

# Report of the Brazilian Committee for Phase Diagrams of Materials 2023 APDIC Meeting (2021 highlights)

## Highlights:

2022 ABM Week Conference was a great success, large number of participants and contributions.  
Technical Coordinators: A.Costa e Silva, F Beneduce, A Vilela.

2023 Two Workshops on Computational Thermodynamics: foreseen for late 2023.

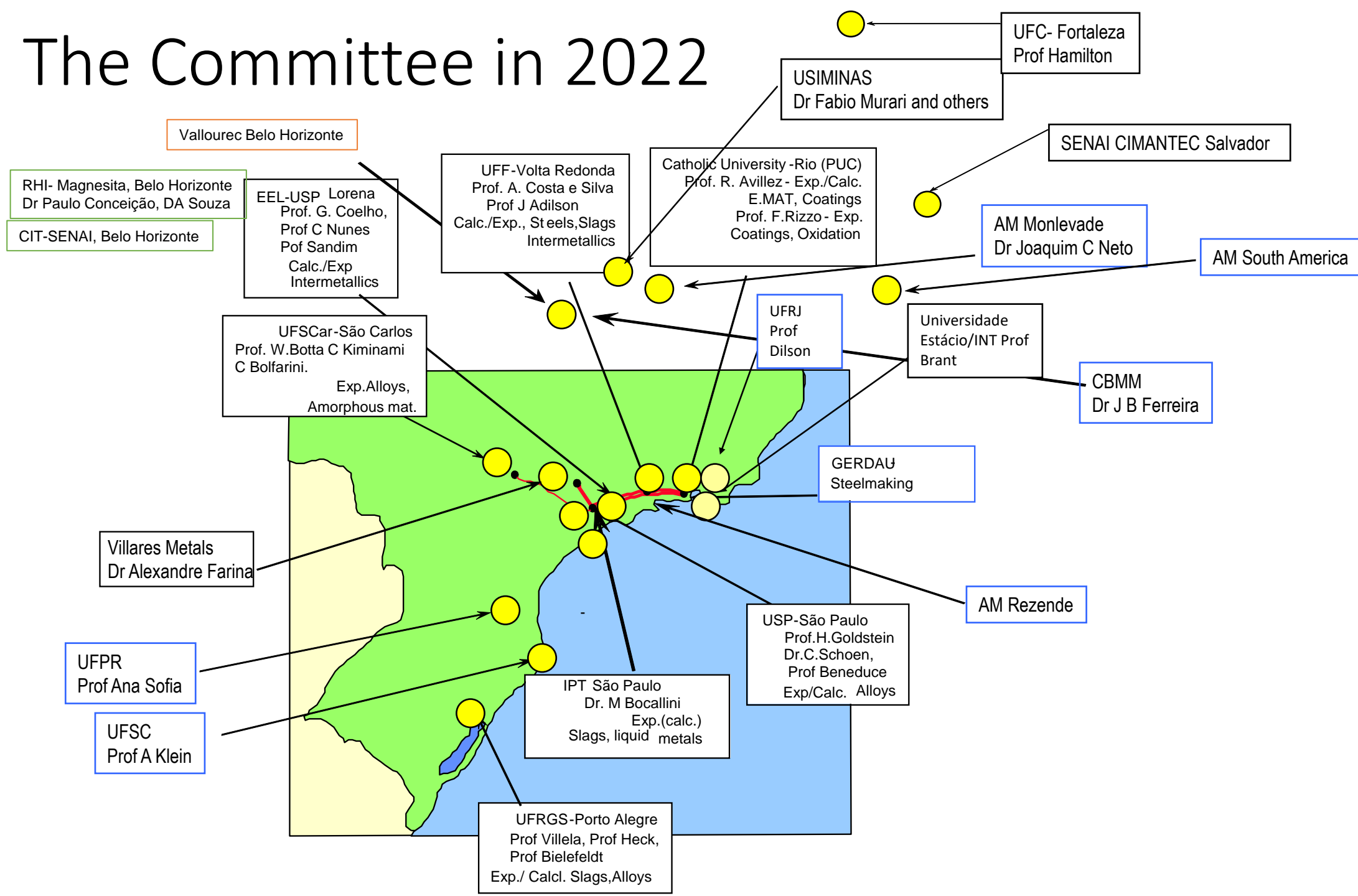
Organizing 2023 ABM Week. Very large number of presentations and participants (>1600)

Prof A Costa e Silva book on Steelmaking published.

Usual activity in Linkedin Phase Diagram Group



# The Committee in 2022



Organization	Researchers	Pub's	Highlights
UFSC-Florianópolis, Santa Catarina	Prof Klein +7, 7PhD, 16MSc +10	+10	controlled wear material, advanced materials for compressor, nanostructured materials. <b>Diffusion and diffusive formation of new materials</b>
UFMG	Prof Wictor Wolf		HEA, Metallic glasses, novel materials
UFSCar, São Carlos SP	Prof Botta, Kiminami, Bolfarini +15	+20	Novel materials, advanced glasses, HEA, borides, low density steel
USIMINAS- Ipatinga, MG	4		Flat steel development. Pipeline, pressure vessels, automotive. DP, HSLA. Slag development, de-P, converter modeling, clogging control in continuous casting
UFRJ- Rio de Janeiro, RJ	Prof Dilson, L Henrique, Leonardo group Prof Payão's group		Hydrogen in materials, oil & gas materials Welding research and simulation, superalloy diffusion and welding, additive manufacturing
USP – São Paulo, SP	Prof Schoen's group Prof Goldstein, Beneduce, Tschiptin		First principles, high entropy Steels, advanced materials, Superalloys. Diffusion modeling in advanced alloys
USP- Lorena, SP	Prof G Coelho, C Nunes, H Sandim +	15	Boron in steel, silicides and other high temperature materials
Vallourec- Belo Horizonte, MG			Steels for sour service, advanced steels
Villares Metals- Sumaré, SP	Dr. A. Farina +5		Development of Ni and Fe based advanced alloys. Solidification, transformation modeling, continuous casting process improvements, database for Ni containing slags.

Organization	Researchers	Pub´s	Highlights
ArcelorMittal Monlevade, MG	8+9 Dr Joaquim Gonçalves	3	Spring steel cleanness,hardenableity. Quenching+distortion control
ArcelorMittal South America (ES)			Environmentally sound steelmaking – Seminar and studies
ArcelorMittal Rezende (RJ)	3, Iury Otaviano	1	B in steel
APERAM, Timóteo, MG	3		Stainless and electrical steel.
CIT-SENAI , Belo Horizonte, MG	2		Precipitation in microalloying steel. Thermodynamics, kinetics and experimental
UNIFEI, São Bernardo, SP	10 Prof Magnabosco		Diffusion and phase transformations in stainless steels. <b>CALPHAD best poster award 2021!</b>
IPT São Paulo, SP	9		
RHI-Magnesita Belo Horizonte, MG	5		Refractory materials development; Slag-Refractory interactions; Inclusion Control and Clean Steel Making; Slag Thermophysical properties
<b>PUC-Rio</b> de Janeiro RJ	Prof Rizzo´s group Prof Avillez´s group	7	Prof Rizzo back in PUC and in the CGEE Research in AHSSsteels Prof Avillez working on molecular dynamics
SENAI CIMANTEC Salvador BA	Dr. Bruna Callegari, Dr. Tiago Lima,		Prof. Dr.-Ing. Rodrigo Coelho, Dr. Luis Fernando Folle, Paulo dos Reis (MSc.), Prof. Dr.-Ing. Rodrigo Coelho Materials development: Cast Al alloy Ferroalloy dissolution in steel
GERDAU			Specialty Steels: non-metallic inclusions, heat treatment
TERNIUM Steelmaking, SantaCruz, RJ	Ricardo Vieira Regis De Almeida Martins, Lorenzo Engel Fornasari, Raissa Santos Salgado, Bruno Suveges Cerchiari		Process development and investigation in melt shop
UNESP- Itapeva SP	Prof Baldan		HEAs computational thermodynamics
UFC- Fortaleza, Ceará	Prof Hamilton +2	7	Maraging steels and high strength materials. Interaction with new steel mill
<b>UFF, Volta Redonda RJ</b>	Prof A. Costa e Silva + Prof J Adilson Prof P.R.Rios group	9 7	Steels and steelmaking. Prof André officially retired in 2022. Work with steel industry continues Kinetics of steelmaking with computational thermodynamics
UFPR- Curitiba, Paraná	Prof Ana Sofia +1		Additive manufacturing
<b>UFRGS - Porto Alegre, RS</b>	Prof Vilela, Bielefelt, Heck	9	Steelmaking, reduction and environment, <b>Steelmaking slag and processing courses. Prof Wagner Bielefelt</b>
UFSC-Florianópolis, Santa Catarina	Prof Klein +7, 7PhD, 16MSc +10	+10	controlled wear material, advanced materials for compressor, nanostructured materials. <b>Diffusion and diffusive formation of new materials</b>
UFMG	Prof Wictor Wolf		HEA, Metallic glasses, novel materials

Appendix for the site, individual reports

# ArcelorMittal Monlevade

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## Researchers

Ângelo Máximo Fernandes Marins  
Carla Regina Ferreira  
Ermani Vinicius de Oliveira Lima  
Fábio Cardoso  
Edgard Ribeiro

Gustavo Henrique Sousa  
Joaquim Gonçalves Costa Neto  
Luciano de Castro Reis  
Rafael Ferreira Delfim Bueno  
Tayná Rayzza Ribeiro

## Engineer Team

Steelmaking 3  
Rolling Mill 1  
Product 6

## Ongoing Projects

- “Heat treatment routes proposition for Quenching and Partitioning (Q&P) for automotive segment spring steel”;
- Computational thermodynamic simulation – Case AISI51B60 steel – Cracks and Banding;
- Computational thermodynamic simulation of SAE 8620 steel

