Overview of research challenges for steel decarbonisation in Knowledge Building Program

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Global Research and Development
Journées annuelles du GDR TRANSINTER II
Juin 2025

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T. Coupez, C. Gauthier (CEMEF)

Smater steel for People and Planet

Towards net-zero steelmaking

Group target:

- 25% reduction in CO_2 equivalent emissions by 2030, Europe target increased to 35%
- Net-zero CO_2 emissions by 2050

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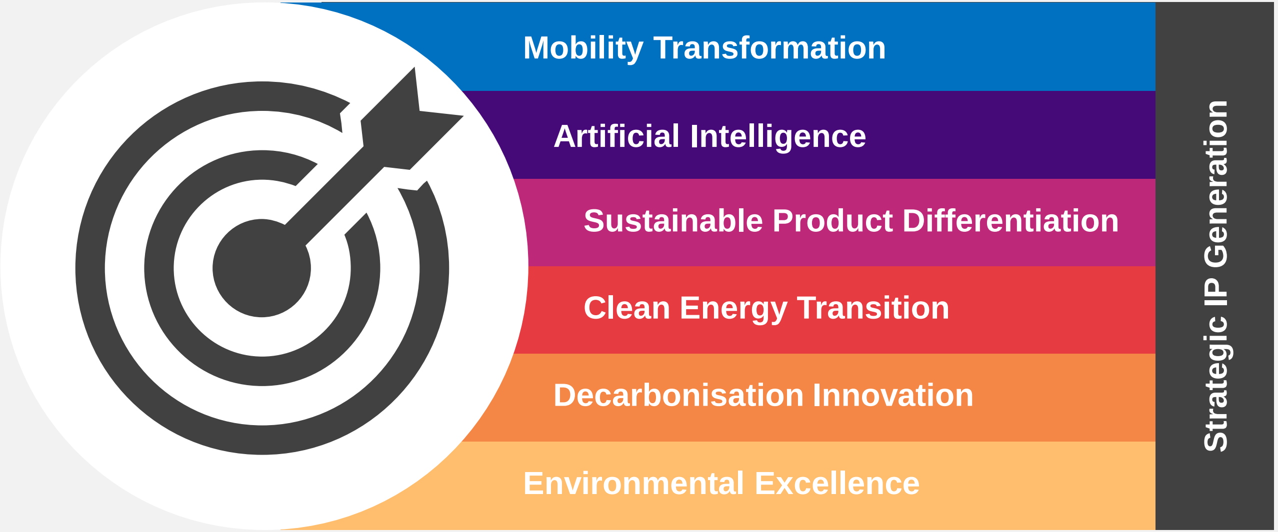
Global Research and Development
Our seven strategic objectives

Aligning innovation and technological advancements with ArcelorMittal's business goals, sustainability efforts, and emerging market trends.



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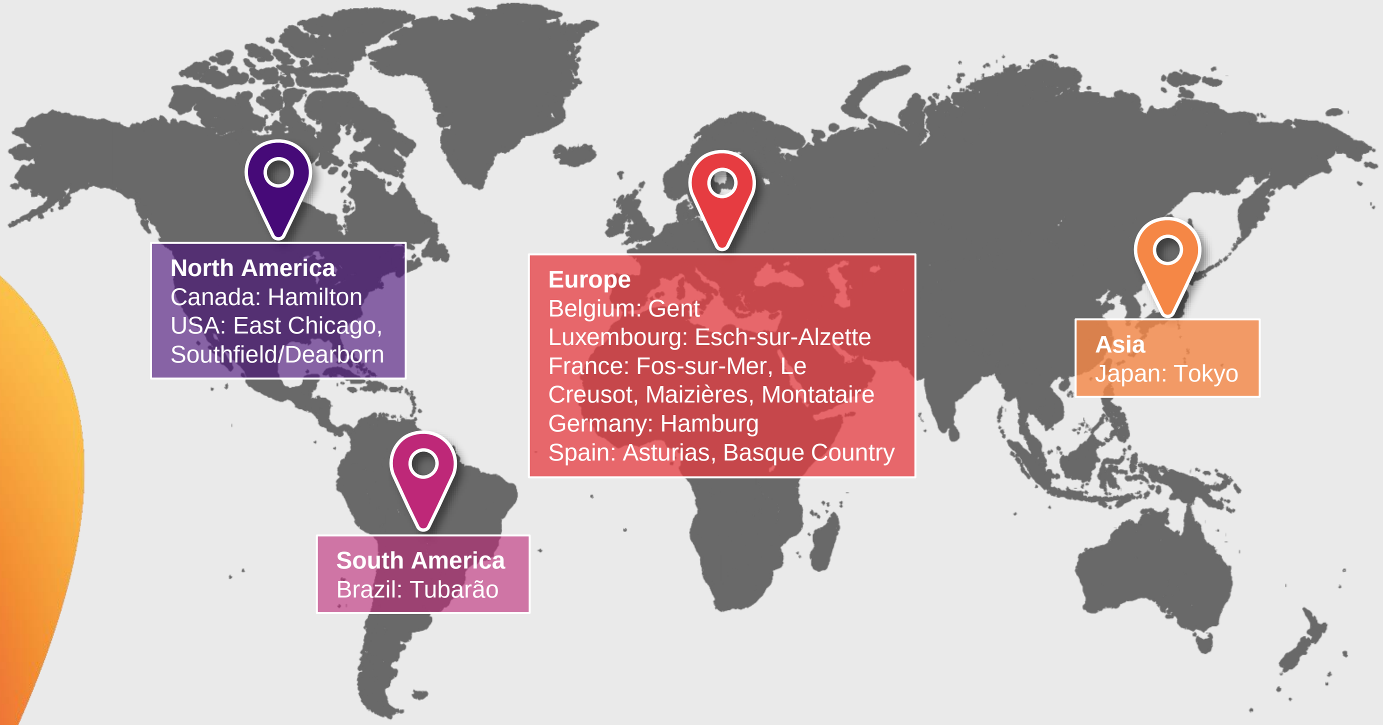
Global Research and Development
Where we are

Presence in 9 countries, 14 geographical sites, including:

- Research centres
- R&D units
- Product and Process deployment centres
- Co-engineering



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Maizières Campus

- ArcelorMittal's largest Research & Development site in the world
- A key asset in Global R&D's organisation

$52\,000\ m^2$

of offices, laboratories and pilot facilities

24

hectares

Maizières Campus | Organisation and staffing

Maizières Process

227

Maizières Products

267

Bars & Wires

52

Shared Services Unit

103

- **Shared Services**:
  78 out of 103 people in direct technical support to researchers: pilot facilities, engineering, machining, cutting, scientific computing.

- **Global R&D Central Team:**
  44 people in Portfolios, Sustainability, Intellectual Property, Quality Management, Controlling, IT, Human Resources, Communication

29/02/2024: 695 permanent - 16 non-permanent - 8 PhDs - 23 interns - 46 apprentices

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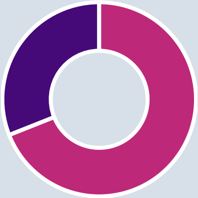
Maizières campus | Our people

695*
researchers

Engineers **48%** **Technicians** **52%**

Female **31%** **Male** **69%**



** 29/02/2024*

A mix of
experienced researchers
and young talented people
(Average age ~ 40)
37 nationalities on the campus

Graduates from the
best universities
and engineering schools

Working with other R&D centres
in result-driven projects
for further cross-fertilization

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Global R&D Research portfolios

Answering to the need of our customers

Products portfolio

- New Products
- Customer Support
- Generic Solutions
- Knowledge Building

Answering to the need of our operations

Process portfolio

Mining portfolio

- New Technologies
- Technical Assistance
- Standard Solutions
- Knowledge Building

Answering to the need our operations, business functions and R&D itself:

Digital portfolio overview

- Differentiating Algorithms
- Techno-economic Models
- Standard Solutions
- Knowledge Building

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Recent research partnerships with academia

- **Chaire Multimine :** Molecular interactions between gas, water and minerals during flotation of iron ore
- **Chaire Métal liquide** (Institut Jean Lamour): Chemical interactions in liquid metals
- **Chaire Solidification** (Institut Jean Lamour):
- **7 on-going CIFRE PhDs with** CEMEF, Georessources, Institut D'Alembert - Sorbonne Université, Technical University of Denmark, Institut Jean Lamour, SIMAP
- **2 on-going CAMEXIA** PhDs (regional initiative in the Grand Est region that aims to promote AI and Digital Skills with ENSAM & LEM3
- **GDR TRANSINTER II, GDR TAMARYS**
- **IFPRI consorsium:** International Fine Particle Research Institute
- **Under preparation**
  - MSCA Earth Project : Energy and Environmental Transition through Radiative Heat Transfer
  - MSCA Les Tenseurs et leur applications
  - PEPR SPLEEN: DEEP-MIN (DEcarbonizing Emissions in mineral and metallurgical Processes: Multi-scale Initiatives)

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Steel production and decarbonisation : A little bit of context

* European average

Two main routes to produce steel

From iron ore

Energy need: **18.7 GJ/ton**
CO_2 : **1808 kgCO2/ton**
71 % of the production worldwide

From scrap steel

Energy need: **6.7 GJ/ton**
CO_2 : **373 kg CO2/ton**
29 % of the production worldwide

→ Saves yearly 800 Mt of CO_2

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* European average

Two main routes to produce steel

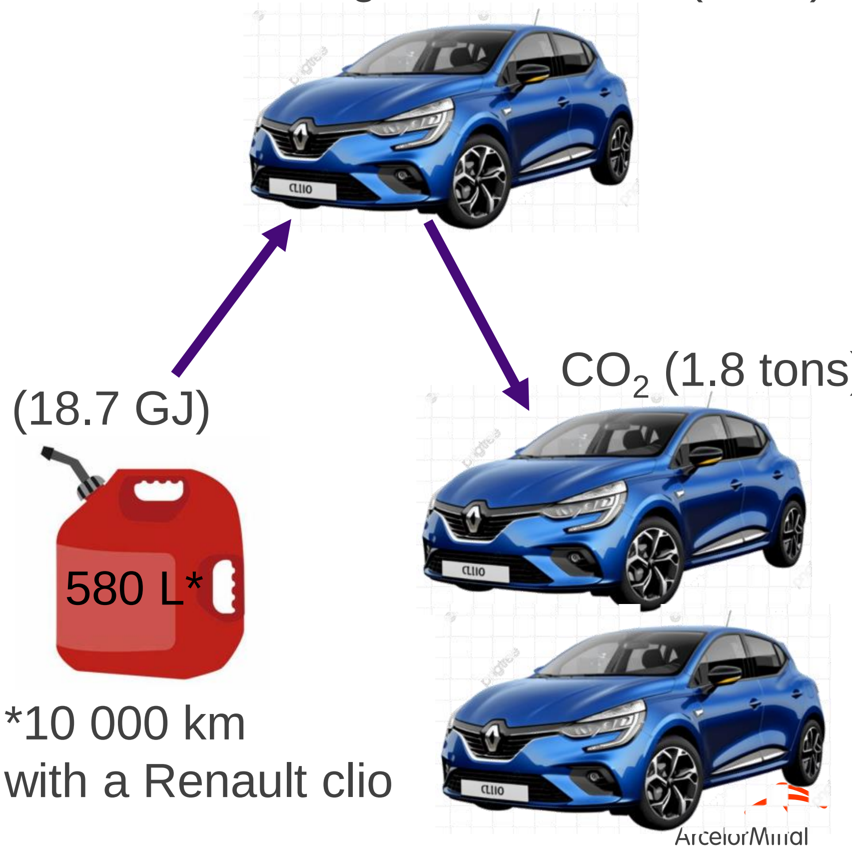
From iron ore

Energy need: **18.7 GJ/ton**
CO2 : **1808 kgCO2/ton**
71 % of the production worldwide

