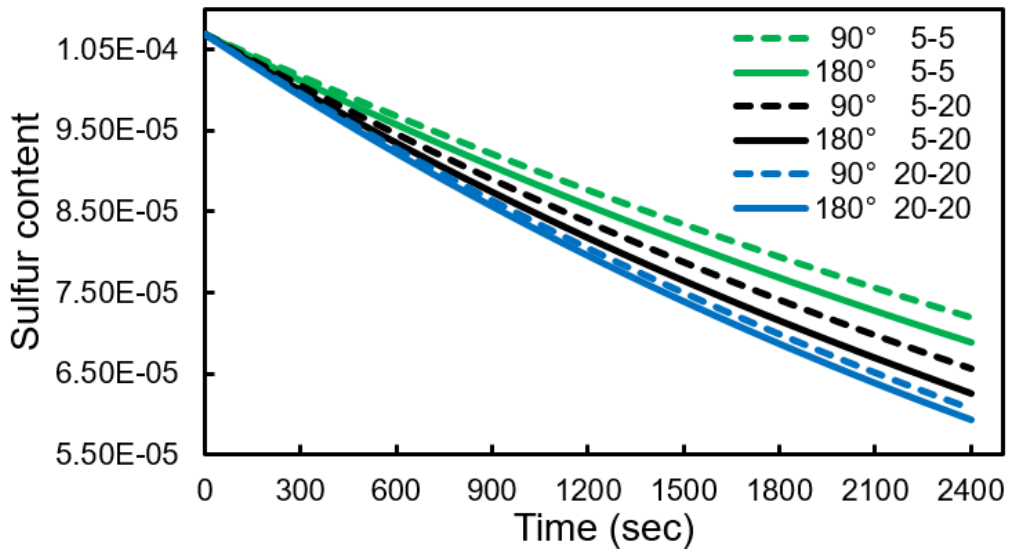
- Case 1: **5.66%**
- Case 2: **3.80%**
- Case 3: **3.19%**

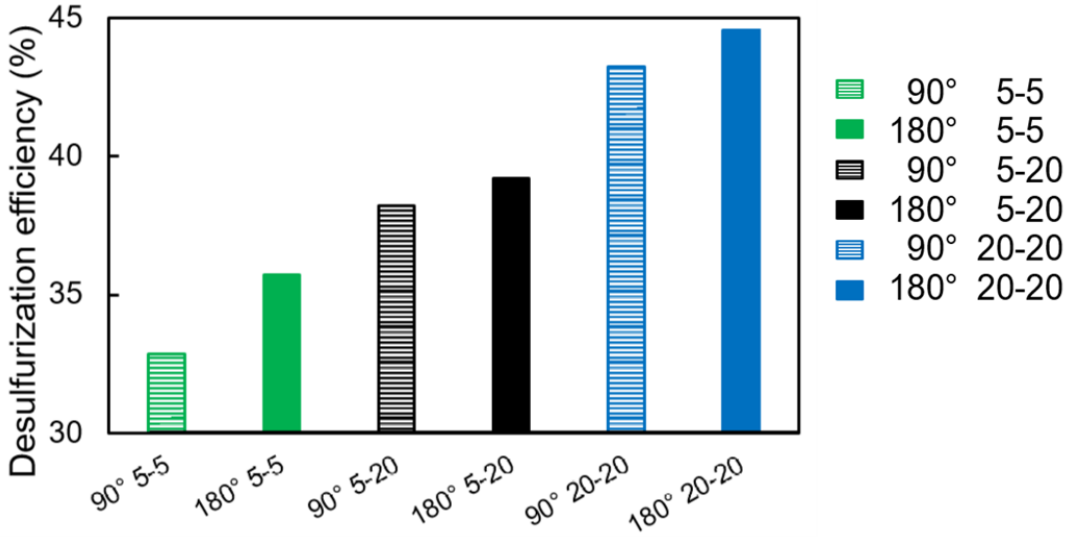
[1] Lou, Wentao, and Miaoyong Zhu. "Numerical simulation of desulfurization behavior in gas-stirred systems based on computation fluid dynamics–simultaneous reaction model (CFD–SRM) coupled model." *Metallurgical and Materials Transactions B* 45.5 (2014): 1706-1722.

Effect of Stirring Condition on Desulfurization

- Model applied to generic industrial ladles
- Stirring condition
  - Plug separation angle: (1) 90°; (2) 180°
  - Argon flow rate: (1) 5/5 SCFM; (2) 5/20 SCFM; (3) 20/20 SCFM
- Plug separation angle on desulf.: 180° > 90°
- Flow rate on desulf.: 20/20 SCFM > 5/20 SCFM > 5/5 SCFM