## Publications

- LIMA EVO. *Limpidez do aço SAE 9254 destinado à indústria automobilística. Dissertação de Mestrado.* UFOP. 2020.
- SOUSA GH. Caracterização microestrutural e mecânica de liga de alta entropia CrMnFeCoNi conformada por laminação. *Dissertação de Mestrado.* UFMG. 2019.
- LIMA, ERMANI VINICIUS DE OLIVEIRA; SOUSA, GUSTAVO HENRIQUE; COSTA NETO, JOAQUIM GONÇALVES; PEIXOTO, JOHNE JESUS MOL; DA SILVA, CARLOS ANTONIO . Thermodynamic Simulations and Industrial Trials Applied to Inclusion Control of SAE 9254 Si-Mn Killed Steel. METALLURGICAL AND MATERIALS TRANSACTIONS B-PROCESS METALLURGY AND MATERIALS PROCESSING SCIENCE, v. 51, p. 1-12, 2020.
- LIMA EVO, SEGEL KT, COSTA NETO JG, SOUSA GH, BUENO RFD, LIMA AJAS, SILVA IA E SILVA CA. *Limpidez do aço SAE 9254 destinado à indústria automobilística.* Artigo aceito. Tecnologia em Metalurgia, Materiais e Mineração. 2020.
- GOMES, GERALDO MAGELA; RIBEIRO, EDGARD MARCOS; CUNHA, MARCOS VINÍCIUS RIBEIRO; MARINS, ANGELO MÁXIMO FERNANDES; MORAIS, GLEISSON; SOUSA, GUSTAVO HENRIQUE; FERREIRA, CARLA REGINA; LIMA, ERMANI VINÍCIUS DE OLIVEIRA; SATO, CESAR TAKACI; CHAVES, ALIN JUNIOR MACHADO. OPTIMIZATION OF PITCH CIRCLE DIAMETER OF LADLE FURNACE. Artigo aceito. In: 51º Seminário de Fusão, Refino & Solidificação de Metais, 2022, São Paulo. Anais do Congresso Anual da ABM.

## Concluded projects

- Optimization of processing parameters to reduce distortion of SAE 1045 steel bars.
- Optimization of the machinability of SAE 1045 used in the manufacture of shock absorber.
- Cleanliness of SAE 9254 steel for the automotive industry.
- RIBEIRO, TAYNÁ RAIZZA; RIBEIRO, SAMYA ESTEVAM; ARAUJO, ATHOS FERNANDES; SOUSA, GUSTAVO HENRIQUE; BUENO, RAFAEL FERREIRA DELFIM; LIMA, ERMANI VINICIUS DE OLIVEIRA. ESTUDO COMPARATIVO DA CORROSÃO DO AÇO INOXIDÁVEL DUPLEX UNS32304 EM SOLUÇÕES ÁCIDAS. Artigo aceito. In: 75º Congresso Anual da ABM, 2022, São Paulo. Anais do Congresso Anual da ABM.
- SOUSA, G.H.; ZEPON, G. ; MAZZER, E.M. . Microstructure evolution and strengthening by cold rolling of CrMnFeCoNi high-entropy alloy processed by spray forming. MATERIALS SCIENCE AND ENGINEERING A-STRUCTURAL MATERIALS PROPERTIES MICROSTRUCTURE AND PROCESSING, v. 793, p. 139814, 2020.
- BRAGA, J. ; LINS, J. ; CASTRO, G. ; JUNIOR, H. ; SANTOS, I. C. ; SOUSA, G. H. ; CRISCUOLO, I. ; SANTANA, C. ; PEREIRA, U. . CORROSION BEHAVIOR OF LOW CARBON STEEL PROCESSED BY EQUAL CHANNEL ANGULAR PRESSING IN NEUTRAL AND ALKALINE ENVIRONMENT. TECNOLOGIA EM METALURGIA, MATERIAIS E MINERAÇÃO, v. 18, p. e2340, 2020.
- ARAUJO, A. F. ; SOUSA, G. H. ; SOUZA, F. V. C. ; BRAGA, C. A. ; BRAGA, J. O. ; SANTOS, I. C. . CORROSION IN WELDED JOINTS BY SMAW PROCESS OF STEEL API5L X70 IN SALINE ENVIROMENT. In: 74º Congresso Anual da ABM, 2019, São Paulo. Anais do Congresso Anual da ABM, 2019. v. 74. p. 224-235.

# ArcelorMittal Monlevade

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## Publications

- ARAUJO, A. F.; SOUSA, G. H.; ARAUJO, G. V.; SANTOS, I. C.; FERNANDES, LOYSLENE RABELO. SYNTHESIS OF MAGNETITA NANOPARTICLES BY COPRECIPITATION. In: 74º Congresso Anual da ABM, 2019, São Paulo. Anais do Congresso Anual da ABM, 2019. v. 74. p. 712-718.
- SOUSA, GUSTAVO HENRIQUE; SANTOS, IGOR CUZZUOL DOS ; ARAUJO, ATHOS FERNANDES ; BRAGA, JORGIMARA DE OLIVEIRA ; ARAÚJO, GUILHERME VITOR DE ; FONSECA, MARCELO ALVES . SEPARAÇÃO DE MATERIAIS METÁLICOS PELO MÉTODO DE FAGULHA: DIAGNÓSTICO DE MISTURAS NO ESTOQUE DE EMPRESAS SIDERÚRGICAS. In: 74º Congresso Anual da ABM, 2019, São Paulo. ABM Proceedings. São Paulo: Editora Blucher, 2019. p. 3317-3327.
- ARAUJO, ATHOS FERNANDES ; GONÇALVES, WALLACE CRISÓLOGO SOUZA ; SOUSA, GUSTAVO HENRIQUE ; FERNANDES, LOYSLENE RABELO ; LINO, RONEY EDUARDO . ANÁLISE DO RENDIMENTO DE FERROLIGAS EM ESTAÇÃO DE RINSAGEM UTILIZANDO O SIMULADOR DE REFINO SECUNDÁRIO DO STEEL UNIVERSITY. In: 50º Seminário de Aciaria, Fundição e Metalurgia de NãoFerroso, 2019, São Paulo. ABM Proceedings. São Paulo: Editora Blucher, 2019. v. 50. p. 128-139.

## Publications

- SOUSA, G. H.; SANTOS, I. C. ; BRAGA, J. O. ; FERNANDES, LOYSLENE RABELO ; ARAUJO, A. F. . HYDROMETALLURGICAL RECOVERY OF MANGANESE FROM BLAST FURNACE SLAG. In: 74º Congresso Anual da ABM, 2019, São Paulo. Anais do Congresso Anual da ABM, 2019. v. 74. p. 236-243.
- SOUSA, G. H.; ARAUJO, G. V. ; FONSECA, G. C. ; PEREIRA, H. T. C. ; ARAUJO, A. F. . EVALUATION OF CORROSION RESISTANCE TO SAE 1080 STEEL IN SULFURIC ACID AND WATER. In: 74º Congresso Anual da ABM, 2019, São Paulo. Anais do Congresso Anual da ABM, 2019. v. 74. p. 702-711.
- FERNANDES, LOYSLENE RABELO ; SOUSA, GUSTAVO HENRIQUE . AVALIAÇÃO DA CORROSÃO NO AÇO 10B22 PARA FIXADORES. In: 73º Congresso Anual da ABM, 2018, São Paulo. ABM Proceedings. São Paulo: Editora Blucher, 2018. v. 73. p. 1573-1583.

## Internal Event

XX Internal Steelmaking Seminar – ArcelorMittal Monlevade, September 2022, João Monlevade – MG- Brazil

# ArcelorMittal Monlevade

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## Publications

- ARAUJO, A. F.; SOUSA, G. H.; ARAUJO, G. V.; SANTOS, I. C.; FERNANDES, LOYSLENE RABELO. SYNTHESIS OF MAGNETITA NANOPARTICLES BY COPRECIPIATION. In: 74º Congresso Anual da ABM, 2019, São Paulo. Anais do Congresso Anual da ABM, 2019. v. 74. p. 712-718.
- SOUSA, GUSTAVO HENRIQUE; SANTOS, IGOR CUZZUOL DOS ; ARAUJO, ATHOS FERNANDES ; BRAGA, JORGIMARA DE OLIVEIRA ; ARAÚJO, GUILHERME VITOR DE ; FONSECA, MARCELO ALVES . SEPARAÇÃO DE MATERIAIS METÁLICOS PELO MÉTODO DE FAGULHA: DIAGNÓSTICO DE MISTURAS NO ESTOQUE DE EMPRESAS SIDERÚRGICAS. In: 74º Congresso Anual da ABM, 2019, São Paulo. ABM Proceedings. São Paulo: Editora Blucher, 2019. p. 3317-3327.
- ARAUJO, ATHOS FERNANDES ; GONÇALVES, WALLACE CRISÓLOGO SOUZA ; SOUSA, GUSTAVO HENRIQUE ; FERNANDES, LOYSLENE RABELO ; LINO, RONEY EDUARDO . ANÁLISE DO RENDIMENTO DE FERROLIGAS EM ESTAÇÃO DE RINSAGEM UTILIZANDO O SIMULADOR DE REFINO SECUNDÁRIO DO STEEL UNIVERSITY. In: 50º Seminário de Aciaria, Fundição e Metalurgia de NãoFerrosos, 2019, São Paulo. ABM Proceedings. São Paulo: Editora Blucher, 2019. v. 50. p. 128-139.