Producing 1 renault Clio (1 ton)

Energy (18.7 GJ)

CO_2 (1.8 tons)



*10 000 km
with a Renault clio

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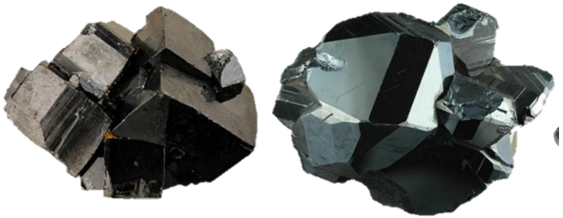
1 ton of steel → 2 tons of CO2 !

Iron Oxide



Coke
(Solid fuel that produces reducing gas : carbone monoxide)

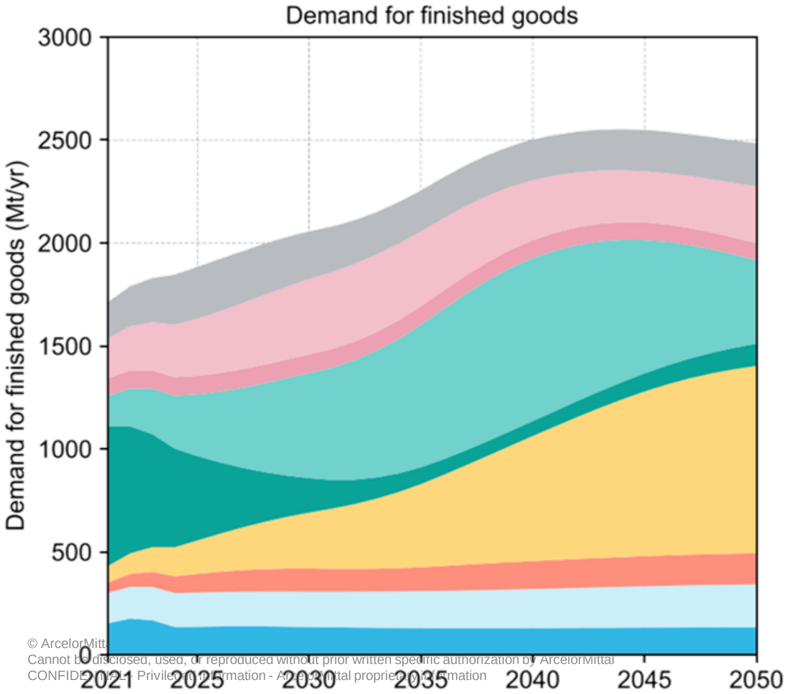
$$Fe_xO_y + CO \longrightarrow Fe + CO_2$$

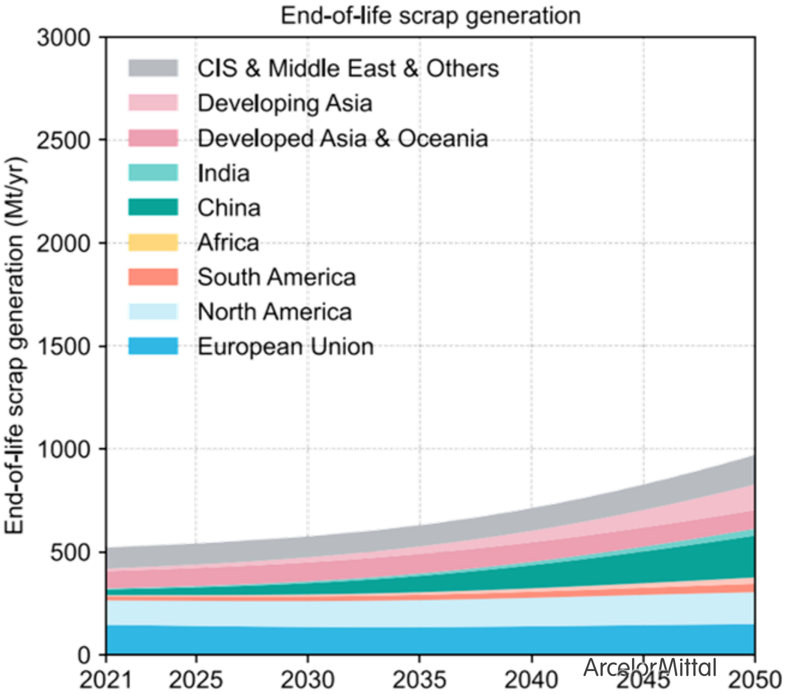
$$Fe_xO_y + H_2 \longrightarrow Fe + H_2O$$

Recycled Steel? Scrap availability vs steel production

Sources
T. Watari et al 2023
Wordsteel Association

Baseline scenario





Sources:
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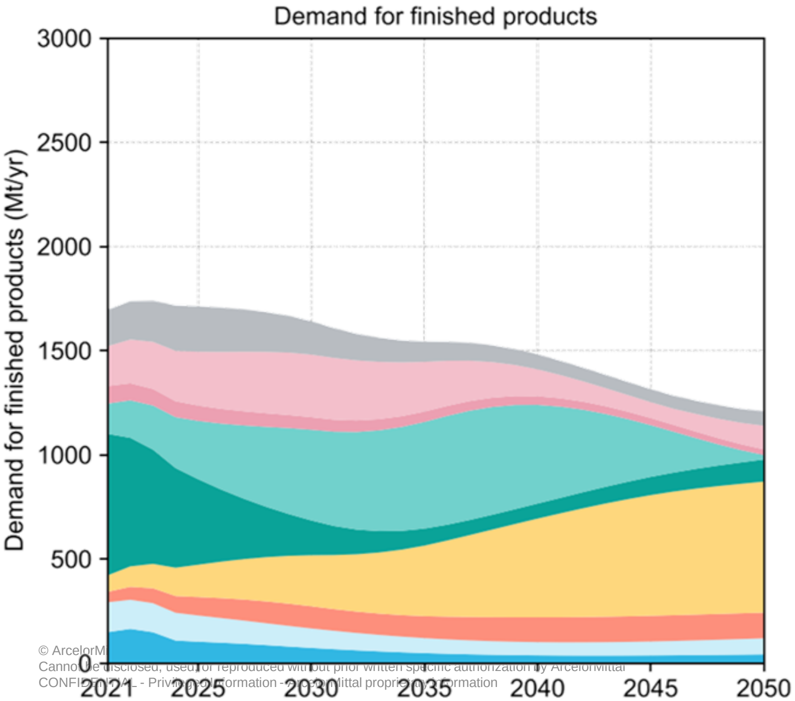
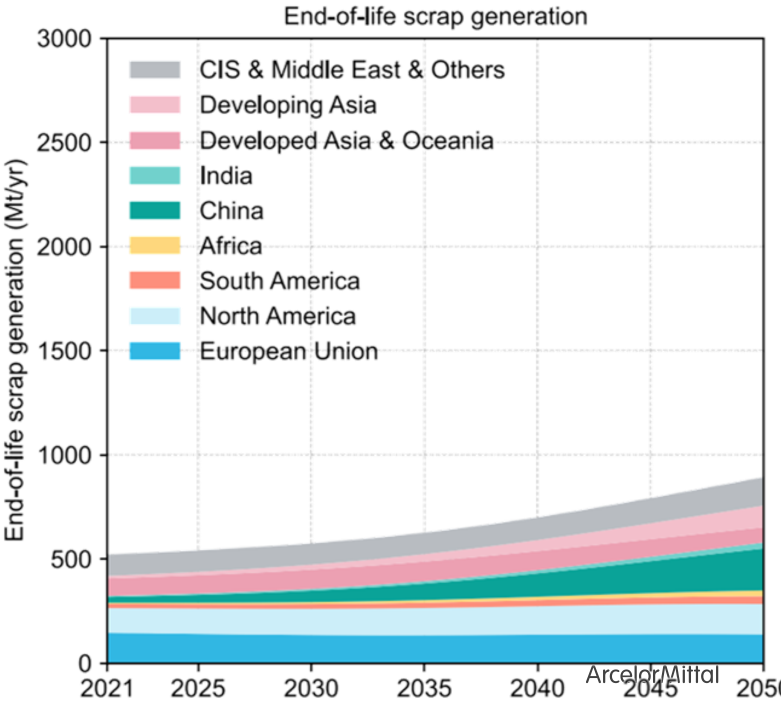
Wordsteel Association