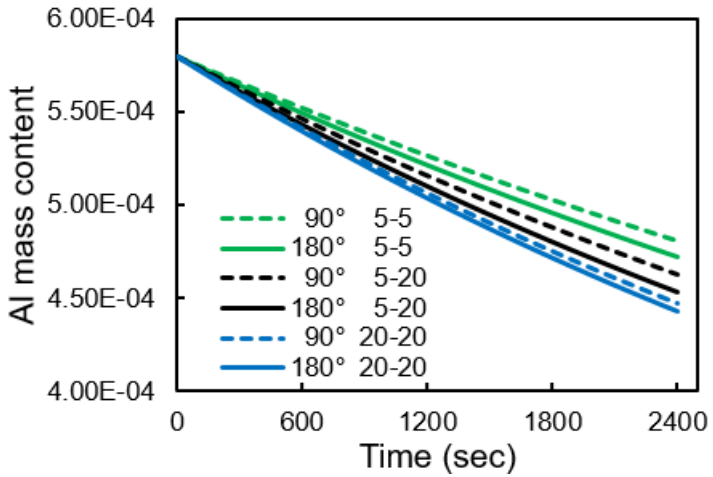


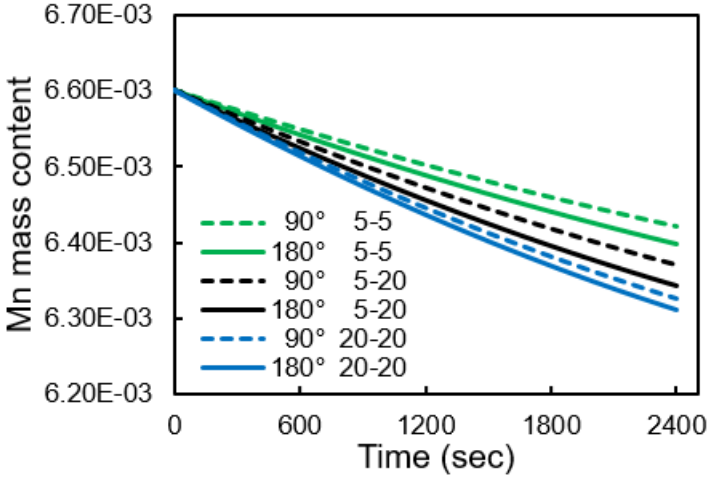


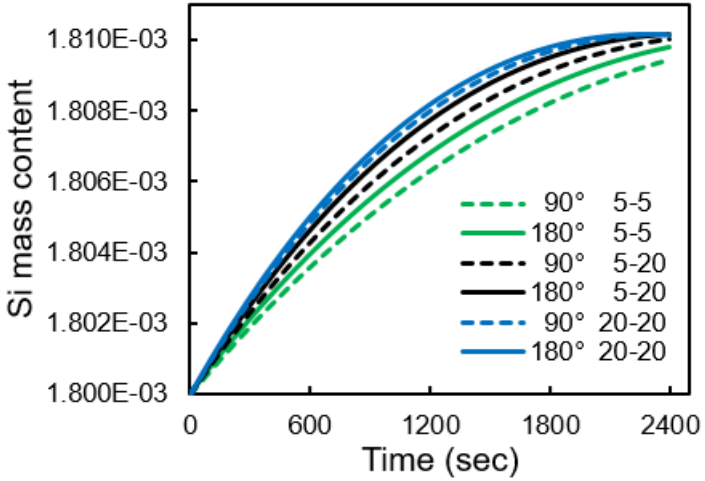


Effect of Stirring Condition on Re-oxidation

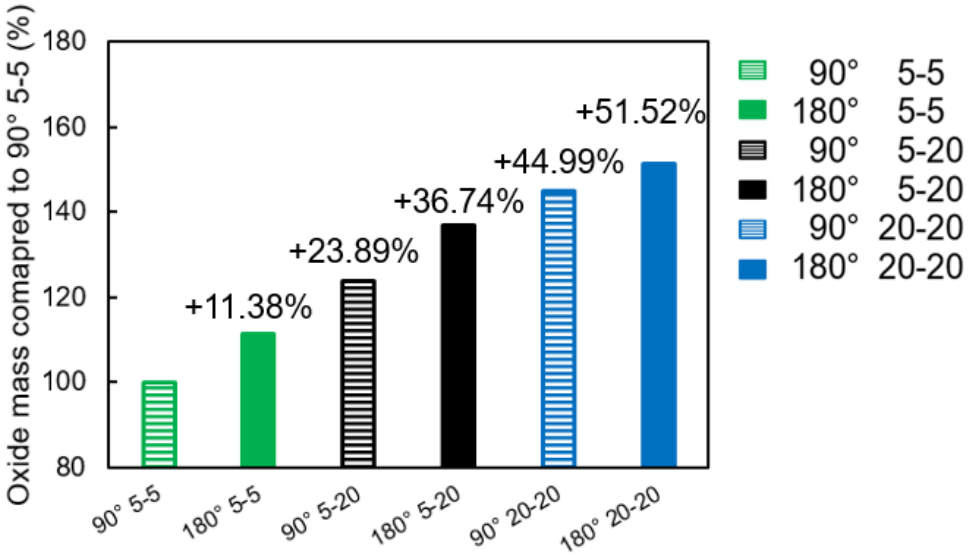
- Al, Mn and Si content with different stirring conditions







- Plug separation angle on re-oxidation: 180° > 90°
- Flow rate on re-oxidation: 20/20 SCFM > 5/20 SCFM > 5/5 SCFM
- Better desulfurization, higher re-oxidation, with inclusion removal model, the best combination can be found



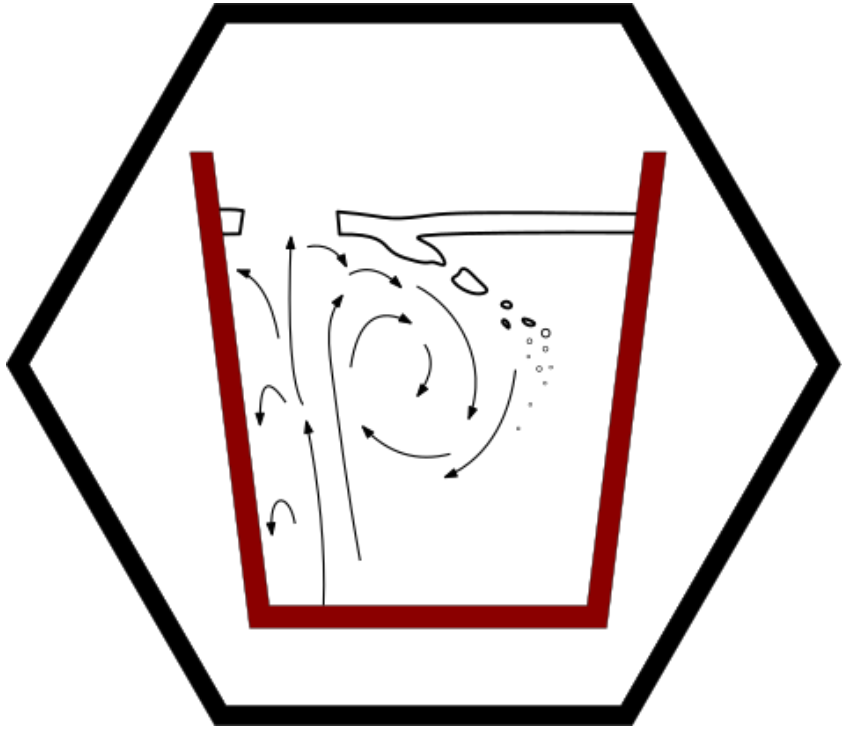
Model Applications

Simulation Capability

- The sulfur mass fraction in different scenarios
  - Plug arrangement
  - Argon flow rate
  - Initial compositions of steel and slag
  - Slag thickness