## Internal Event

XIX Steelmaking Seminar – ArcelorMittal Monlevade, September 2021, João Monlevade – MG- Brazil

## Publications

- SOUSA, G. H.; SANTOS, I. C. ; BRAGA, J. O. ; FERNANDES, LOYSLENE RABELO ; ARAUJO, A. F. . HYDROMETALLURGICAL RECOVERY OF MANGANESE FROM BLAST FURNACE SLAG. In: 74º Congresso Anual da ABM, 2019, São Paulo. Anais do Congresso Anual da ABM, 2019. v. 74. p. 236-243.
- SOUSA, G. H.; ARAUJO, G. V. ; FONSECA, G. C. ; PEREIRA, H. T. C. ; ARAUJO, A. F. . EVALUATION OF CORROSION RESISTANCE TO SAE 1080 STEEL IN SULFURIC ACID AND WATER. In: 74º Congresso Anual da ABM, 2019, São Paulo. Anais do Congresso Anual da ABM, 2019. v. 74. p. 702-711.
- FERNANDES, LOYSLENE RABELO ; SOUSA, GUSTAVO HENRIQUE . AVALIAÇÃO DA CORROSÃO NO AÇO 10B22 PARA FIXADORES. In: 73º Congresso Anual da ABM, 2018, São Paulo. ABM Proceedings. São Paulo: Editora Blucher, 2018. v. 73. p. 1573-1583.



## WEBINAR | Green Steel



### PROGRAMME

▶ Tuesday, February 15, 2022

▶ 10:00 AM – 12:00 PM

### JOIN US

Live Stream on Youtube

<https://www.youtube.com/watch?v=ysGS2sHEO2M>

- ▶ **10:00 Welcome and Opening Session**  
Jorge Oliveira – CEO ArcelorMittal Aços Planos América do Sul
- ▶ **10:10 Presentation: Green Steel Research at the Max Planck Institute**  
Prof. Dr. Dierk Raabe – Managing Director, Max-Planck-Institut für Eisenforschung GmbH  
Dr. Isnaldi Souza Filho – Max-Planck-Institut für Eisenforschung GmbH, Group Leader Sustainable Synthesis of Materials
- ▶ **11:00 Panel Discussion mediated by**  
Prof. Andre Costa e Silva – Professor, EEIMVR-UFF, Director IBQN
- ▶ **11:30 Q&A mediated by**  
João Bosco Silva – General Manager – Sustainability and Institutional Relations
- ▶ **11:50 Closing Remarks**  
Erick Torres – Operations Vice-president ArcelorMittal Aços Planos América do Sul

PARTNERSHIP



# The Effect of Boron on Low Carbon Steel

Author: Iury Otaviano

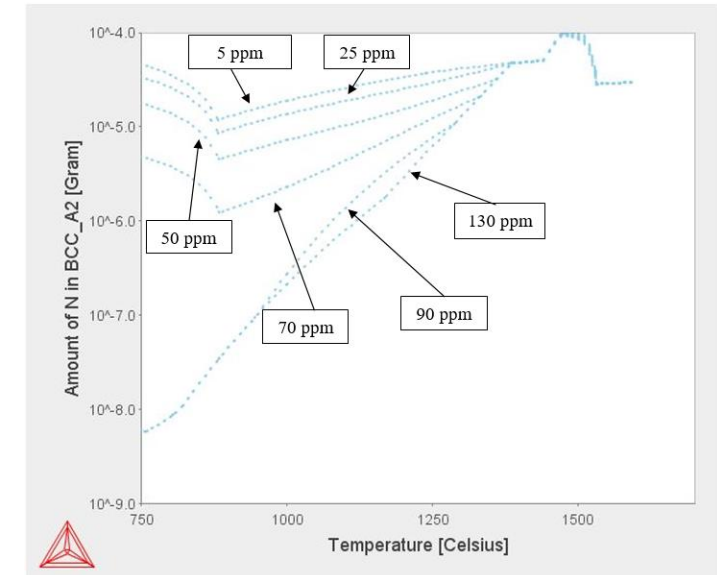
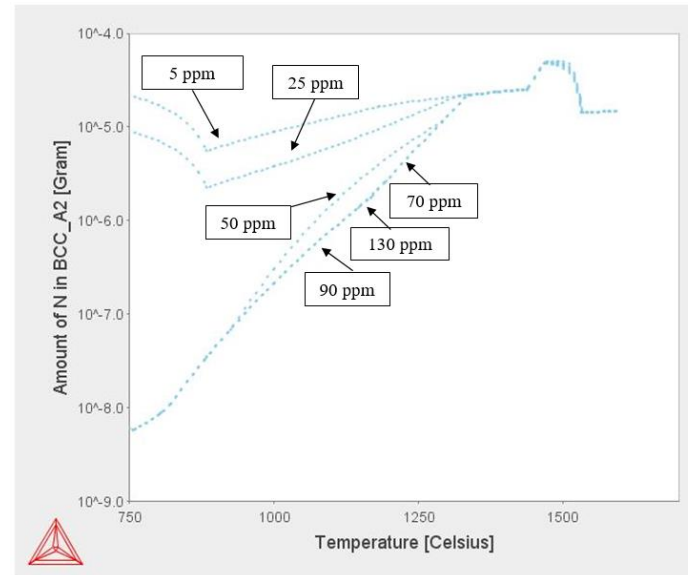
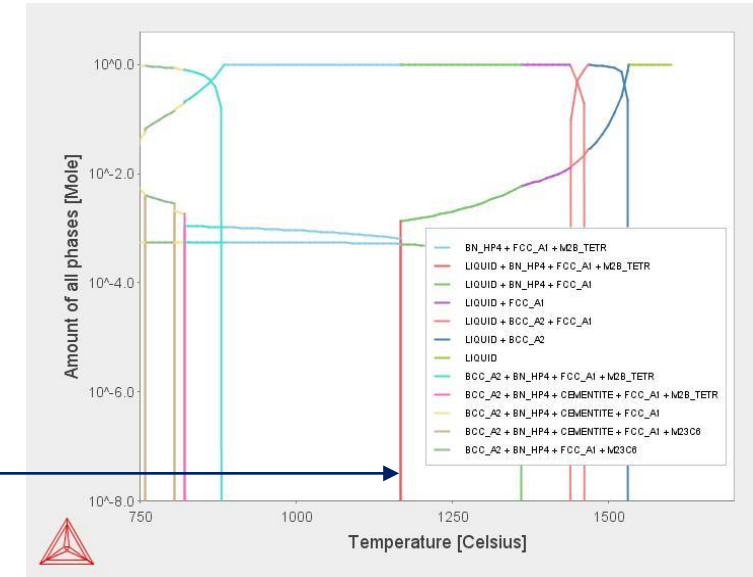
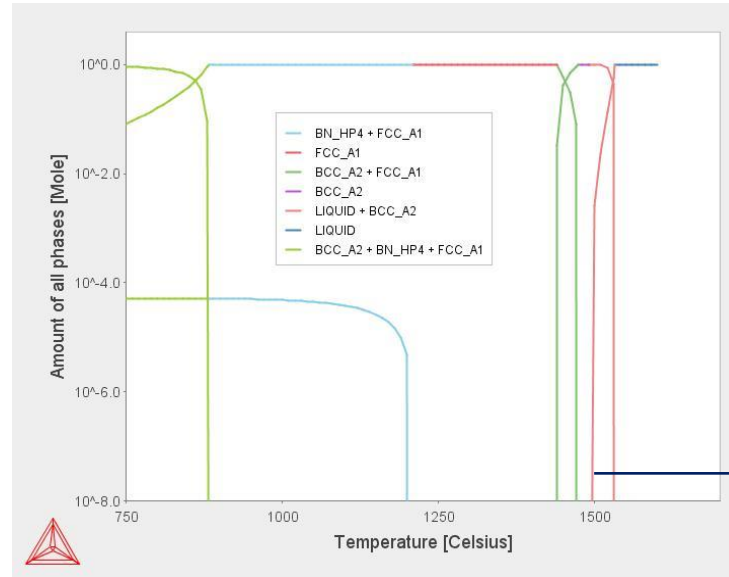
Organization Name: Arcelormittal

Team: Pedro Coutinho / Bruno Veiga

Team Size: 3

Advisor: André Costa e Silva

At Resende plant to minimize the aging effect on low carbon steels we have a boron addition in order to create boron nitride. The usage of boron have to be very well controlled because of his negative effects at the continuous casting machine. To better understand this effects we used thermodynamics computations. With some simple computations we could understand the effect of boron on the solidification shell. It was possible to notice that, as the relationship between boron and nitrogen grows a compound with boron and iron with low melting point is created and the solidification will finish in lower temperatures. We could also evaluate what was the best relationship between boron and nitrogen using the amount of Nitrogen remaining at BCC for different amounts of boron



# Gerdau Specialty Steels Brazil (Pindamonhangaba Plant)

## Control of Liquid Inclusion Window for SBQ Steels

Team: **Marcelo Carboni**, **Marcos Vinicios Garcia Neves**, **Marivaldo Junior Oliveira**, **Eduarda Zangrandi**, **Henrique Morales Zaggo**

Highlights: Calculation of liquid inclusion window (Holappa model) for all steel grades to be cast on the new continuous casting machine. Offline Mapping of a set of liquid inclusion windows using macro processing on FactSage covering all typical conditions during the refining stages of each steel grade. Based on these calculations, development of a statistical model for calculation of CaSi injection to achieve liquid inclusions for each steel grade on real time, during the production of the heat. More than 80 different steel grades were cast with this model: zero occurrences of clogging.