Recycled Steel? Scrap availability vs steel production

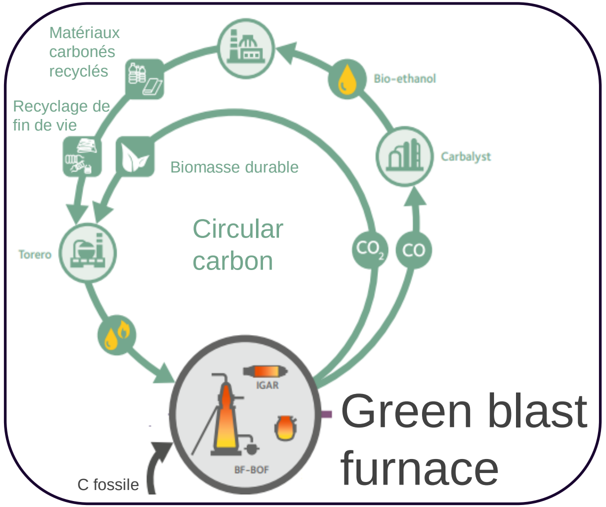
Material efficiency scenario

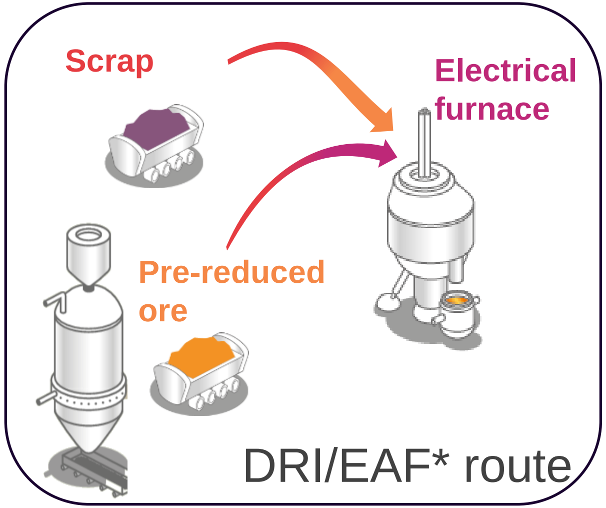


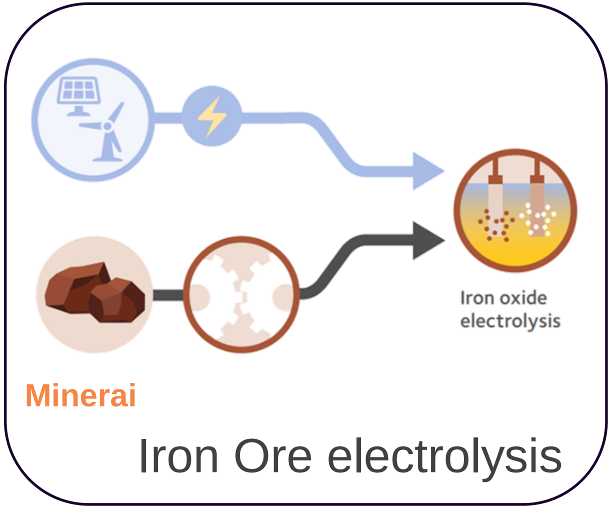


Steel production decarbonization

- Biosourced/Circular Carbon
- Hydrogen based reduction
- Electrification







*DRI/EAF = Direct Reduced Iron/ Electric Arc Furnace

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Challenges of the steel Industry

Slower-Than-Expected Hydrogen Transition Poses Challenges and Opportunities

September 16, 2024 | 0 | By ANGIE BERGENSON

Green hydrogen: Short-term scarcity, long-term uncertainty

However, historic analogues suggest that emergency-like policy measures could foster substantially higher growth rates

Date: September 8, 2022

Source: Potsdam Institute for Climate Impact Research (PIK)

L'Europe montre les dents pour sauver la production d'acier sur son sol

Ce contenu est réservé aux abonnés

La Commission européenne prend un virage protectionniste assumé, et compte réduire les importations d'acier sur son sol. Le commissaire européen Stéphane Séjourné détaille son plan, qui consiste aussi à taxer les exportations de déchets d'acier.

Steel and Metals Action Plan unveiled

Published 21st March, 2025 by Matthew Moggridge

The Steel and Metals Action Plan, unveiled today by the European Commission on Wednesday 19 March, provides the right diagnosis to the existential challenges facing the European steel industry, according to the European Steel Association (EUROFER).

Tarifs imposés le 2 avril par Trump: certains secteurs pourraient être exclus

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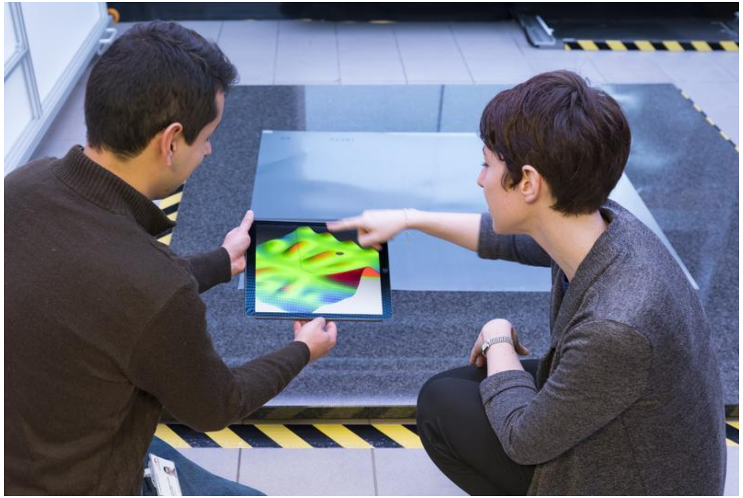
Scientific ! Challenges of the steel Industry

Some of the



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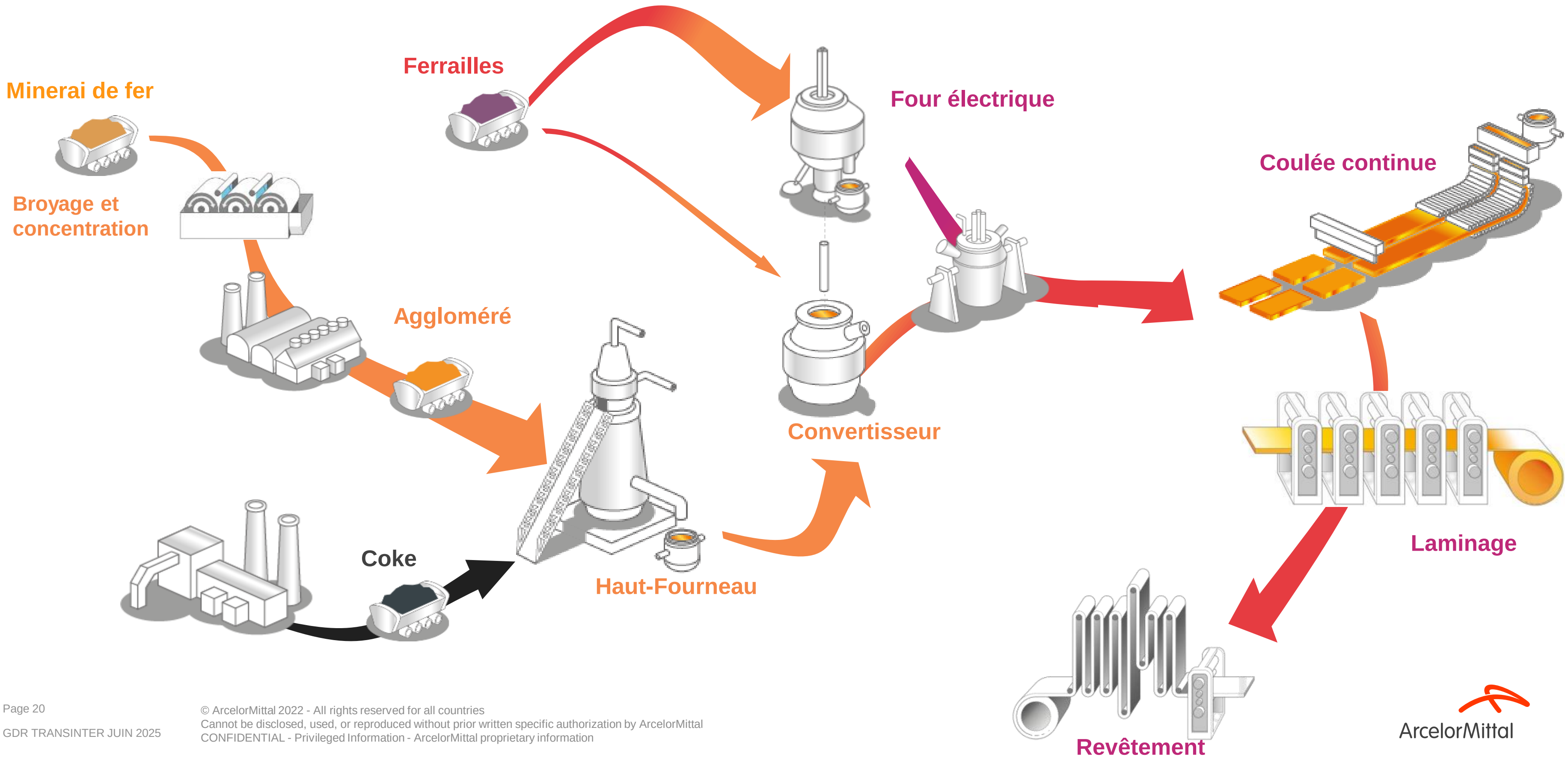
Les challenges industriels et thématiques de recherches
Décarbonation, différentiation produit et digitalisation



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Les challenges industriels et thématiques de recherches
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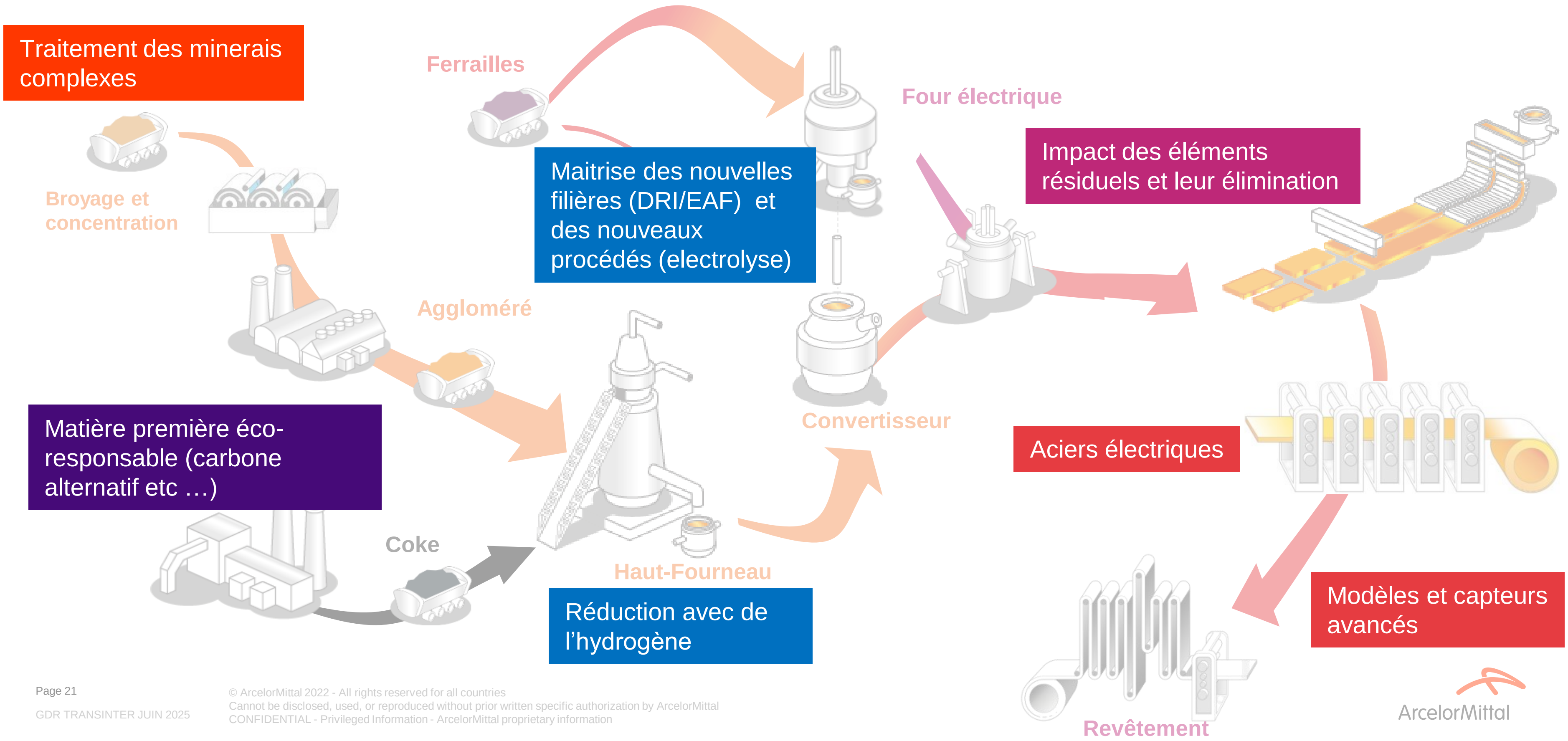