Industry Implementation

- Sulfur control
  - Sulfur content prediction
- Ladle design optimization
  - Layout improvement for lower sulfur content
- Cost reduction
  - Treatment time estimation



Project 16:

Microscale Inclusions and Alloy Mixing (NSF GOALI)

Site: Nucor/SSAB
Start: September 2021

Alloy Mixing Study

- **Motivation**
  - Effectiveness of mixing and homogenization of alloying materials is critical to comparing stirring procedures
- **Objective**
  - To accurately model the addition and stirring of alloying materials
  - Develop model to compare stirring methods and ladle designs for ability to homogenize added alloys
- **Potential Impact**
  - Improved steel quality
  - Better understanding of stirring time requirements for different alloying materials

Alloy Mixing Methdology

Ferroalloy injection

- DPM particle injection at slag eye
- Single continuous phase (steel only) with frozen flow

Steel shell formation and dissolution

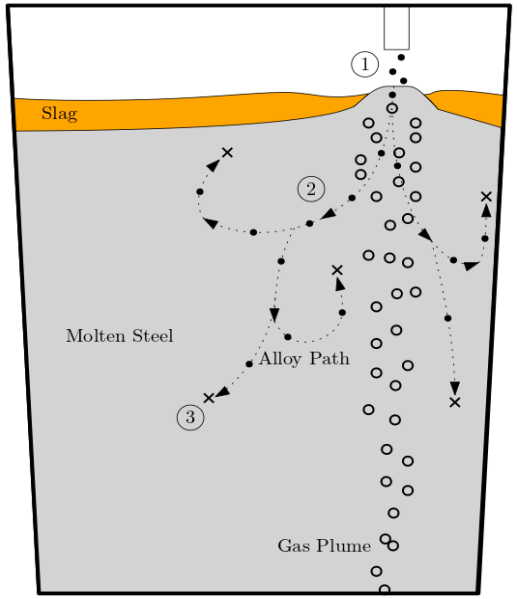
- Fixed DPM particle lifetime
- Conversion to species source term after lifetime exceeded