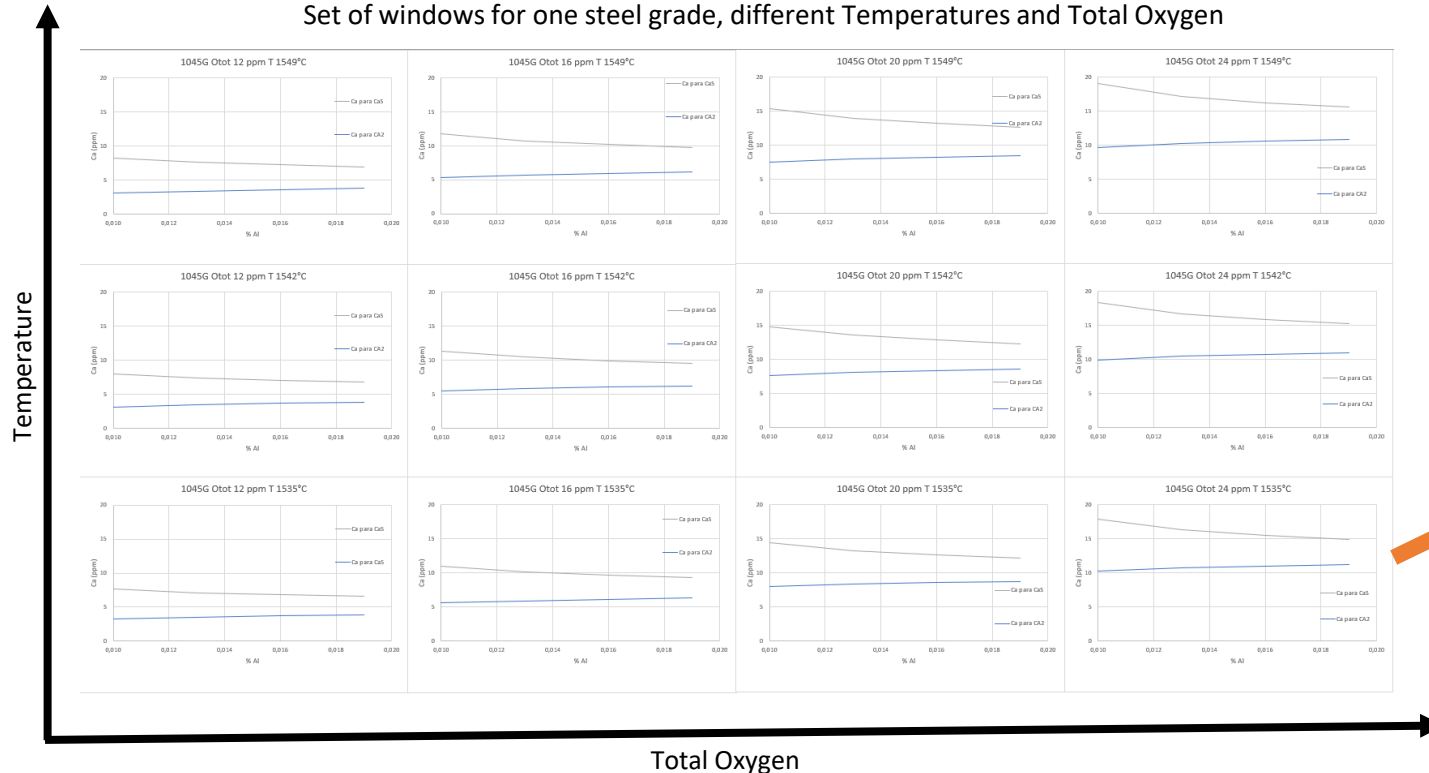
Collaborations:

**Bruno Laidens** (RHI): template for liquid window calculation

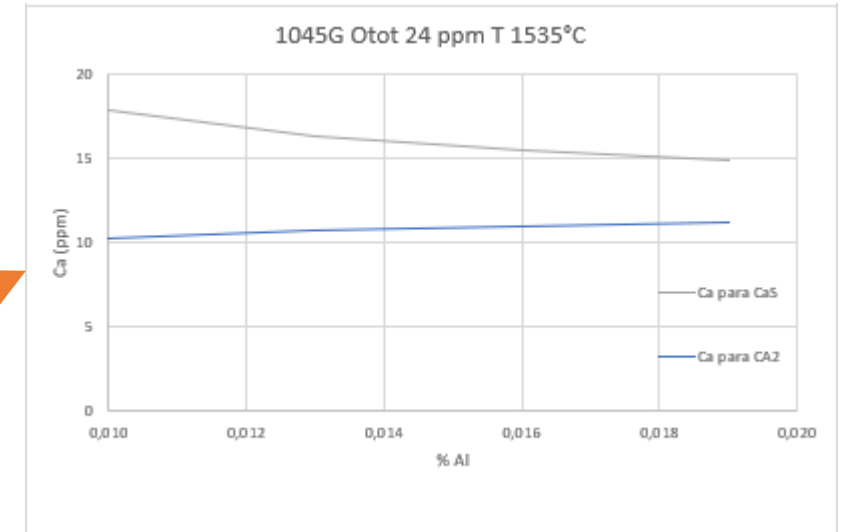
**Prof. Wagner Bielefeldt** (UFRGS – Federal University of Rio Grande do Sul): template for liquid window calculations and FactSage training of the team.

**Prof. Marie-Aline Van Ende** (Seoul National University): Webinar on Macro processing and contacts via LinkedIn for questions.

Set of windows for one steel grade, different Temperatures and Total Oxygen



Single windows for one steel grade, fixed Temperature and Total Oxygen (previous solution)



# Gerdau Specialty Steels Brazil (Pindamonhangaba Plant)

## Refining Slag Monitoring and Control

Organization: Gerdau Specialty Steels Brazil (Pindamonhangaba Plant)

Team: **Marcelo Carboni, Bruno Laidens (RHI), Marcos Vinicios Garcia Neves, Marivaldo Junior Oliveira, Eduarda Zangrandi**

Highlights: Evaluation of refining slags on ladle furnace and vacuum degassing, aiming for the protection of refractories (MgO saturation), optimizing C/S and C/A relations to guarantee inclusion cleanliness and control of viscosity of the slag. Daily report analysing all production heats from previous day (offline, using macro processing of FactSage) Adjument of slag recipes and practices.

Colaborations:

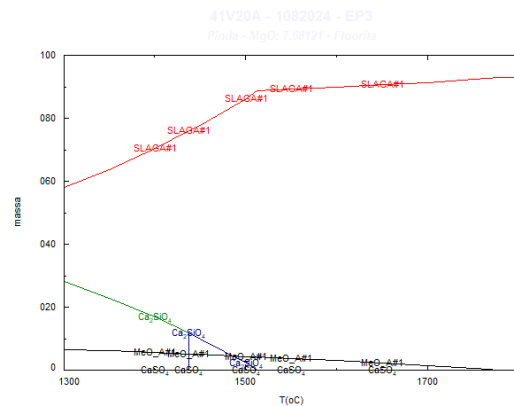
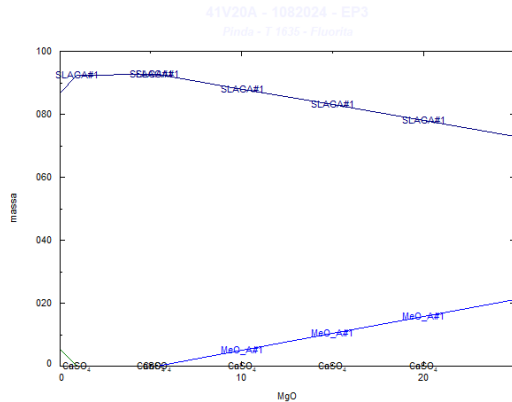
**Prof. Wagner Bielefeldt** (UFRGS – Federal University of Rio Grande do Sul): template for slag calculations and FactSage training of the team.

**Prof. Marie-Aline Van Ende** (Seoul National University): Webinar on Macro processing and contacts via LinkedIn for questions.

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	CaF <sub>2</sub>	1
	CaO	4
	FeO	5
	MgO	6
	MnO	1
	S	C
	SiO <sub>2</sub>	2
	T Calc	1
	g-MgO(SLAGA#1)	(% em massa MgO da fase liq)
MgOSat	(MgO total para precipitação de fase sólida rica em MgO)	10,
Xliq	(fração de fase líquida no sistema)	92
visc. (Pa.s)	Calculado no módulo Viscosity do FactSage	0
Xsol	Xsol	0
$\mu_{Fe}^{[1]}$	(Correção considerando fração de fase sólida conforme referências literatura - precisa verificar)	0
$\eta_e$ (Roscoe-Einstein) <sup>[2]</sup>		0

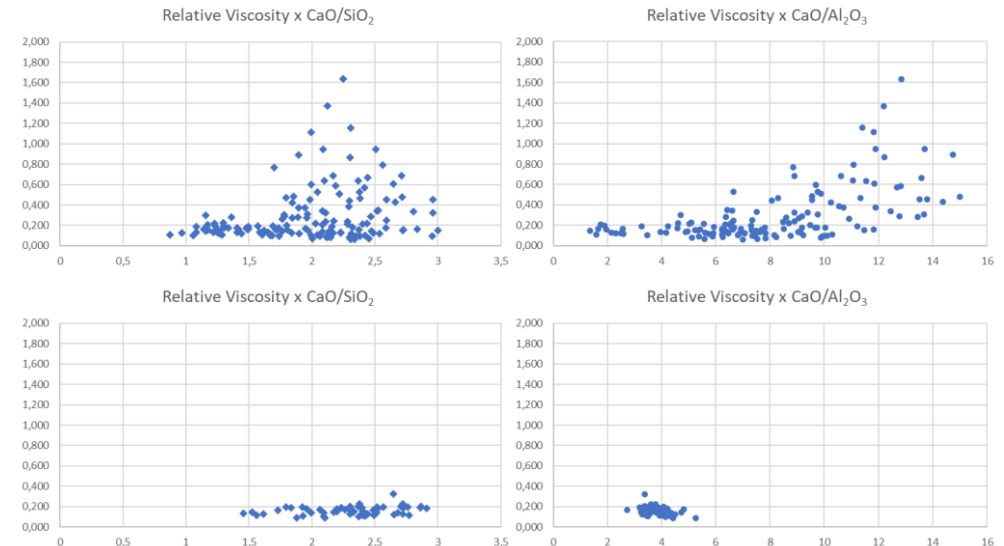
Inputs

Results (FactSage and Slag Model)



Standard Practice  
(before project)

Adjusted Chemistry  
(using FactSage)



The logo for the Center of Innovation and Technology (CIT), featuring the letters 'CIT' in a bold, white, sans-serif font on a dark blue rectangular background.