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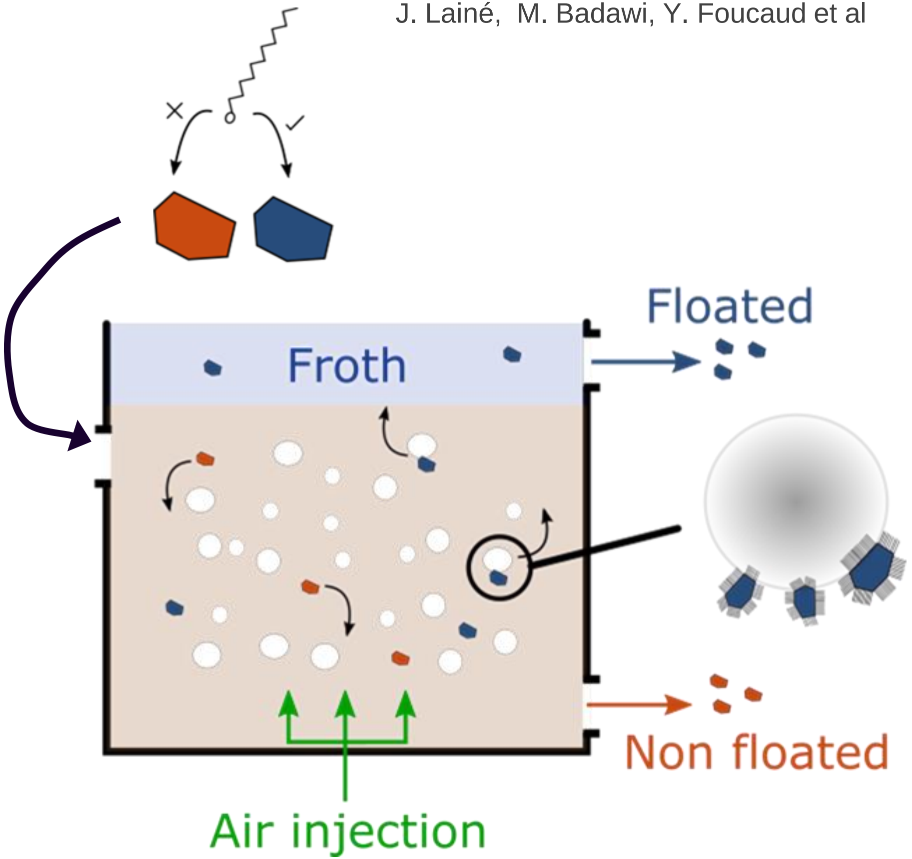
Flotation : the basics

- Flotation is becoming crucial for ore beneficiation
  - Need for better quality (for DRI*: $SiO_2 + Al_2O_3 < 3$ %)
  - More complex ores : decrease of quality + finer liberation sizes + gangue complexity
- Separation based on contrast of wettability of mineral surfaces:
  - Hydrophobic particles are carried by bubbles upwards
  - Hydrophilic particles do not attach to air bubbles and sink to the bottom
- Addition of selective reagents to modify surface properties
  - Collectors (amines): render particles hydrophobic (quartz)
  - Depressants (starch): render particles hydrophilic (iron oxide)



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Flotation performance

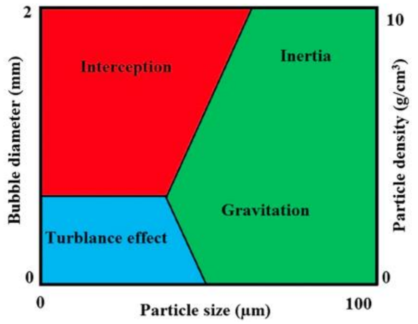
$$\frac{dN_p}{dt} = -\mathbf{k}.N_p = -\frac{3\,Q\,h_{cell}\,P_{collection}}{2\,d_{bubble}\,V_{cell}}N_p$$

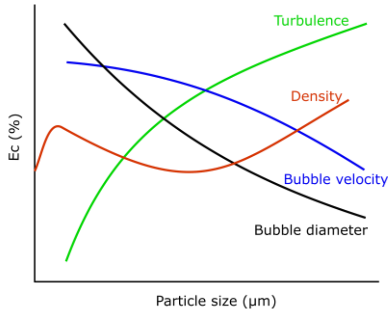
$$P_{collection} = P_{collision}\;P_{attachment}\,(1 - P_{detachment})$$

Hydrodynamics and interaction with turbulence

Physico-chemical surface reactions

Turbulence shearing and gravity





Effect of turbulence, density, bubble velocity, bubble diameter on particle/bubble encounter
Source: A. Hassanzadeh, M. Firouzi, B. Albijanic, M. Celik, 2018

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Flotation: Overview of modelling approaches

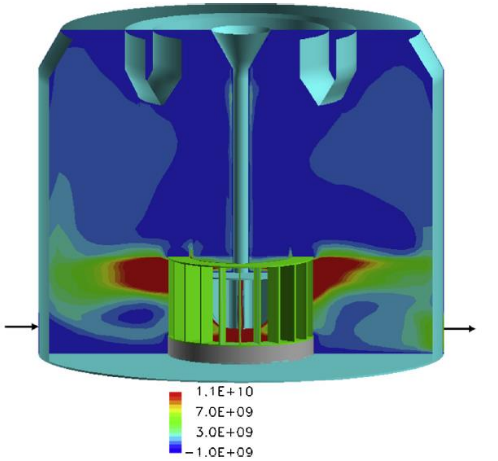
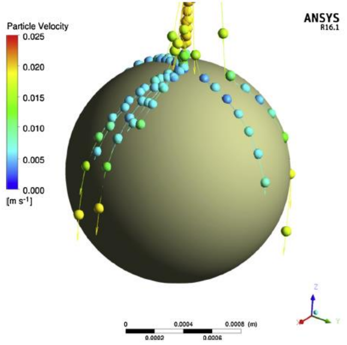
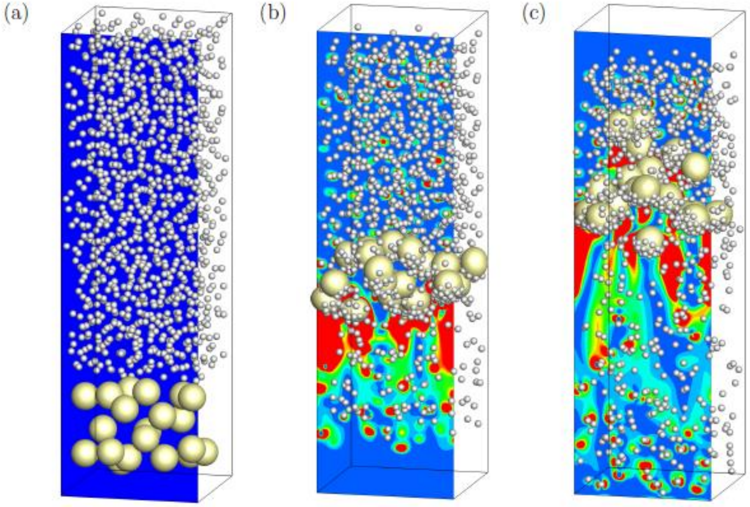


Fig. 3. Net attachment rate predicted by CFD model of an OK 150 type cell, operating at 106 rpm. The scale indicates number per m^3 per sec.