Ferroalloy diffusion

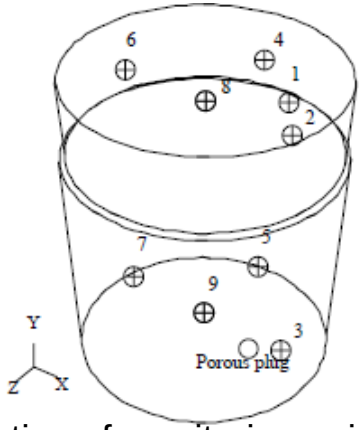
- Species diffusion via flow field

Mixture homogeneity

- Tracking of homogeneity via monitoring points



1. Alloy injection
2. Shell formation and melting
3. Alloy dissolution

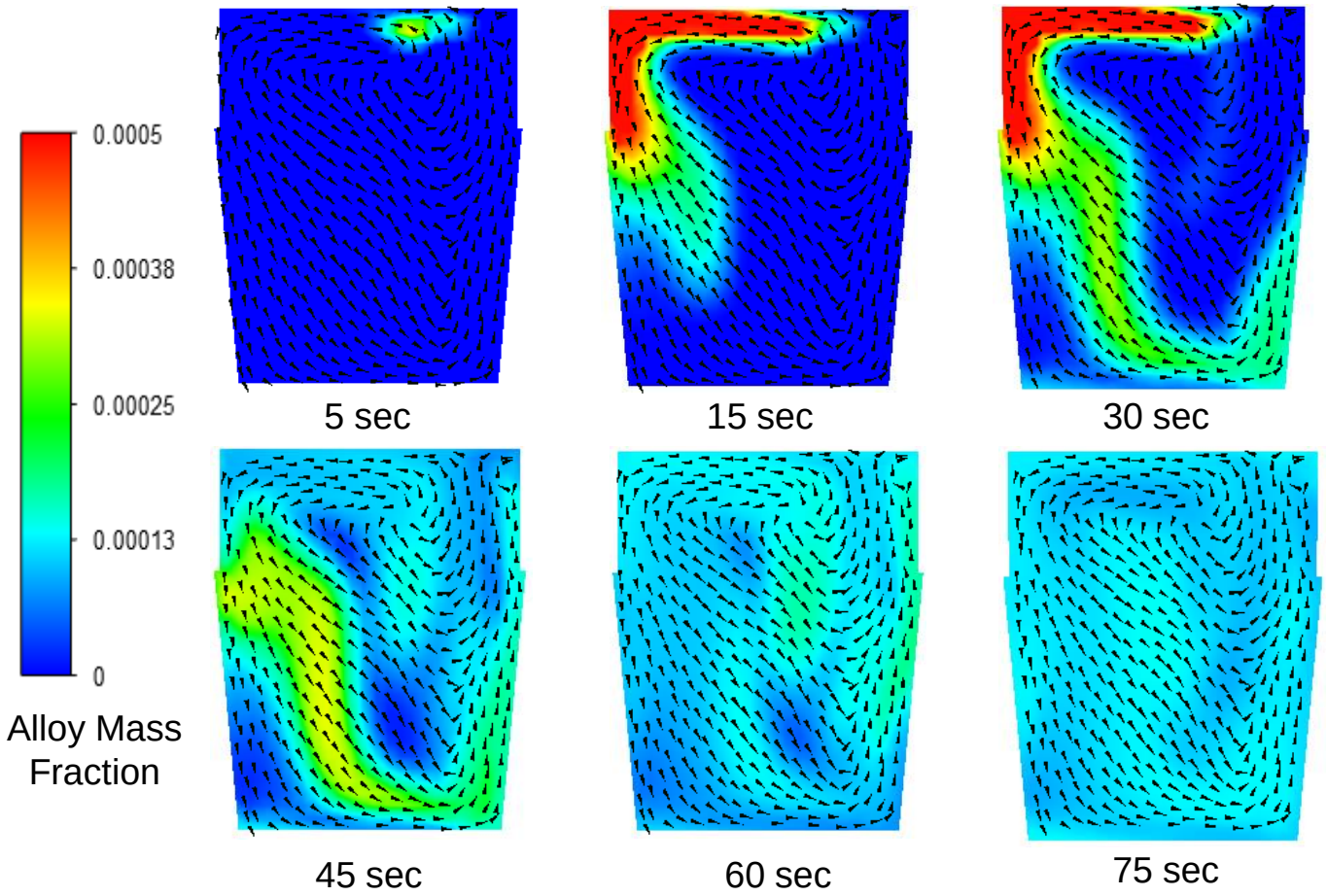


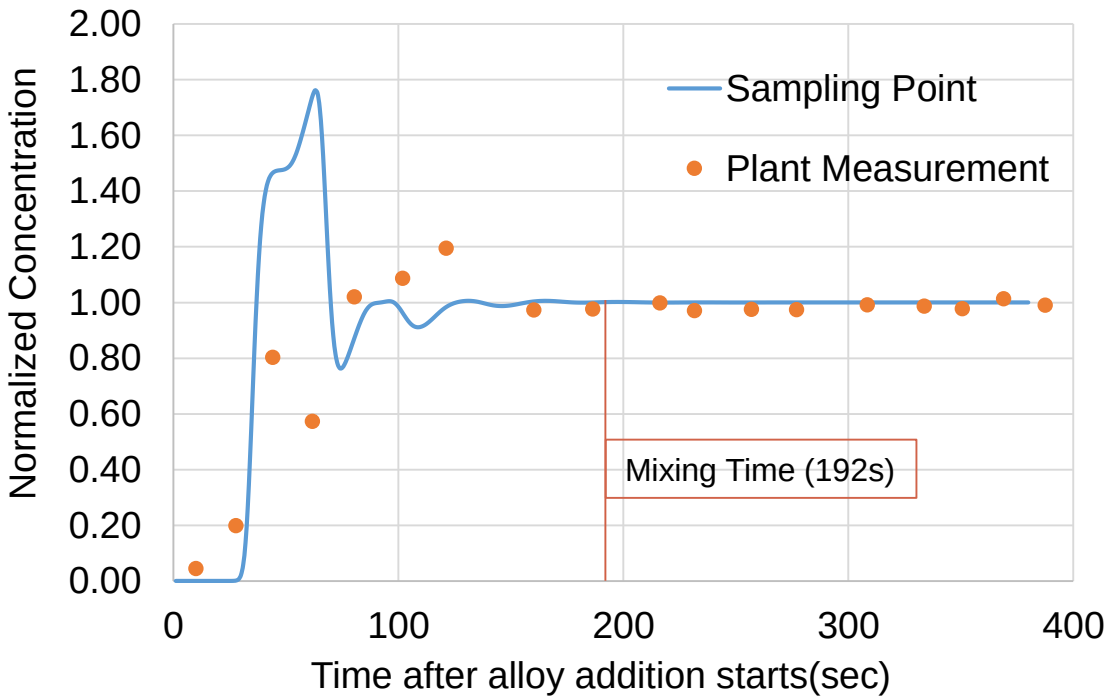
Location of monitoring points [1]

[1] J. Aoki, BG. Thomas, J. Peter, and KD. Peaslee, "Experimental and Theoretical Investigation of Mixing in a Bottom Gas-Stirred Ladle." AISTech Proceedings, 2004.

Injection Mixing Method

- DPM alloy particles injected for 37 seconds with a dissolution time of 4.5 seconds
- Particles follow flow before dissolving
  - Results in early bias of concentration to one side of ladle