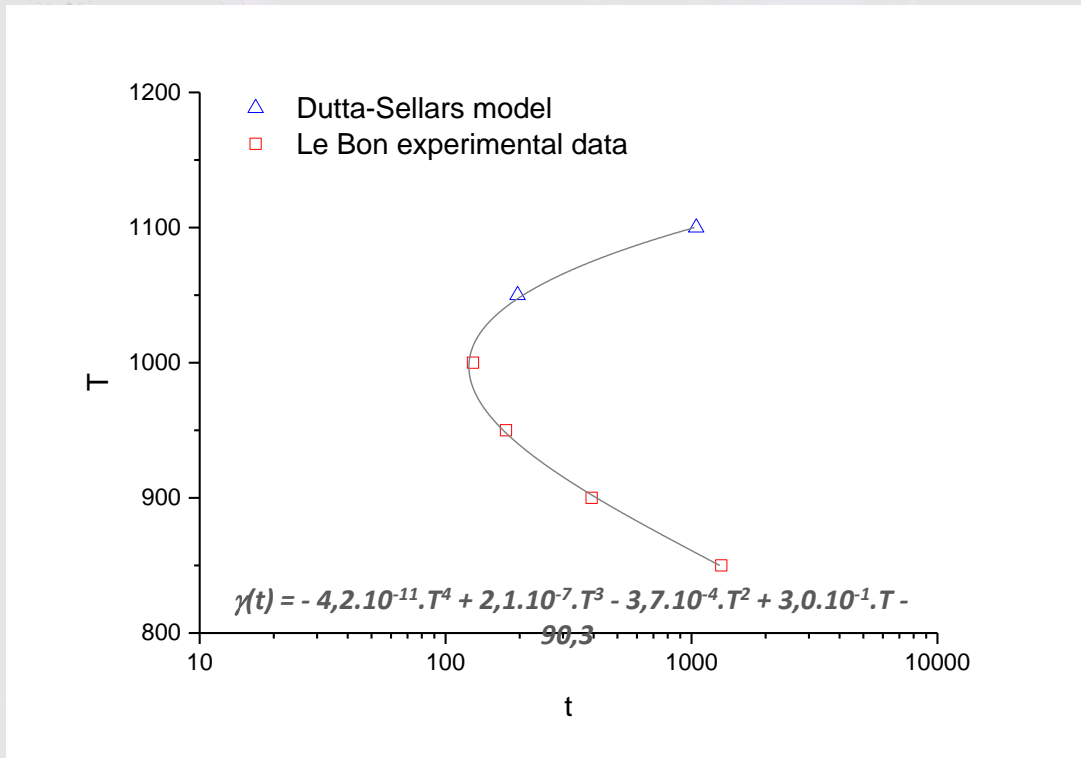
CENTRO DE  
INOVAÇÃO E TECNOLOGIA

A smaller version of the CIT logo, consisting of the letters 'CIT' in white on a dark blue background, located in the top right corner of the slide.

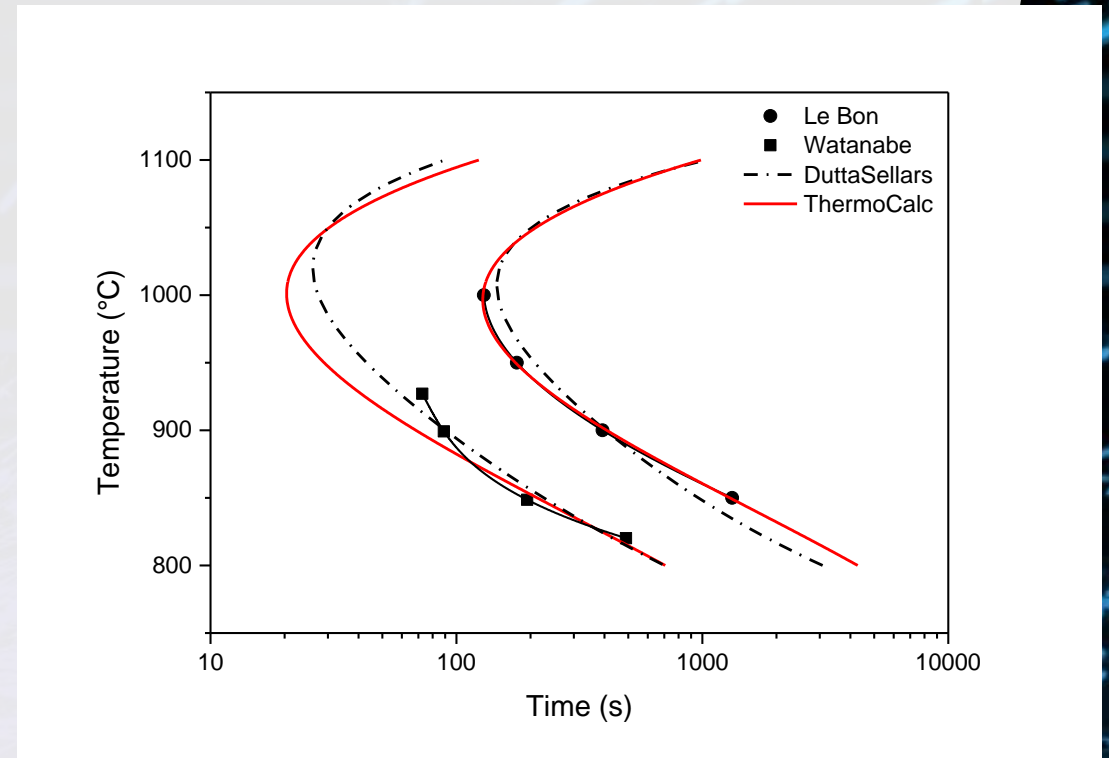
***Modeling Nb(C,N)  
precipitation kinetics after the  
roughing of thick plates***

- **Project:** Modeling Nb(C,N) precipitation kinetics after the roughing of thick plates
- **Participants (10):** Ricardo N. Carvalho<sup>(1)</sup>; Neice F. Santos<sup>(1)</sup>; Cynthia S. B. Castro<sup>(1)</sup>; Clélia R. Oliveira<sup>(1)</sup>; Anderson C. Jesus<sup>(1)</sup>; Ronaldo Barbosa<sup>(3)</sup>; Paulo Haddad<sup>(2)</sup>; Ed J. M. Taiss<sup>(2)</sup>; Daniel B. Matsubara<sup>(2)</sup>; André L. V. Costa e Silva<sup>(4)</sup>
- **Organizations:** (1) CIT-Senai; (2) CBMM; (3) Gerdau; (4) UFF
- **Publications:** only internal reports by now, a paper is being written
- **Highlights:** Nb(C,N) precipitation kinetics was modeled by ThermoCalc/Prisma to support decisions on physical simulations by Gleeble and industrial experiments. The main goal was to adjust processes parameters (furnace temperature and waiting time after roughing) to maximize the amount of Nb in solid solution available for finishing steps. Both decreasing waiting time and temperature showed efficient to prevent Nb(C,N) precipitation after roughing and, therefore, increasing the driving force for strain induced precipitation at finishing steps and/or interphase precipitation during final cooling.

# Calibration of $\gamma(t)$



# Validation of $\gamma(t)$



Calibration: 0,17C; 0,0110N; 0,040Nb steel,  $d\gamma = 250 \mu\text{m}$  (Le Bon et al.)

Valiation: 0,063C; 0,0058N; 0,084Nb steel,  $d\gamma = 25 \mu\text{m}$  (Watanabe et al.)

# CSN – Volta Redonda

- Steel products development for automotive and infrastructure: solidification, precipitation and phase transformation.
- Melt shop: development of slags and coupling with refractories
- Researchers involved with the use of phase diagrams and computational thermodynamics: 9
- Publications: 2



# SENAI CIMATEC Computational Thermodynamics for RD&I projects

June/2023

# Informação/Information

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# Casting aluminum alloys: Alloy design

- Institution: SENAI CIMATEC – Integrated Campus for Manufacture and Technology (Salvador, Ba, Brazil)
- Main team: Dr. Bruna Callegari, Dr. Tiago Lima, Prof. Dr.-Ing. Rodrigo Coelho
- Full team size (from management to research): 07
- Problem: automotive cast aluminum alloy design for property optimization
- Employed Thermo-Calc tools:
  - DICTRA and PRISMA modules; TCAL8 and MOBAL7 databases
  - Equilibrium calculations, hot tearing susceptibility calculation, Scheil simulation (conventional and back-diffusion), simulation of phase dissolution, simulation of isothermal precipitation (aging)
- Outcome: new alloy with improved strength (+18%)

# Study of dissolution behavior of ferroalloy

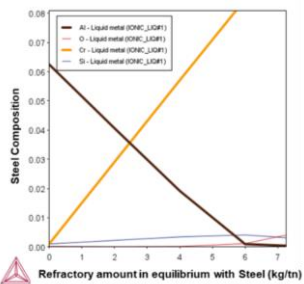
- Institution: SENAI CIMATEC – Integrated Campus for Manufacture and Technology (Salvador, Ba, Brazil)
- Main team: Dr. Bruna Callegari, Dr. Tiago Lima, Dr. Luis Fernando Folle, Paulo dos Reis (MSc.), Prof. Dr.-Ing. Rodrigo Coelho
- Full team size (from management to research): 07
- Problem: need to understand dissolution behavior of ferroalloys with varying granulometries in molten steel
- Employed Thermo-Calc tools:
  - Thermo-Calc 2023a (incl. DICTRA module); TCFE12 and MOBFE7 databases
  - Equilibrium calculations, Scheil simulation (conventional and back-diffusion), simulation of particle dissolution, simulation of homogeneization heat treatment
- Ongoing project

# Non-contamination related chromium pick-up in RH degasser: Chromium based refractory ternary phase diagrams, thermodynamic and kinect analysis