Peter Koh, Michael P. Schwarz et al

Lei Zeng, Jiacai Lu, and Grétar Tryggvason 2025

J. Lainé, M. Badawi, Y. Foucaud et al

Chaire Multmimine
A 5 year industrial chair to study molecular interactions at mineral surface during flotation

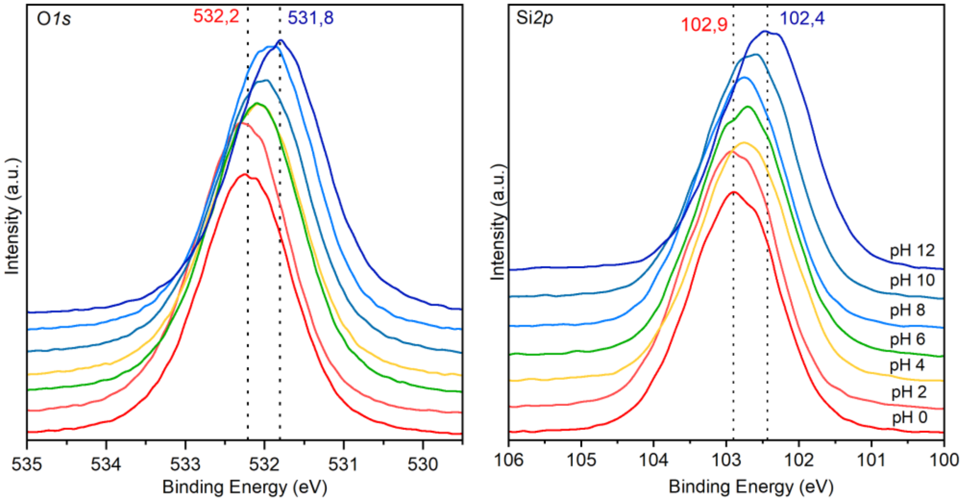
- A multi-scale approach of flotation, from quantum chemistry to machine-learning modelling of molecular interactions, passing by adsorption, flotation, and surface analysis experiments, to finally get the most realistic models of molecular interactions at mineral surface, i.e., with water and flotation reagents, and suggest innovating approaches for mineral extraction accordingly

- Objectives
  - Understand the interaction between mineral surfaces, water, and flotation reagents.
  - Enhance the flotation technics with scientific approaches of surface chemistry to understand the stabilization of the adsorption layer in different experimental conditions.
  - Allow the beneficiation of complex, depleted iron ores in the context of increasing demand on steel and a lower quality of iron ore
  - Reinforce the scientific leadership of University of Lorraine in mineral processing and in surface chemistry of froth flotation
  - Maintain a high-level of formation and employment in this domain in the Grand-Est region, providing ArcelorMittal new possibilities in terms of recruitment

J. Lainé, M. Badawi, Y. Foucaud et al

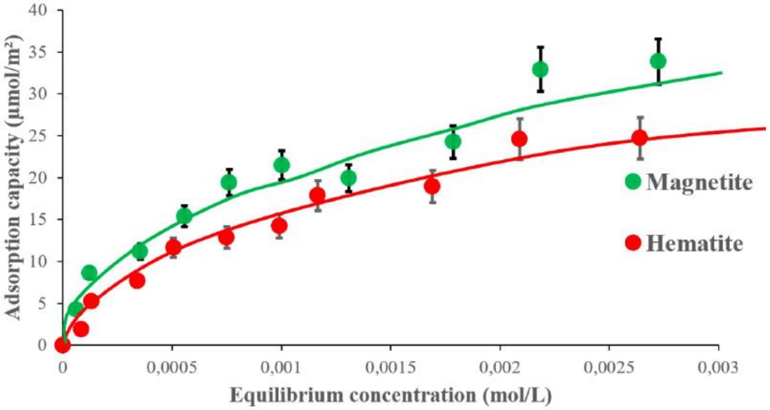
Flotation: adsorption mechanisms and interactions with mineral surfaces

Experimental caractersation of mineral surfaces by XPS, DRIFTS and titration



O1s and Si2p XPS spectra of quartz samples treated to different pH conditions (O. Gamba, M. Badawi et al, 2025)

Understanding interactions between reageant and minerals



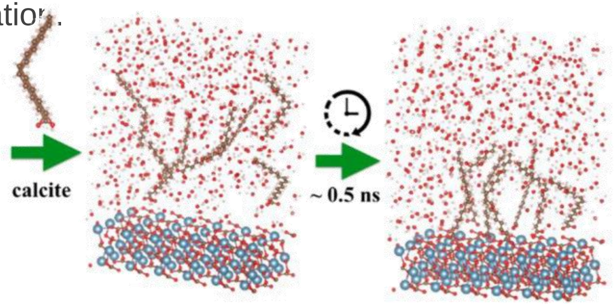
Adsorption of depressants by iron oxides (J-W Hounfodji, M. Badawi et al, 2025)

Flotation: Machine learning Force Field a cutting edge description of mineral-water interfaces

MULTIMINE
APPROCHES MULTI-ÉCHELLES POUR LA SÉPARATION DES MINÉRAUX

- Development of an efficient numerical method for modeling mineral interfaces and their surface reactivity: Artificial intelligence coupled with molecular modeling and possible applications in flotation.

- Machine Learning ForceFields (MLFF)
  - Machine learning force fields (MLFF) based on AIMD (Ab Initio Molecular Dynamics)
  - Reduce computation times by 100
  - Possible to manage large molecules



A first attempt at modeling the adsorption of the collector on mineral surface

THE JOURNAL OF PHYSICAL CHEMISTRY C

pubs.acs.org/JPCC Article

Machine Learning Force Field beyond the Limits of Classical and First-Principles Molecular Dynamics Simulations: The Case of Kaolinite Hydration

David Dell'Angelo,* Juliette Lainé, Halima Said, Yann Foucaud,* and Michael Badawi*

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journal homepage: www.elsevier.com/locate/mineng

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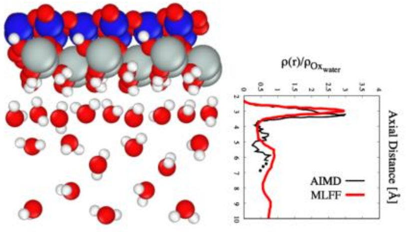
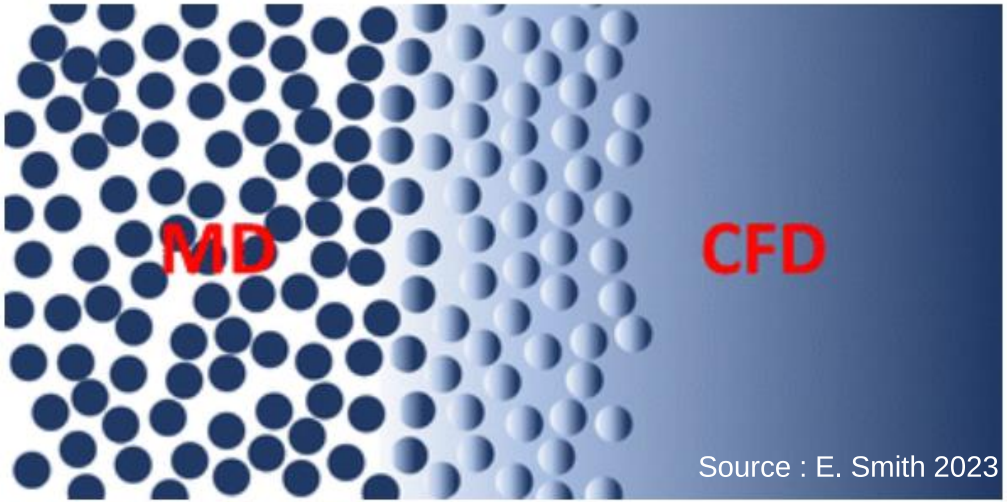
Enhanced Machine Learning Molecular Simulations for optimization of flotation selectivity: A perspective paper

D. Dell'Angelo[a], Y. Foucaud[b], J. Mesquita[c], J. Lainé[c], H. Turrer[c], M. Badawi[a,*]



Water layering snapshot at the kaolinite slab using both AIMD and MLFF techniques

Flotation: future work



Combining ML-AIMD simulations (atomic and particle scales) with CFD (process scale)

Instrumentation of pilot scale flotation cells

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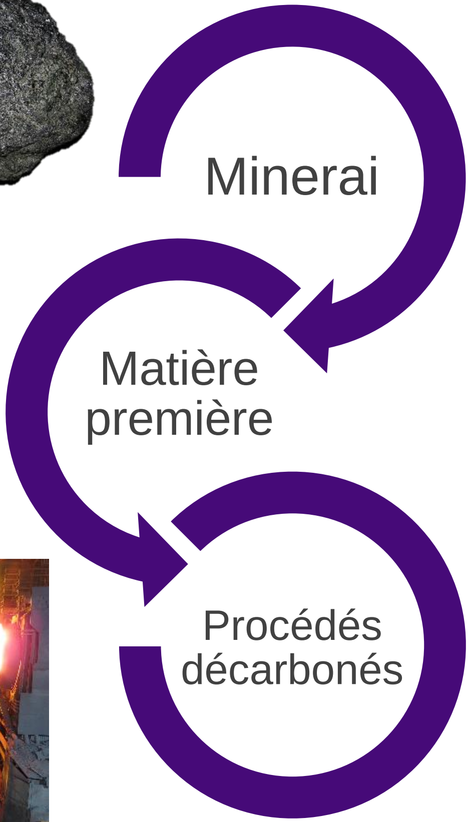
Les enjeux de la décarbonation de l’acier



- La décarbonation de l’industrie sidérurgique nécessite une adaptions importante des procédés voire la création de nouveaux procédés.

- La qualité et les propriétés du minerai de fer impacte fortement les procédés de production de la matière première (pellets de DRI ou le rendement faradique dans l’électrolyse) En aval, le fonctionnement des procédés métallurgiques et la réussite des filières décarbonées dépend fortement de la qualité de cette matière première.

- En parallèle, il est important d’optimiser les procédés de préparation de la matière première pour réduire leur impact environnemental, leur consommation d’énergie et les résidus des transformations.

- Plusieurs questions fondamentales se posent concernant des mécanismes élémentaires à l’échelle du grain (minerai, pellet, briquette)
  - Interactions solide/gas, solide/liquide
  - Physico-chimie aux interfaces
  - Transferts de chaleurs et de masse
  - Thermodynamique et réactions chimiques
  - Comportement mécanique

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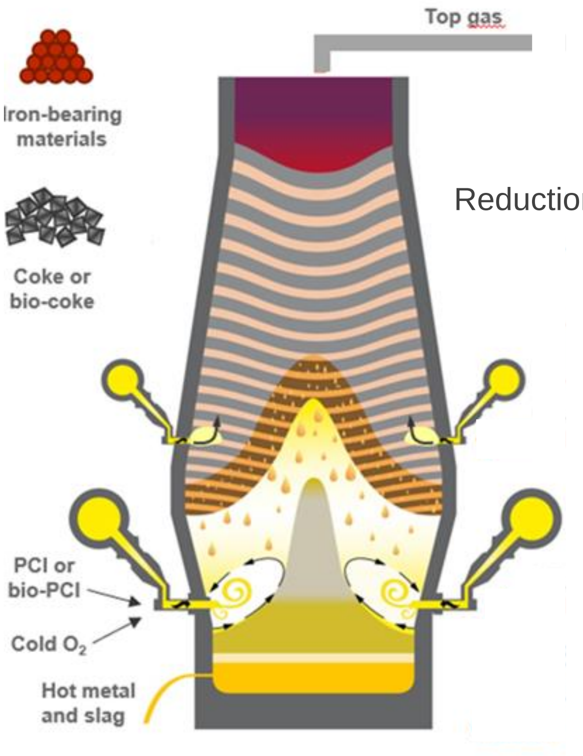
Reactive solid-gas flows in Blast Furnace (BF) and Direct Reduction Process (DRP)