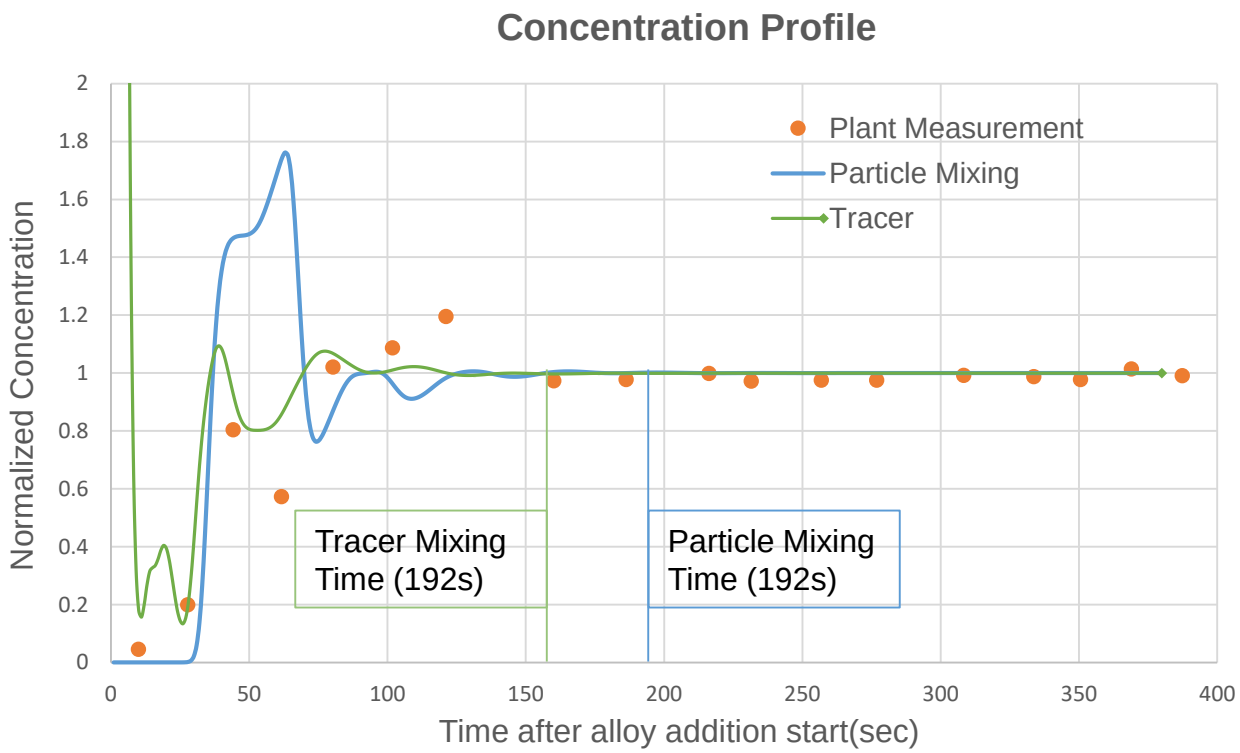


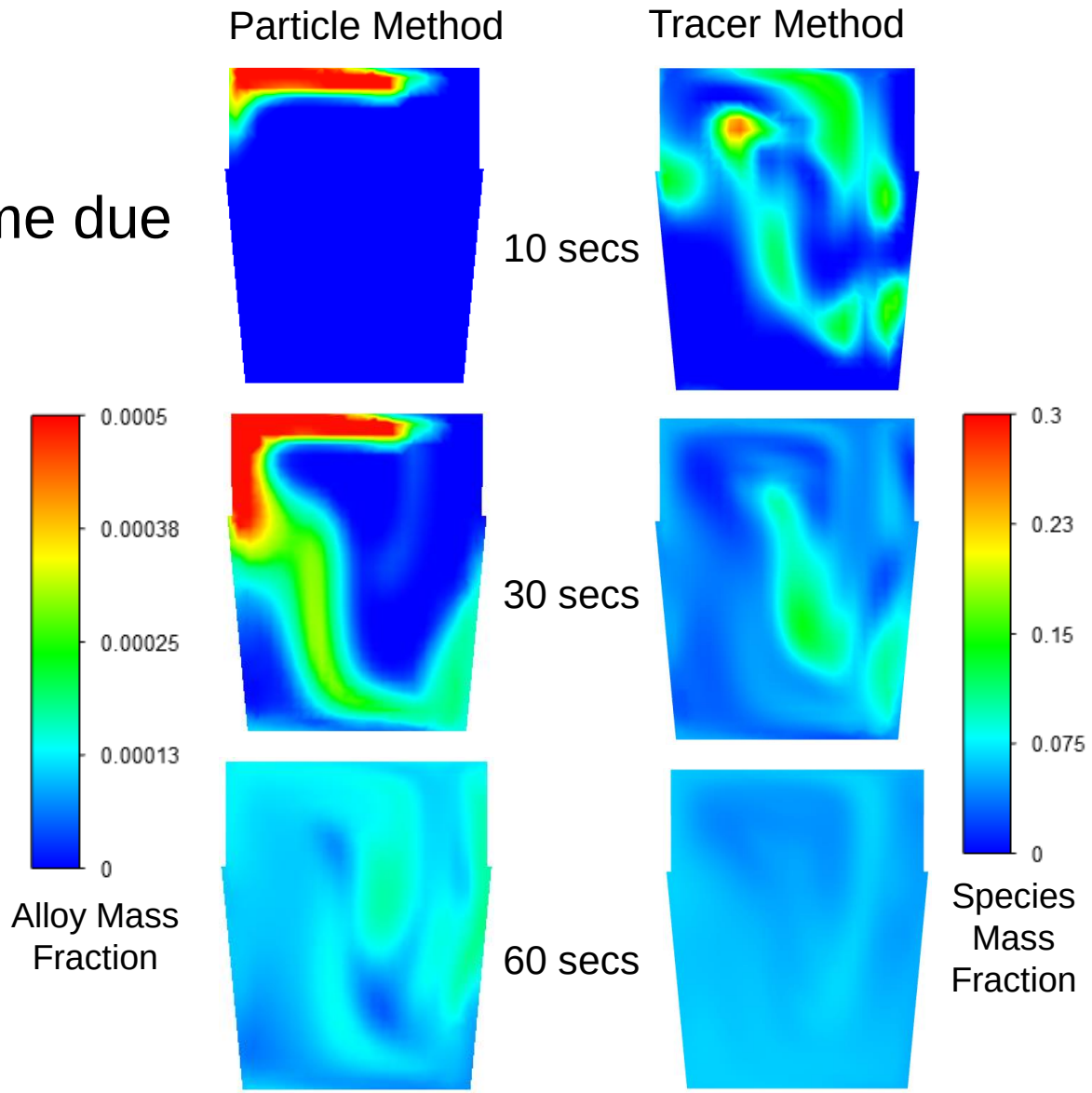


[1] J. Aoki, BG. Thomas, J. Peter, and KD. Peaslee, “Experimental and Theoretical Investigation of Mixing in a Bottom Gas-Stirred Ladle.” AISTech Proceedings, 2004.