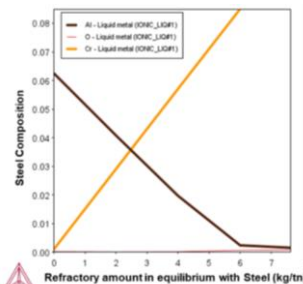
## The problem

- Cr pick-up in RH vessel in ULC steels with Si > 0,3%
  - Fenômeno não ocorre para UBC convencional
  - Exauridas as possibilidades do Cromo vir de contaminação
  - Foi investigado pelo Thermocalc o efeito do Si no Refratário do Vaso, que contêm 20% de Cromita

UBC + 0,3% Silicon



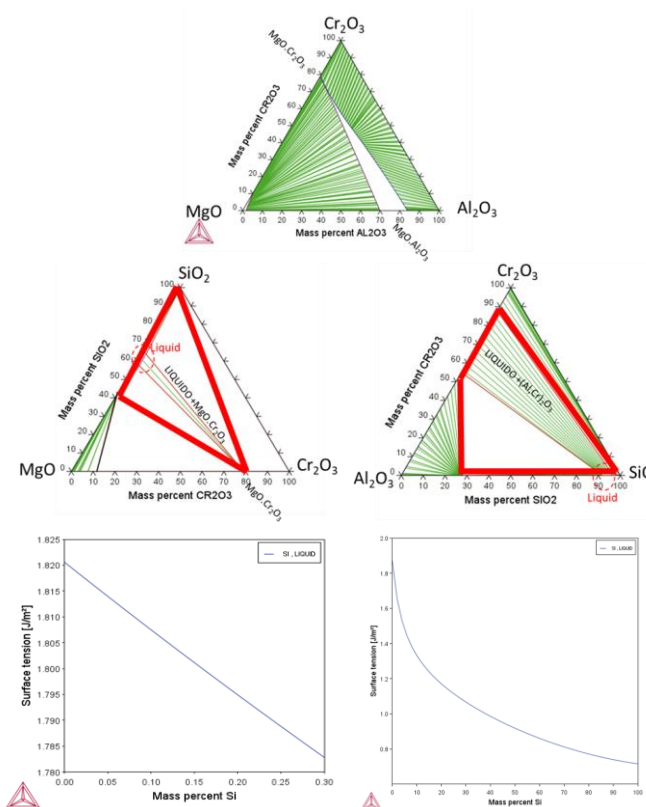
UBC



- Pelo Thermocalc Viu-se que a Cromita não é Estável para ambos os sistemas
- Iniciou-se a investigação do efeito catalizador do Silício

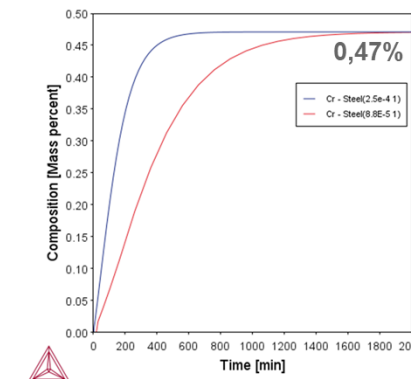
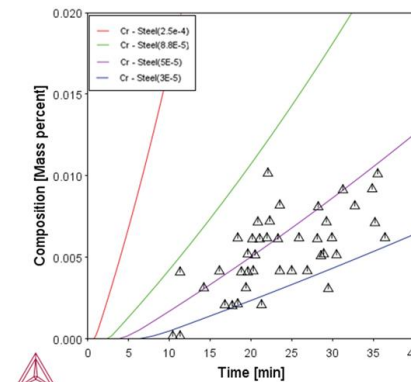
## Analysis

- Análise das fases do Refratário a 1600° C antes e após interação com o Silício
  - Formação de fases líquidas
- Aumento da Área de contato Aço-Refratário com a adição de Silício



## Solution

- Previsão do Pick-up por modelamento do transporte de Massa
- Sucesso no Controle da Composição Química



- R&D Team
  - Alexandre Bellegard Farina, PhD (R&D Manager)
  - Daniel Pallos Fridman, MsC
  - Eduardo Netto de Souza, PhD
  - Hendrew de Souza Giroto
  - Luiz Henrique Martinez Antunes, MsC
  - Mario César Mantovani, PhD
  - Luiza Pessoa Moreira, PhD
  - Roberto Tibúrcio Canito Frota Júnior, MsC

# Works in Progress

- Development of new Ni-based and Fe-based alloys using thermodynamic simulations with Thermo-Calc software. TCFE12, TTNI8 and TCNI12 thermodynamic databases and its validation with experimental tests (DTA, DSC, Dilatometry).
- Kinetic simulations using DICTRA for Fe-based and Ni-based alloys to predict heat treatments and phase transformations.
- Simulations of the solidification process with dedicated software coupled with thermodynamic data extracted from Thermo-Calc software using TCFE12 and TTNI8 thermodynamic databases.
- Definition of parameters for continuous casting process using data from thermodynamic simulations with Thermo-Calc software coupled with SLAG4 and TCFE12 database.
- Thermodynamic modeling of slag/metal reactions for non-metallic inclusions control and process optimization using Thermo-Calc software coupled with TCFE12, SLAG4 and TTNI8 thermodynamic databases.
- Thermomechanical modeling of rolling and forging process of alloys with dedicated software coupled with thermodynamic simulations of alloys using Thermo-Calc software and TCFE12 and TTNI8 thermodynamic databases.

# Unesp Itapeva/SP

Main researcher: Renato Baldan

Team: 5

Highlights: Research on HEAs using computational thermodynamics. Collaboration with UFSJ (Universidade Federal de São João del Rei), UNICAMP-Limeira, USP.



## Witor Wolf – Professor of the Metallurgical and Materials Department – Federal University of Minas Gerais.

Researchers involved:

-PhD students: Maria Helena Teles Lopes, Miguel Leite Lapér

-Master's students: Luiz Paulo Mendonça e Silva (defended), Guilherme Cardeal Stumpf (defended), Alisson Silva Winther.

-Undergrad students: Arthur Diniz Silveira (defended), Thiago Cezar Drumond de Oliveira (defended), Nicassio Silva Franca, Abraao Fonseca Martins, Julia Santos Hobl, Pablo de Souza Miguel.

-Collaborators: Prof. Roberto Braga Figueiredo (UFMG), Prof. Dagoberto Brandão Santos (UFMG), Prof. Eduardo Henrique Martins Nunes (UFMG), Prof. Marcelo Araújo Câmara (UFMG), Prof. Eric Marchezini Mazzer (UFSCar), Prof. Francisco Gil Coury (UFSCar), Prof. Guilherme Yuuki Koga (UFSCar), Prof. Guilherme Zepon (UFSCar), Prof. Walter José Botta Filho (UFSCar), Prof. Claudemiro Bolfarini (UFSCar), Prof. Claudio S. Kiminami (UFSCar), Prof. Jan Schroers (Yale University).

In the last 5 Years we have been developing quasicrystal-forming Al-based alloys and High Entropy Alloys. Most of our work makes use of thermodynamic calculations for predicting phase formation in the alloys that we fabricate. We often associate the use of Calphad with tools for predicting high resistant alloys, by use of precipitation, grain size control and solid solution strengthening.

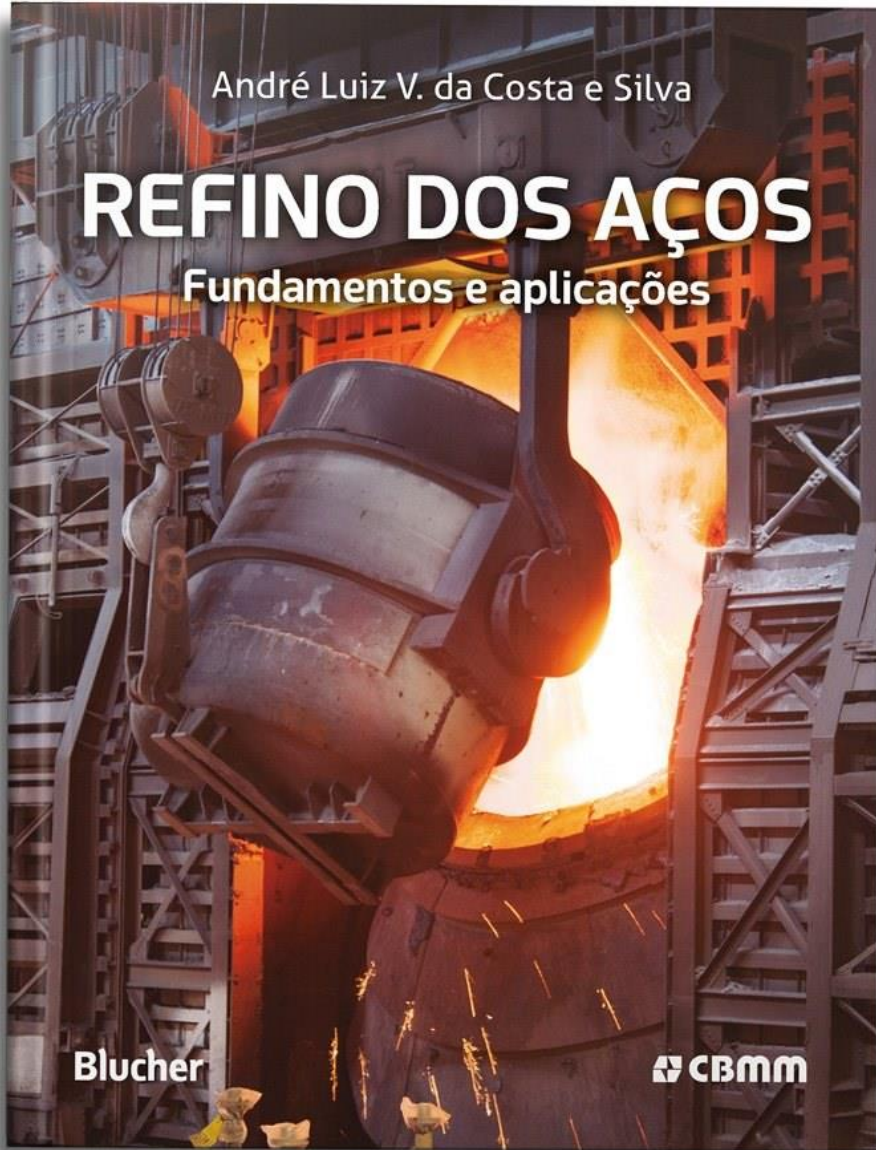
We have been able to accurately use High Entropy alloys databases for predicting phase formation and stability as well as for selecting alloying additions to promote carbide precipitation that has shown to be promising for grain growth control during thermomechanical processing of these materials. The thermodynamic calculation of quasicrystal-based alloys are more challenging due to lack of appropriate databases.