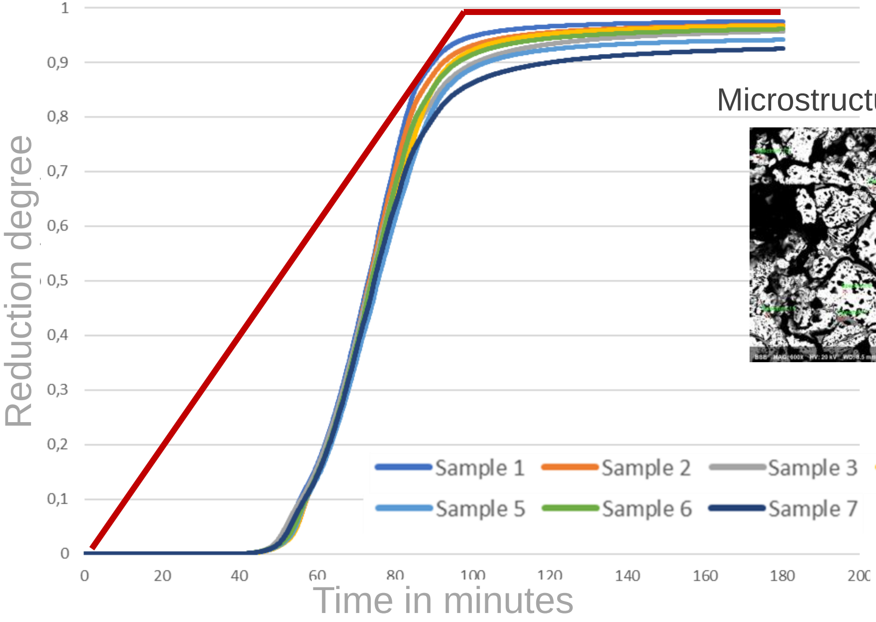


Reduction zone

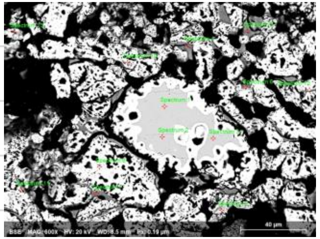
$Fe_2O_3 \rightarrow Fe_3O_4 \rightarrow FeO \rightarrow Fe$

Reduction behavior of pellets is affected by the presence of gangue materials

Silica can react with wustite and form an olivine phase with the composition Fe2SiO4 which will be very difficult to reduce (Y. Graz et al 2023)



Microstructure of sample 5



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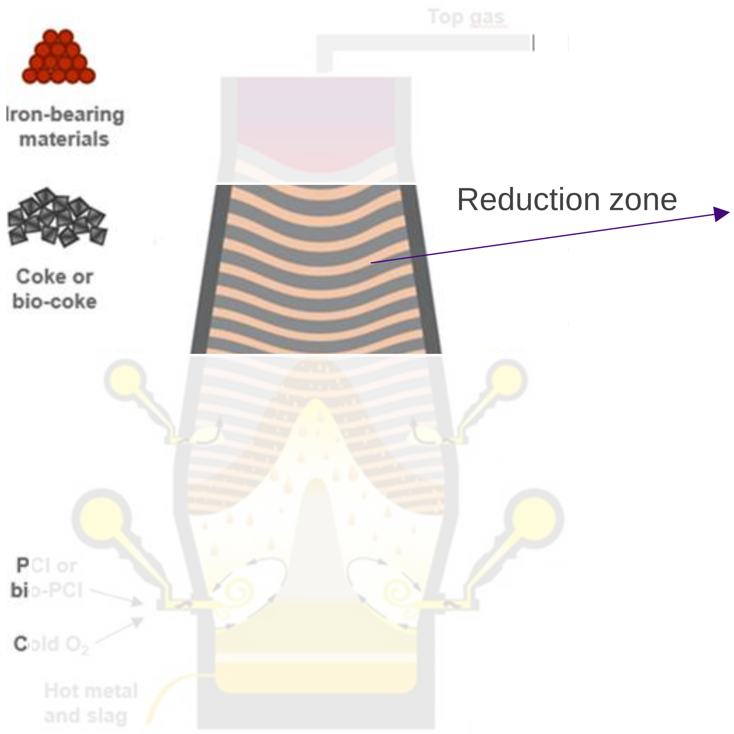

$Fe_2O_3 \rightarrow Fe_3O_4 \rightarrow FeO \rightarrow Fe$

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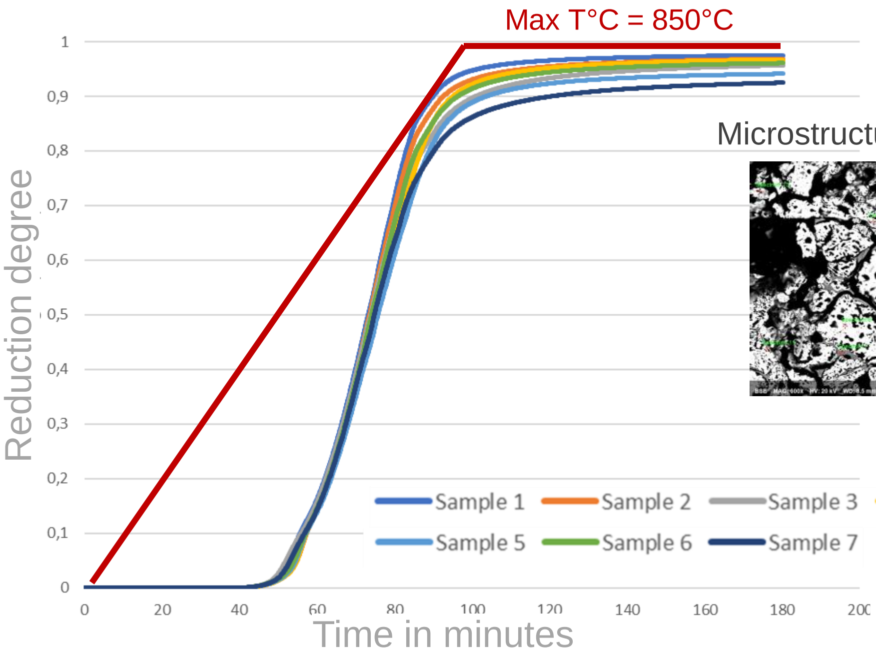
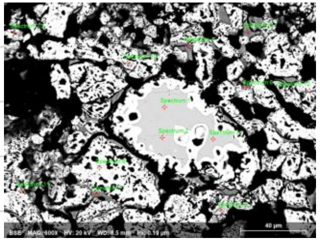


Microstructure of sample 5



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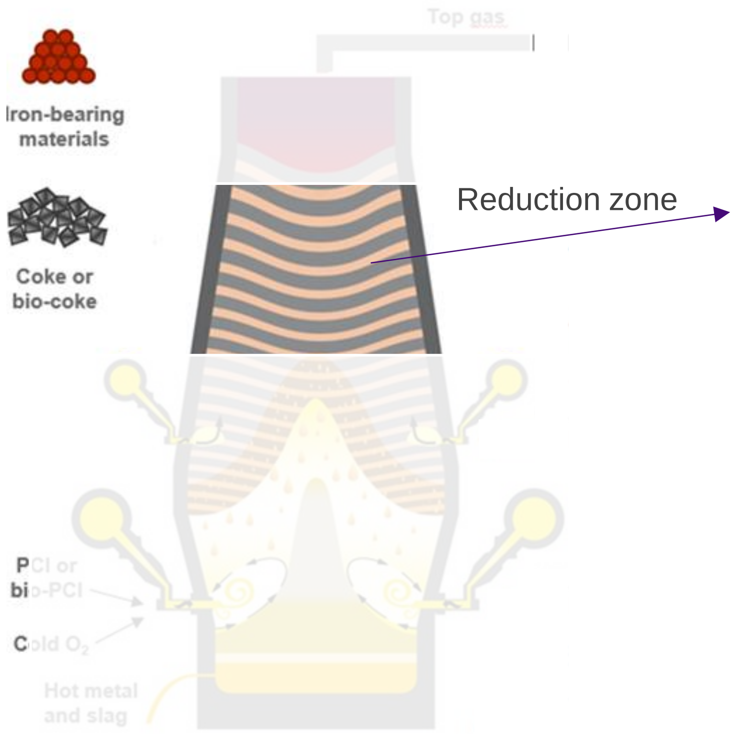
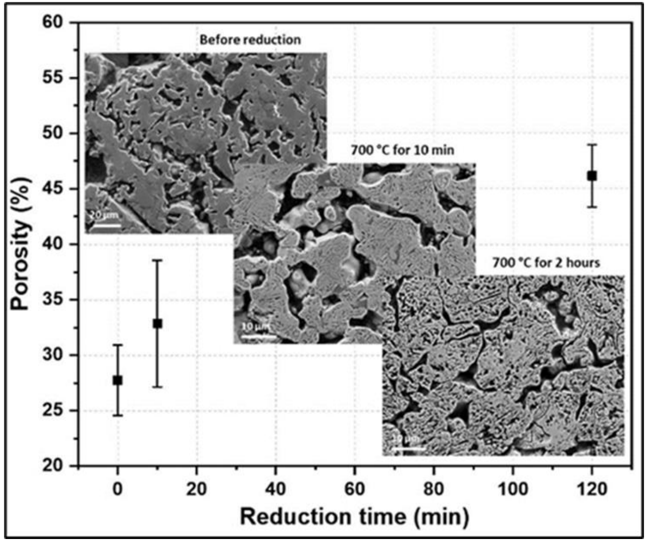
Reactive solid-gas flows in Blast Furnace (BF) and Direct Reduction Process (DRP)



$Fe_2O_3 \rightarrow Fe_3O_4 \rightarrow FeO \rightarrow Fe$

Reduction phenomenon also generates new porosities, because the ferrous phases transform and change shapes and volumes.