Method Comparison

- Particle injection method reflects physical distribution of alloy particles
- Tracer approach may under-predict mixing time due to more-homogenous initial distribution





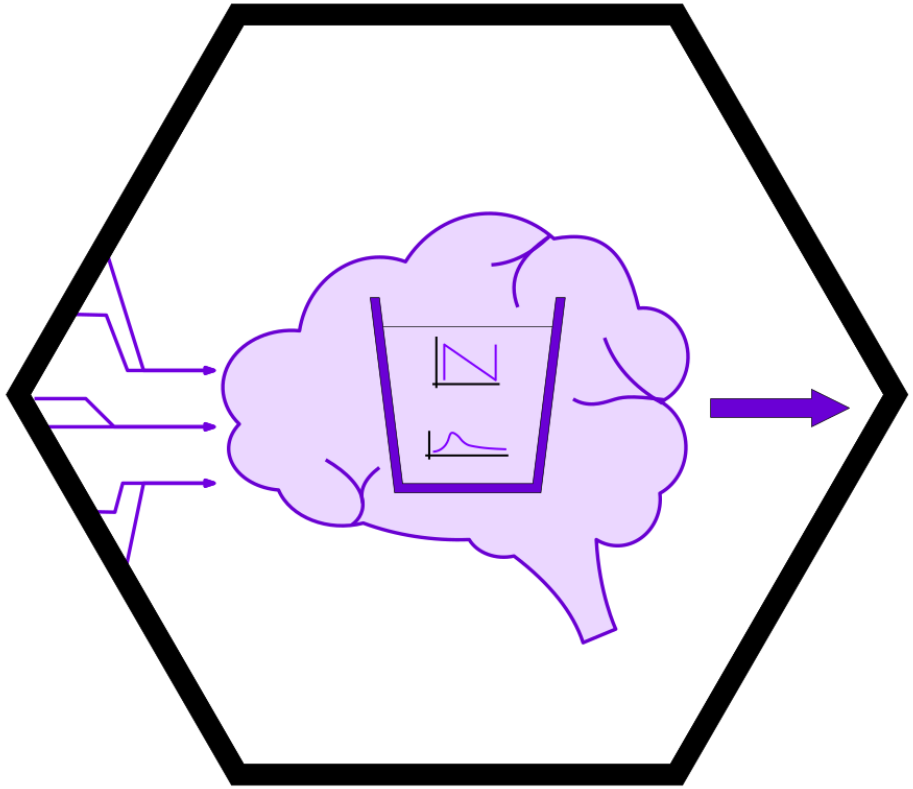
Model Applications

Simulation Capability

- Alloy penetration and homogenization
  - Plug positions
  - Stirring strength
  - Particle properties
  - Alloy injection location

Industry Implementation

- Process Optimization
  - Identify best-practices for stirring time, alloy addition location, etc.
- Ladle Design Optimization
  - Improve mixing efficiency via plug placement and ladle shape
- Product Quality Improvement
  - Improve homogeneity
  - Reduce slag entrainment



Project 9:

Smart Ladle AI-Based Tool

Site: SDI Butler Division
Start: September 2019

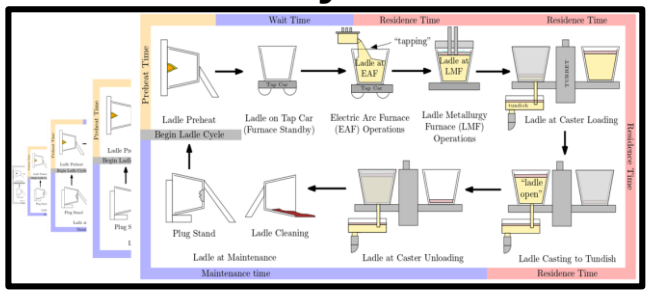
Overview

- **Issue:**
  - Operators must predict future temperature requirements using limited information
- **Approach:**
  - AI model using real-time and historic process data to predict future casting temperature
- **Potential Impacts:**
  - Improved operational responses for casting temperature control
  - Recognition of special circumstances

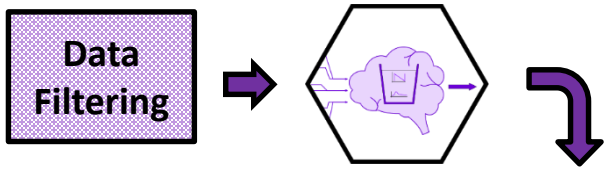
Smart Ladle Usage

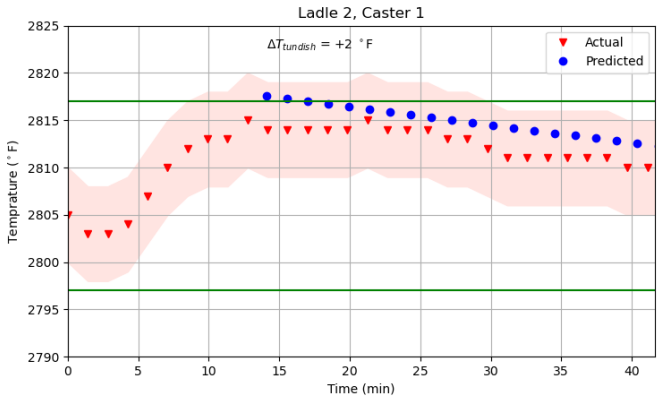
- Smart Ladle executed on ladle at LMF (or pre-cast)
- Trained using industry data
  - Varies per-site, e.g. SDI is 25 inputs
  - Steel contact time, number of heats on ladle, temperature measurement, etc.
- Model makes three predictions:
  - Time until ladle will be half-empty at caster
    - using time-to-open, ladle tonnage, and avg. casting speed
  - Tundish midpoint temperature
  - Temperature slope at midpoint
- Inputs and results stored to database for query and display