### • Main publications:

- A wear-resistant Al<sub>85</sub>Cu<sub>6</sub>Fe<sub>3</sub>Cr<sub>6</sub> spray-formed quasicrystalline composite. *Materialia*, v. 21, p. 101367, 2022.
- Al-matrix composites reinforced with quasicrystals consolidated at room temperature using HPT. *MATERIALS LETTERS*, v. 317, p. 132107, 2022.
- Effect of grain size on strength and strain rate sensitivity in the CrMnFeCoNi high-entropy alloy. *Journal of Materials Research and Technology-JMR&T*, v. 20, p. 2358-2368, 2022.
- Microtexture evolution of sigma phase in an aged fine-grained 2205 duplex stainless steel. *MATERIALS CHARACTERIZATION*, v. 171, p. 110802, 2021.
- The influence of particle size and heat treatments on the transformation energies of a gas atomized Cu-Al-Ni-Mn shape memory alloy. *THERMOCHIMICA ACTA*, v. 707, p. 179107, 2021.
- Designing new quasicrystalline compositions in Al-based alloys. *JOURNAL OF ALLOYS AND COMPOUNDS*, v. 823, p. 153765, 2020.
- Wear-resistant boride reinforced steel coatings produced by non-vacuum electron beam cladding. *SURFACE & COATINGS TECHNOLOGY*, v. 386, p. 125466, 2020.
- Single step fabrication by spray forming of large volume Al-based composites reinforced with quasicrystals. *SCRIPTA MATERIALIA*, v. 181, p. 86-91, 2020.
- Wear and Corrosion Performance of Al-Cu-Fe-(Cr) Quasicrystalline Coatings Produced by HVOF. *JOURNAL OF THERMAL SPRAY TECHNOLOGY*, v. 29, p. 1195-1207, 2020.
- Formation and stability of complex metallic phases including quasicrystals explored through combinatorial methods. *Scientific Reports*, v. 9, p. 7136, 2019.
- Fabrication of Al-matrix composite reinforced with quasicrystals using conventional metallurgical fabrication methods. *SCRIPTA MATERIALIA*, v. 173, p. 21-25, 2019.
- Effect of boron addition on the solidification sequence and microstructure of AlCoCrFeNi alloys. *JOURNAL OF ALLOYS AND COMPOUNDS*, v. 775, p. 1235-1243, 2018.
- Corrosion and wear properties of FeCrMnCoSi HVOF coatings. *SURFACE & COATINGS TECHNOLOGY*, v. 357, p. 993-1003, 2018.

# UFF

Published 2023



Work on kinetic modeling of ladle furnace with industry (two projects)  
Work in slags, refractories and insulating materials, most with industry  
Precipitation in HSLA steels

GOULART, LLO ; CASTRO, JA ; Costa e Silva, A. Development of a computational thermodynamics EERZ model for the improvement of hot rolled light steel profiles steel refining. CALPHAD, v. 81, p. 102550, 2023.

Costa e Silva, A Second phases in steel: a review of the concept, origin, and their relevance for properties. TECNOLOGIA EM METALURGIA, MATERIAIS E MINERAÇÃO, v. 19, p. e2753, 2022.

GOULART, LLO ; SILVA, E. P. ; ALVES, CLM; CASTRO, J. A. ; COSTA E SILVA, A. APPLICATION OF A COMPUTATIONAL THERMODYNAMICS EFFECTIVE EQUILIBRIUM REACTION ZONE (EERZ) TO DESCRIBE THE PROCESSES FROM TAPPING TO ARRIVAL AT THE LADLE FURNACE. In: 51º Seminário de Fusão, Refino & Solidificação de Metais, part of the ABM Week 6th edition, June 7th-9th, 2022, São Paulo, SP, Brazil., 2022, São Paulo. Editora Blucher, 2022.

COSTA E SILVA, A. SOME ASPECTS OF THE MODELING OF AUSTENITIC GRAIN SIZE CONTROL IN MICROALLOYED STEELS. In: 57º Seminário de Laminação e Conformação de Metais, part of the ABM Week 6th edition, June 7th-9th, 2022, São Paulo, SP, Brazil, 2022, São Paulo. Anais do 57º Seminário de Laminação e Conformação de Metais, part of the ABM Week 6th edition, June 7th-9th, 2022, São Paulo, SP, Brazil, 2022

COSTA E SILVA, A. Applications of Thermo-calc to steelmaking and processing. 2023. Stockholm.

OLIVEIRA, J. ; RAABE, D. ; SOUZA FILHO, I. ; SILVA, J. B. ; TORRES, E. ; COSTA E SILVA, ANDRÉ . Green steelmaking and green-making steel. 2022. Presentations and discussion online, sponsored by ArcelorMittal Brasil.

# UFRJ

- Professors: Dilson Silva dos Santos; Leonardo Sales Araujo; Luiz Henrique de Almeida
- Areas of Research
- **Microstructural evolution of cast, high temperature steels for pyrolysis furnaces (HP steels):** the cast HP steels operate under high temperature ( $> 900^{\circ}\text{C}$ ) for long periods ( $> 10$  years) and its microstructural evolution through time can influence its creep properties. Important alloying additions, like Nb and Ti, improved its properties and slowed degradation, but it is important to have better knowledge of the phases formed and its transformations.
  - - Phase diagrams and isopleths;
  - - Step cooling phase formation;
  - - precipitation;
  - - Scheil calculations;
- **Phase formation during weld of austenitic clads:** the austenitic clads can be deposited over ferritic steels for protection against corrosion and hydrogen embrittlement for offshore applications. However, due to the thermal cycle and compositional gradients, it is key to investigate the phases formed over different conditions (kinetic and thermodynamic)
  - - Phase diagrams and isopleths;
  - - Step cooling phase formation;
  - - Solidification (Scheil calculations);
  - - Diffusion;
- **Alloying influence and phase transformation in superalloys:** nickel-base superalloys are complex materials, congregating various alloying elements that provide its remarkable properties. However, an improper control or processing can promote brittle phases formation and degradation of properties.
  - - Phase diagrams and isopleths;
  - - Solidification (Scheil calculations);
  - - Step cooling phase formation;
  - - Precipitation;
- **Titanium alloys for biomedical applications:** titanium alloys are candidate materials for biomedical components like stem prosthesis. However, the alloying is very limited to elements that promote no harm to the human body. At the same time, it is important to control phases formations to tailor mechanical properties.
  - - Phase diagrams and isopleths;
  - - Step cooling phase formation;

# Universidade Federal do Rio Grande do Sul - UFRGS

- **Research Staff**

- Prof. Dr. Wagner V. Bielefeldt – LaSid (<http://www.ct.ufrgs.br/lasid>)
- Prof. Dr.-Ing. Antônio C. F. Vilela – LaSid coordinator
- Dr. Julio Morales
- Dr. Daniel R. Silva
- MSc. Anderson Kempka
- MSc. Sharon Kempka

- **Research Themes**

- Steelmaking and processing: Engineering steel, Free cutting steel; nonmetallic inclusions; secondary refining slags, mould slags.

# UFRGS - Publications

FERREIRA, FELIPE BUBOLTZ ; KLUG, JEFERSON LEANDRO ; PEREIRA, JULIO ANIBAL MORALES ; Bielefeldt, Wagner Viana ; VILELA, Antônio Cezar Faria . Laboratory Evaluation of Tundish Covering Powders and Rice Hull Ash on Cleanliness for a SAE 1055 Modified Steel. MATERIALS RESEARCH, v. 26, p. e20220216, 2023.

BACCARIN, L.I.P. ; BIELEFELDT, W.V. ; BRAGANÇA, S.R. . Evaluation of thermodynamic simulation (FactSage) for the interpretation of the presence of phases and the firing behavior of triaxial ceramics. CERAMICS INTERNATIONAL, v. 47, p. 21522-21529, 2021.

CUNHA ALVES, PEDRO ; CARDOSO DA ROCHA, VINICIUS ; MORALES PEREIRA, JULIO ANÍBAL ; Bielefeldt, Wagner Viana ; VILELA, Antônio Cezar Faria . Evaluation of Thermodynamic Driving Force and Effective Viscosity of Secondary Steelmaking Slags on the Dissolution of Al<sub>2</sub>O<sub>3</sub>-Based Inclusions from Liquid Steel. ISIJ INTERNATIONAL, v. 61, p. 2092-2099, 2021.

PEREIRA, JULIO ANÍBAL MORALES ; ROCHA, VINICIUS CARDOSO DA ; ALVES, PEDRO CUNHA ; Bielefeldt, Wagner Viana ; VILELA, Antônio Cezar Faria . Analysis of Spinel Based Inclusions During the Last Stage of The Steelmaking Process of SAE 52100. MATERIALS RESEARCH, v. 23, p. 1-11, 2020.

FERREIRA, F. B. ; ROCHA, V. C. ; BIELEFELDT, W.V. ; VILELA, ANTÔNIO C. F. . ANALYSIS AND VERIFICATION OF PROCESS VARIABLES AS CAUSES FOR MACROINCLUSIONS AND SCRAPPING IN A SPECIAL STEEL MELT SHOP. TECNOLOGIA EM METALURGIA, MATERIAIS E MINERAÇÃO (IMPRESSO), v. 17, p. 1-7, 2020.