Porosity evolution during reduction (Kim et al., 2021)

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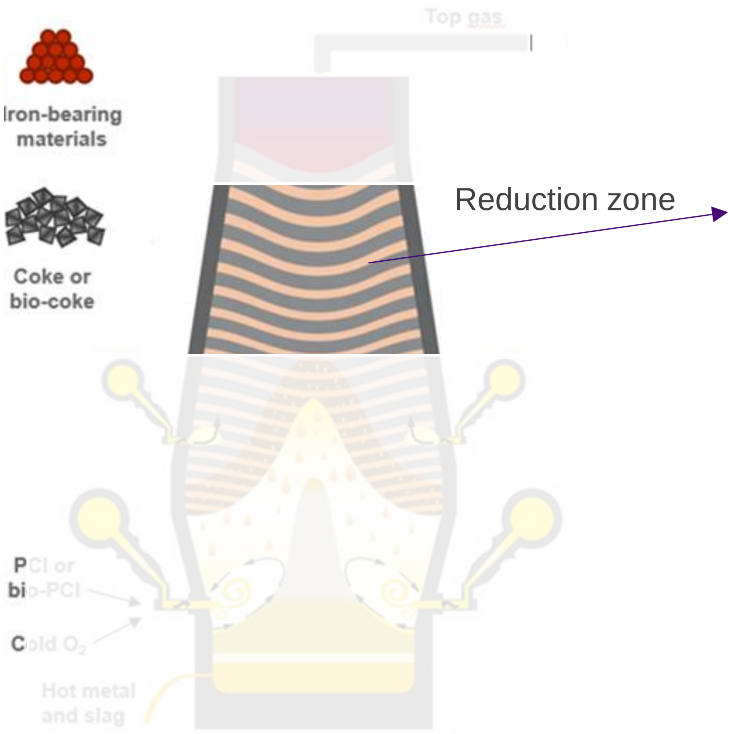
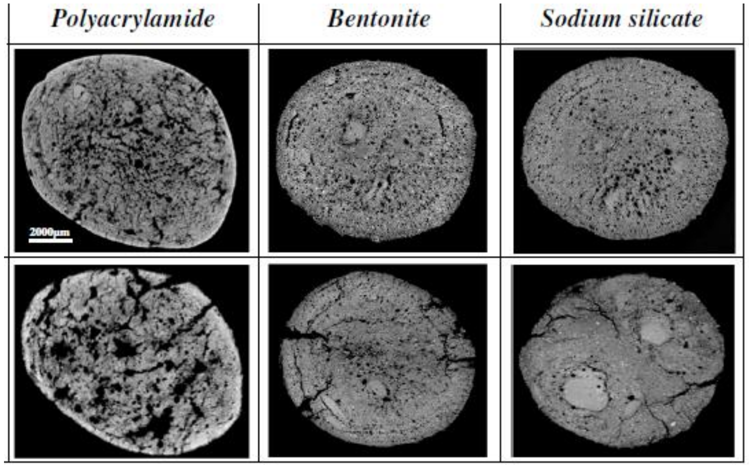
Reactive solid-gas flows in Blast Furnace (BF) and Direct Reduction Process (DRP)



Pelletizing impact: Bentonite offers the best compromise (mechanical strength and porosity to ensure effective reduction vs dust-related issues observed with organic binders) [1]

Unreduced pellet

Reduced pellet



[1] Ben Hassine, Mirgaux, Quatravaux, Graz, Effect of Binder Type on the Reducibility, Microstructure, and Mechanical Properties of Iron Ore Pellets under a High-Hydrogen Atmosphere, *Métallurgie quel avenir*, 2025

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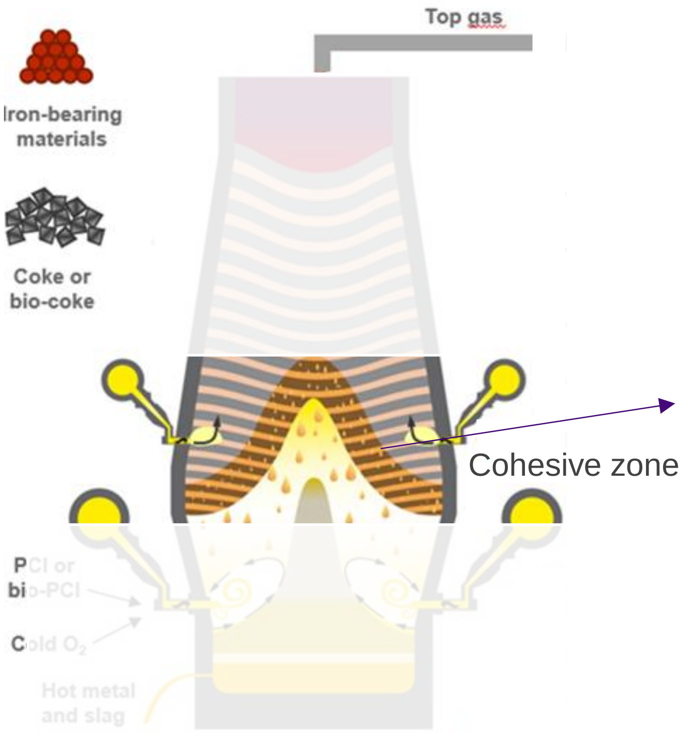


Acid Pellet :

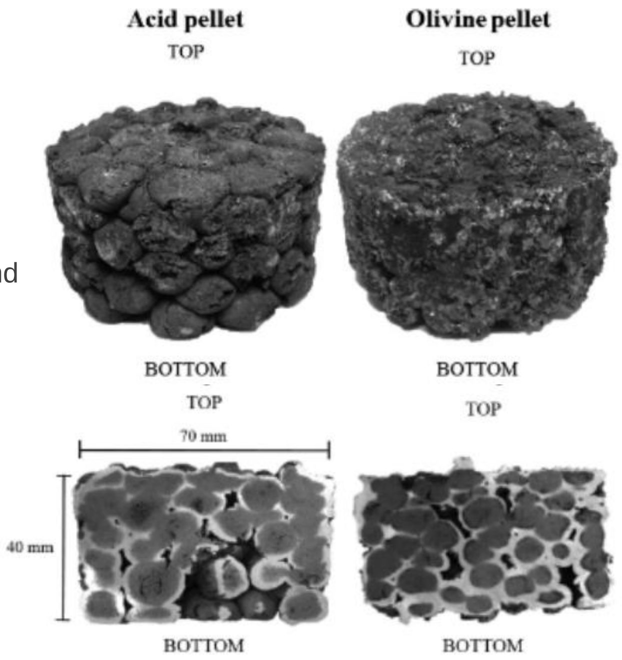
High degree of metalization

High softening and deformation

High quantity of FeO rich SLAG

Permeability loss

High direct reduction of FeO



Basic pellet :

Higher degree of metalization

Lower softening and deformation

Lower quantity of FeO rich SLAG

Higher Permeability

Lower direct reduction of FeO

Llana, Kemppainen et al, Evaluating the Reduction-Softening Behaviour of Blast Furnace Burden with an Advanced Test, *ISIJ International, 2016*

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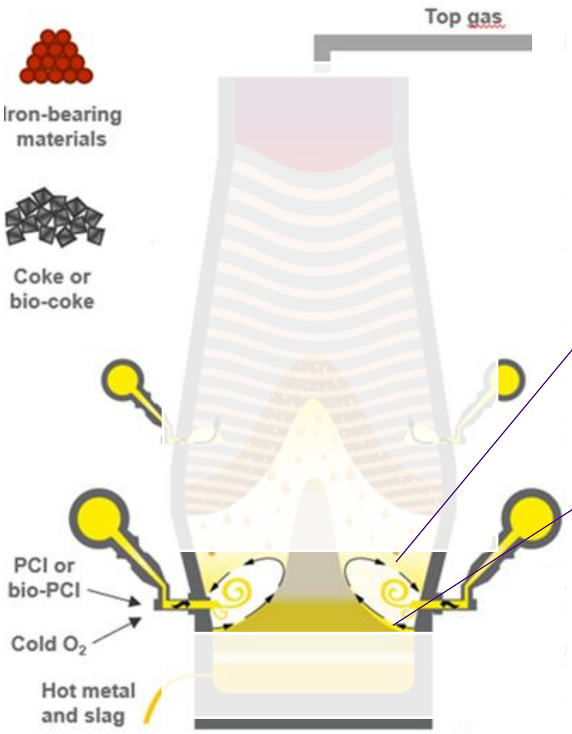
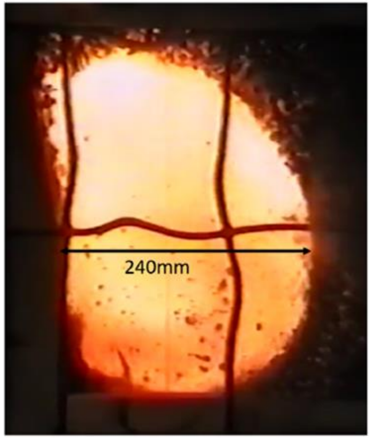
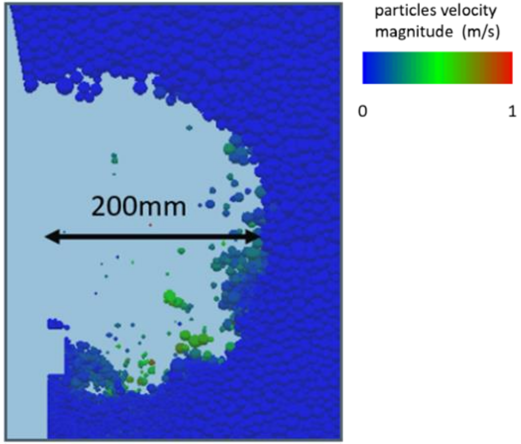
Reactive solid-gas flows in Blast Furnace (BF) and Direct Reduction Process (DRP)



Simulation of a hot pilot-scale BF [1]





CFD/DEM modelling represents well raceway dynamics when cohesion forces due to the softening of particles are added.