Ladle Process & History Data



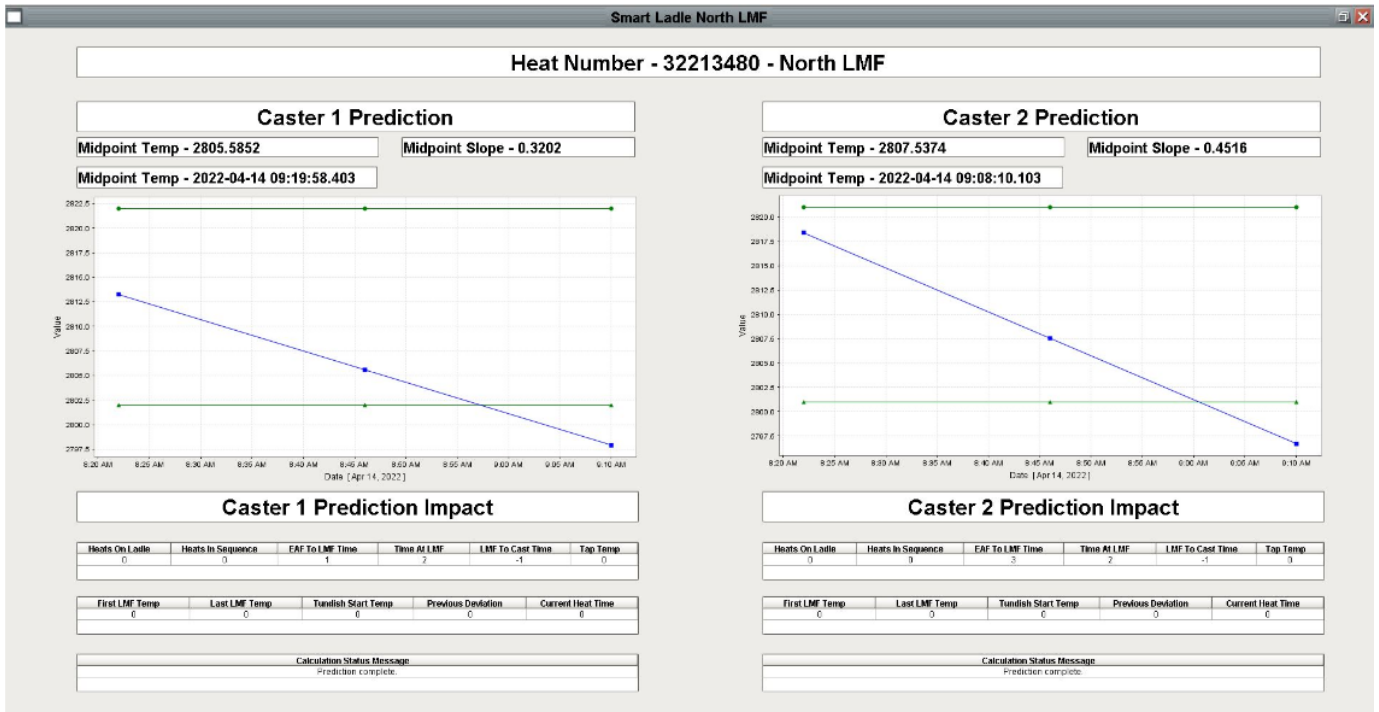
Smart Ladle





Smart Ladle Implementation Status

- Fully implemented at SDI Butler Division
  - Automatic execution on LMF temperature sample
  - Uses dedicated input/output tables
    - Faster processing
    - Better recordkeeping
- Early model trained for Nucor
  - Accuracy around +/- 5 degrees error
  - More training to be done
- Planning phases for Tata Steel, SSAB, Gerdau, and Cleveland-Cliffs

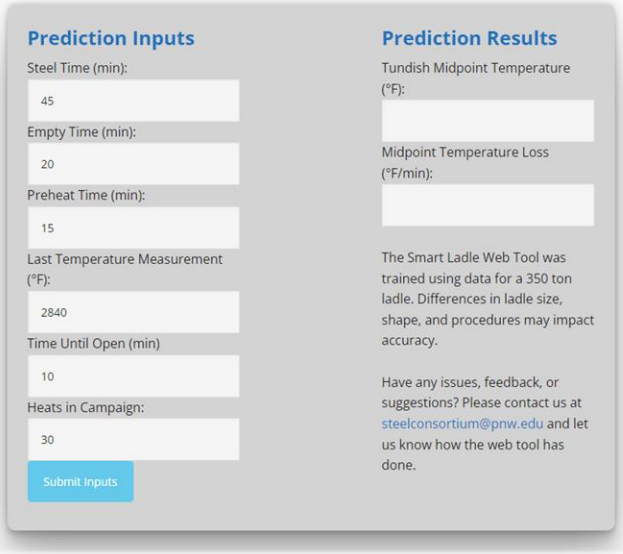


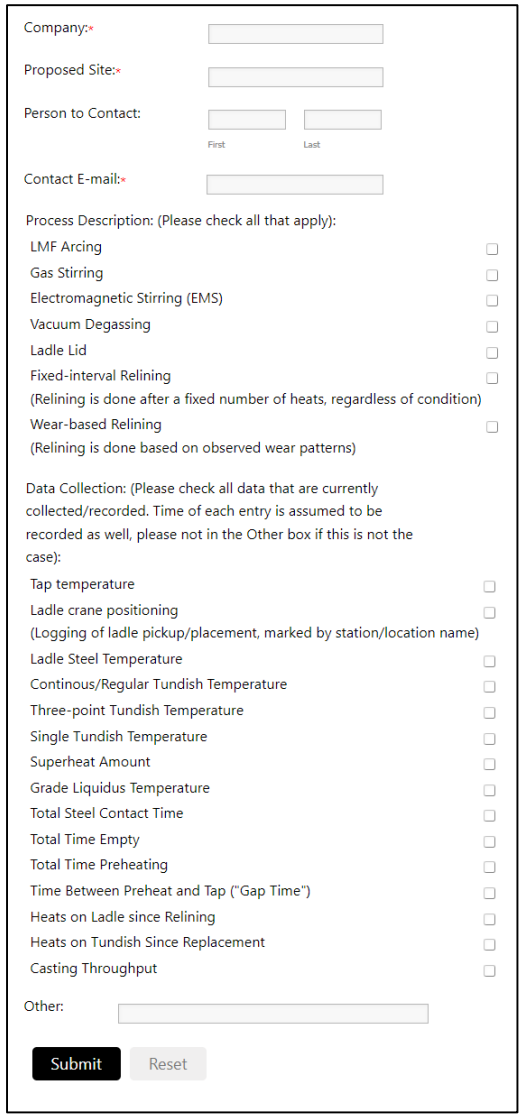
Smart Ladle Level 2 Interface at SDI Butler Division