LEÃO, PABLO B. P. ; KLUG, JEFERSON L. ; DE ABREU, HAMILTON F. G. ; CARNEIRO, CARLOS A. R. ; FERREIRA, HILDER C. ; BIELEFELDT, Wagner V. . Sliver defects in an ultra-low carbon Al-killed steel caused by low steel level in the tundish. IRONMAKING & STEELMAKING, v. 1, p. 1-8, 2020.

LEÃO, PABLO B. P. ; KLUG, JEFERSON L. ; CARNEIRO, CARLOS A. R. ; CALDAS, HILDER ; BIELEFELDT, Wagner V. . Castability and Inclusions in a Low Sulfur Ca-Treated Peritectic Steel for Two Deoxidation Techniques. steel research international, v. 90, p. 1900151, 2019.

# USIMINAS Product development

## Team

Fábio Dian Murari

Jean Viana Bahia

Tadeu Messias Donizete Borba

Used computational thermodynamics to design and development the thermo-mechanical processing of a new alloy to reach class 450 HB wear resistance with hot strip mill

# Usiminas - Hot metal treatment and steelmaking

Usiminas – Werner Arede Matos, Pedro Henrique Resende Vaz de Melo, Rafael Fernandes Reis

UFRGS – Wagner Viana Bielefeldt

UFF - Andre Costa e Silva

Uso dos softwares FactSage e Thermo-Calc:

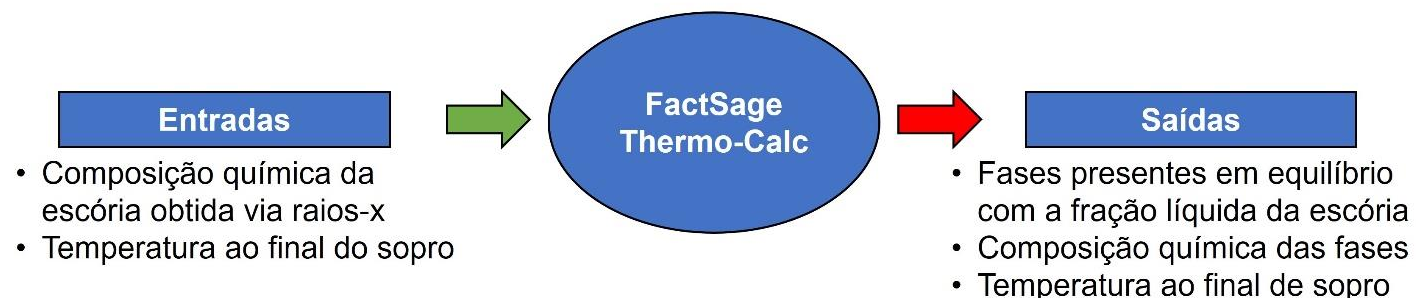
- Auxiliar os processo de produção de aços de baixo e ultra baixo fósforo;
- Verificar o distanciamento que os processos se encontram do equilíbrio termodinâmico;
- Auxiliar na modelagem termodinâmica do processo.

## Publicações

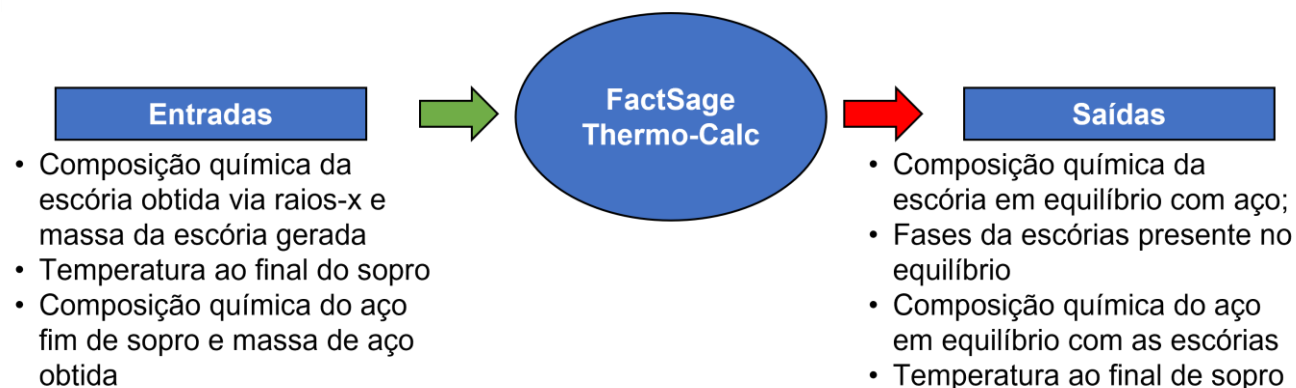
1. EVALUATION OF PHOSPHORUS PARTITION AT THE END OF BLOW IN LD CONVERTER (ABM WEEK – 2023)
2. PHOSPHOROUS PARTITION AT THE END OF BLOW IN BOF STEELMAKING – A THERMODYNAMIC STUDY OF P DISTRIBUTION BETWEEN SLAG AND METAL AND WITHIN THE SLAG (CALPHAD -2023)
3. DISSERTAÇÃO MESTRADO – WERNER AREDES MATOS / DESFOSFORAÇÃO EM CONVERTEDORES DO TIPO LD: UMA ANÁLISE VIA TERMODINÂMICA COMPUTACIONAL E MODELAGEM DO PROCESSO (PREVISÃO DE DEFESA ATÉ AGOSTO DE 2023).

## Tipos de simulações

Determinação das fases sólidas em equilíbrio com as escórias ao fim do sopro nos convertedores:



## Determinação do equilíbrio termodinâmico



# Usiminas - Hot metal treatment and steelmaking

## Members:

Usiminas – Werner Aredes Matos, Pedro Henrique Resende Vaz de Melo, Rafael Fernandes Reis  
UFRGS – Wagner Viana Bielefeldt  
UFF - Andre Costa e Silva

## The use of FactSage and Thermo-Calc software:

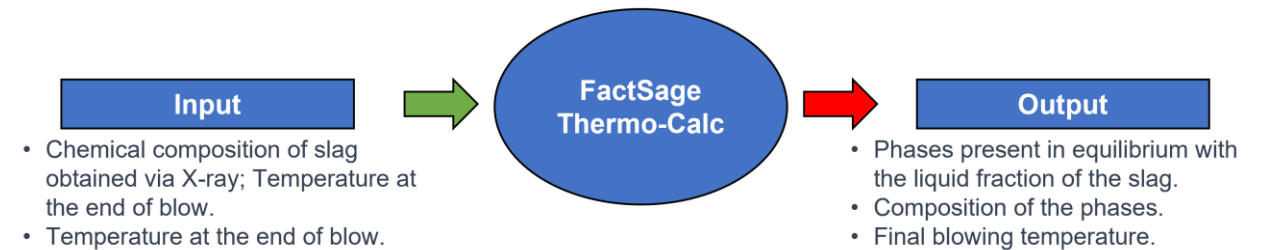
1. To assist in the production processes of low and ultra-low phosphorus steels;
2. To assess the deviation of the processes from thermodynamic equilibrium;
3. To support thermodynamic modeling of the process.

## Publications:

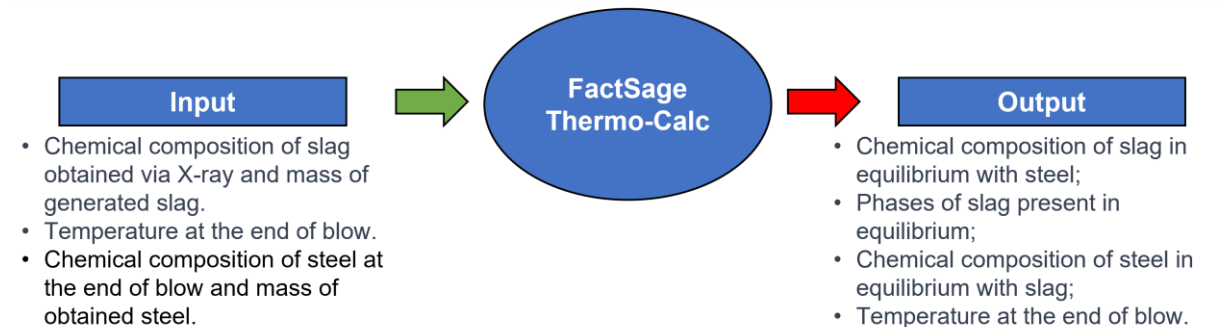
1. EVALUATION OF PHOSPHORUS PARTITION AT THE END OF BLOW IN LD CONVERTER (ABM WEEK – 2023)
2. PHOSPHOROUS PARTITION AT THE END OF BLOW IN BOF STEELMAKING – A THERMODYNAMIC STUDY OF P DISTRIBUTION BETWEEN SLAG AND METAL AND WITHIN THE SLAG (CALPHAD -2023)
3. DISSERTAÇÃO MESTRADO – WERNER AREDES MATOS / DESFOSFORAÇÃO EM CONVERTEDORES DO TIPO LD: UMA ANÁLISE VIA TERMODINÂMICA COMPUTACIONAL E MODELAGEM DO PROCESSO (PREVISÃO DE DEFESA ATÉ AGOSTO DE 2023).

## Types of simulations

Determination of solid phases in equilibrium with molten slag at the end of blow in converters.



Thermodynamic equilibrium determination of slag/metal at the end of blow





# USIMINAS Secondary Steelmaking

1. Nome da organização: USIMINAS S.A.
2. Researchers: Pedro Henrique Resende Vaz de Melo, Werner Aredes Matos, Rafael Fernandes Reis, Hélio Alexandre Alves
3. Using *software* Thermo-Calc to deal with (1) Castability Windows to avoid clogging by proper adjustment of Ca addition (2) Slag calculations: liquidus temperature, phases formed. Aim is reducing slag viscosity to improve de-S