Smart Ladle At Your Site

- Smart Ladle can be adapted to your facility
  - **We** adapt to **your** process
- Smart Ladle Survey Form added to SMSCV Members Ladle PTC page
  - Contact info, process description
- Smart Ladle Simplified Web Demo
  - Demonstration of Smart Ladle concept
  - Trained using reduced inputs
  - More features to come

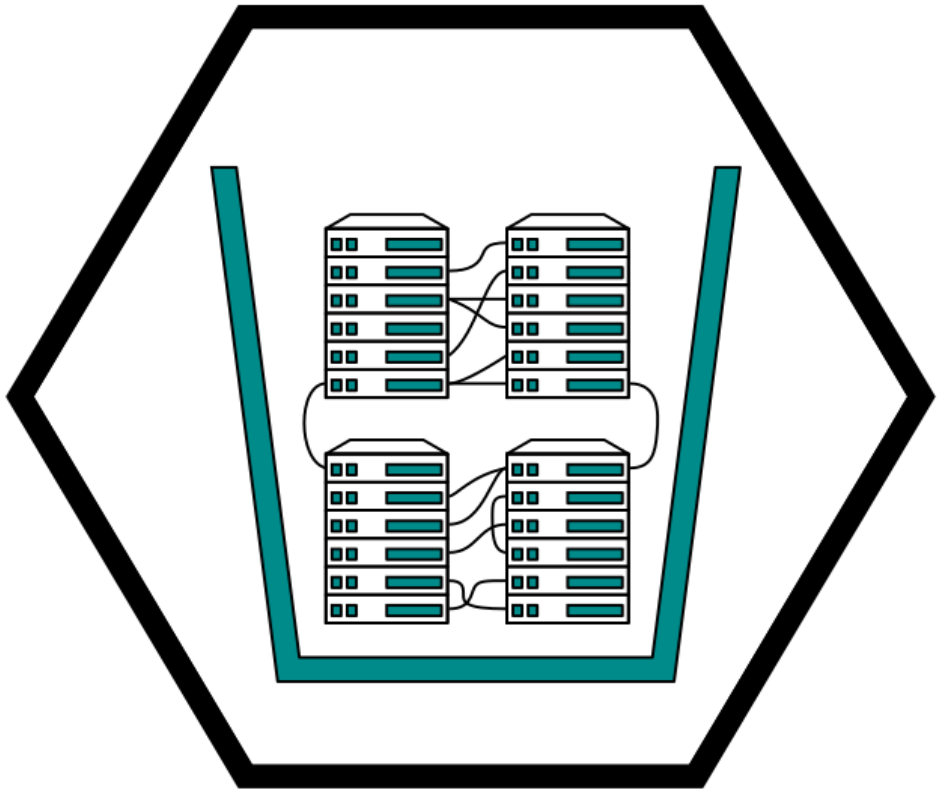
Smart Ladle Web Demo





Smart Ladle Survey

Find out more at:
https://steelconsortium.org/sponsor-access/ladle-ptc/



Project 17:

Reduced Order Modeling and Performance Prediction (HPC Ladle)

Start: May/June 2022

Overview

- **Issue:**
  - Excessive time at refining stage leads to unnecessary heat loss and therefore expense
  - Improper mixing can result in out-of-tolerance product
  - There is no reliable online method to adjust operations for inclusion removal
- **Approach:**
  - Simulations using HPC to generate a Reduced Order Model of the steel refining process
  - ROM used to create responsive performance predictions for operational control
- **Potential Impacts:**
  - Energy, productivity, and operational transformations through the use of HPC and reduced order modeling

Summary

Summary

- Project #8: Desulfurization and Re-oxidation
  - Developed and validated re-oxidation model for Al and Mn
  - Impacts of stirring conditions on desulfurization rate
- Project #9: Smart Ladle
  - Implemented at SDI Butler Division
  - Planning and training at several other sites
- Project #10: Hot Metal Desulfurization
  - Validated CaC_2/CaO desulfurization model
  - Effects of penetration ratio, particle size and temperature
- Project #16: Microscale Inclusions and Alloy Mixing (NSF GOALI)
  - Developed alloy mixing model with injection and tracer methods
  - Developed flow field with frozen and normal flow

Future Work

- Project #8: Steel Desulfurization & Re-oxidation
  - To develop and validate the re-oxidation model for other elements including Si and Fe
  - To explore the influence of ladle parameters on desulfurization & re-oxidation rates
- Project #10: Hot metal desulfurization
  - To develop and validate the Mg desulfurization model with industrial data
  - To investigate the impact of different stirring conditions
- Project #12: Shipping Temperature and Superheat Control
  - To expand implementation to other sites
- Project #16: Microscale Inclusions and Alloy mixing (NSF GOALI)
  - To investigate the mixing process with other prominent alloy elements
  - To develop the mixing model with multiphase cases
  - To identify the impact of temperature profile
- Project #17: Reduced Order Modeling and Performance Prediction (HPC Ladle)
  - To identify target variables for Reduced Order Model
  - To build baseline simulation

Comments from Industry Collaborators

Judy Li

Thank You
Questions and Comments

Additional Potential Applications

- **Refining Process Improvements:**
  - Stirring time minimization
  - Gas flow rate selection
  - Ladle heat loss reduction
  - Refractory life extension/wall shear stress reduction
  - Inclusion removal effectiveness/speed
  - Slag opening minimization

- **Ladle Design:**
  - Ladle shape
    - Height, diameter, wall taper angle
  - Plug parameters
    - Plug number, separation angle, distance
  - Lance positioning/flow

- **Industry 4.0:**
  - Smart Ladle AI prediction
  - Superheat suggestion and control