[1] Romano, Izard, Fede, Mechanical Analysis of the Forces Involved in a Pilot-Scale Blast Furnace Raceway Formation by Means of CFD/DEM Simulations, *Processes* 12 (2024) 637

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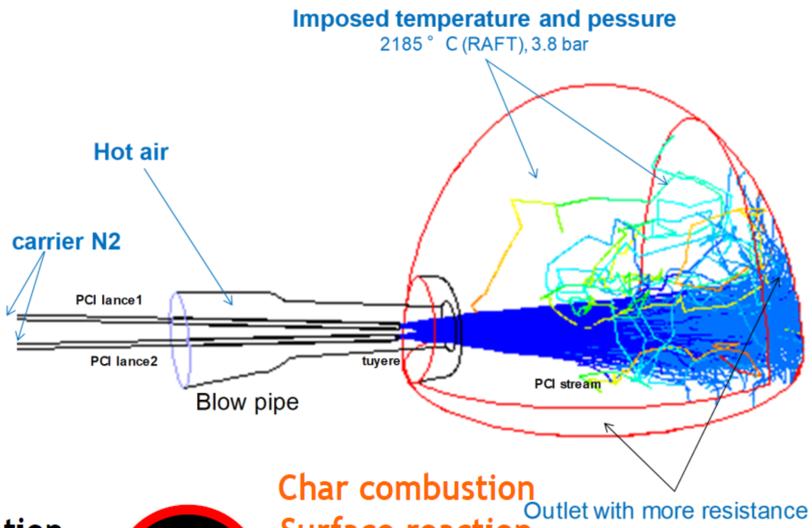
Reactive solid-gas flows in Blast Furnace and DR shaft

Coal combustion in BF raceway :
A coupled problem including: Radation, turbulent fluid flow, particle tracking, solid/gas reactions and gaseous combustion



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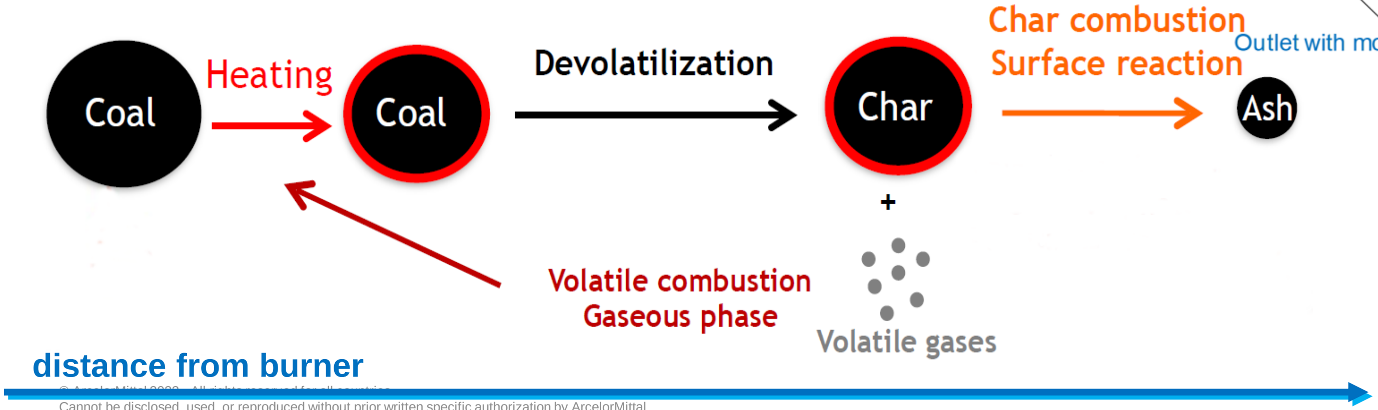

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Coal combustion in BF raceway

Two competing rates model for Devolatilisation

Coal → α_1 volatiles$_1$ + $(1-\alpha_1)$char$_1$ (low temperatures)
Coal → α_2 volatiles$_2$ + $(1-\alpha_2)$char$_2$ (high temperatures)

$$\frac{dv}{dt} = (K_1 Y_1 + K_2 Y_2) C_0 \qquad K_1 = A_1 exp\left(\frac{-E_1}{RT_p}\right)$$

Kinetic & diffusion rate model for coal

Surface reation	Relative rate	Reaction Enthalpy
$C + CO_2 \rightarrow 2CO$	1	173.04
$C + H_2O \rightarrow CO + H_2$	3	131.88
$C + 2H_2 \rightarrow CH_4$	$3x10^{-3}$	-75.18
$C + O_2 \rightarrow CO_2$	10^5	-395.22

Endothermic reactions

Exothermic reactions

Gaseous combustion

Eddy Dissipation Model **(chemical reaction rates are controlled by the rate of turbulent mixing)**

$Vol + O_2 \rightarrow xCO + yCO_2 + zH_2O + wN_2$
$CO + 1/2\ O_2 \rightarrow CO_2$
$H_2 + ½\ O_2 \rightarrow H_2O$ (COG)
$CH_4 + 2\ O_2 \rightarrow CO_2 + 2\ H_2O$ (NG)

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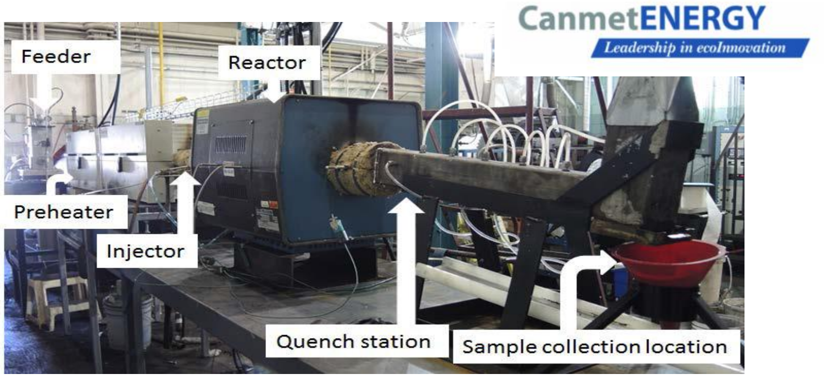
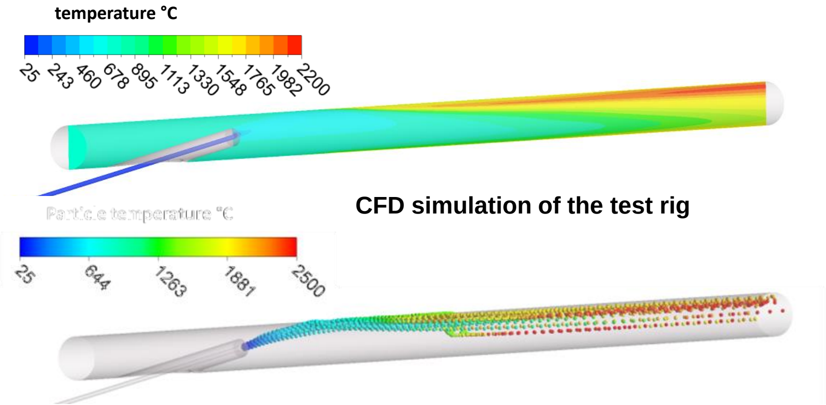
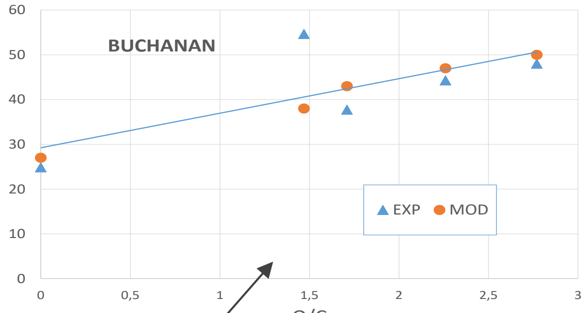
Coal combustion model validation

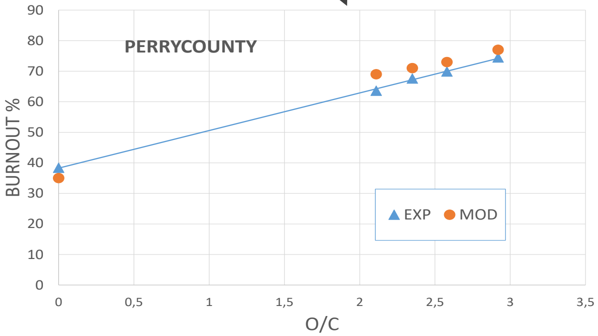




CFD simulation of the test rig



Measured vs calculated burnout
for a **low** and **high** volatile coal



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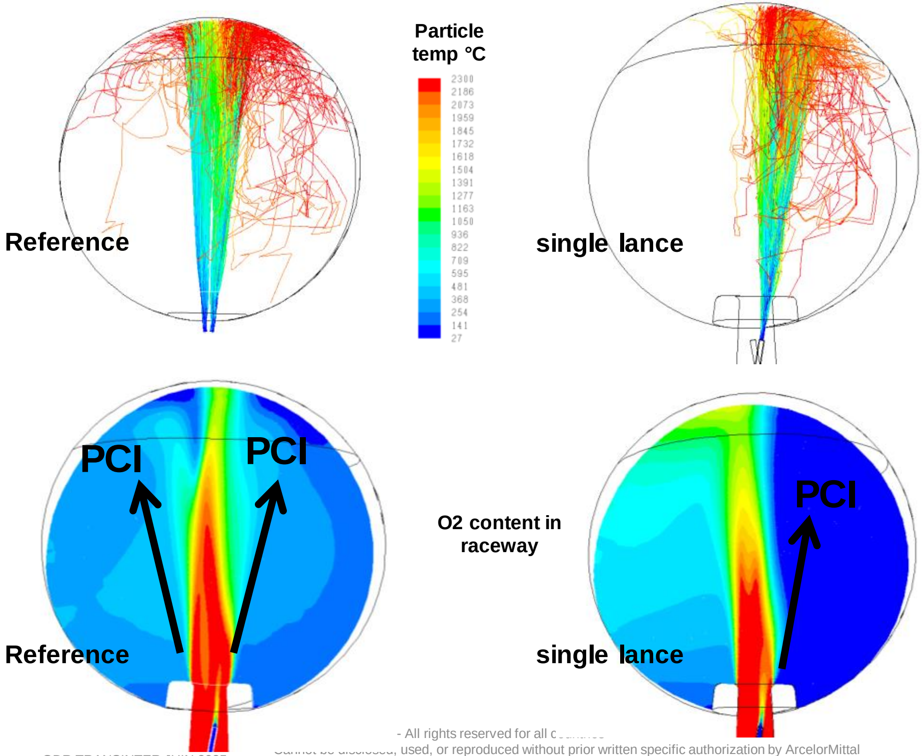
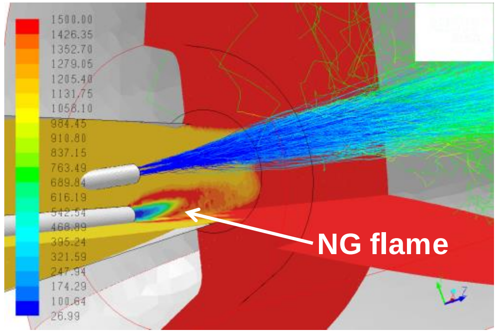
Coal combustion model results

Double vs Single Lance

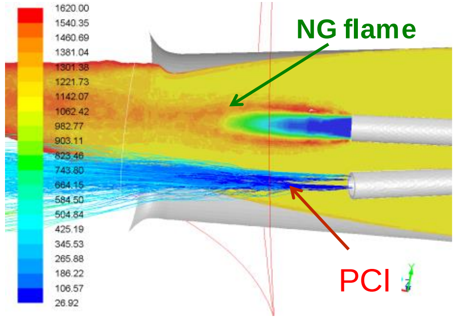


Where to position NG lance ?

NG at bottom lance



NG at top lance



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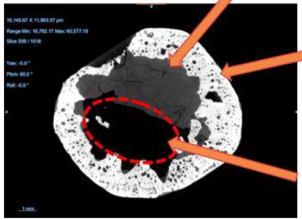
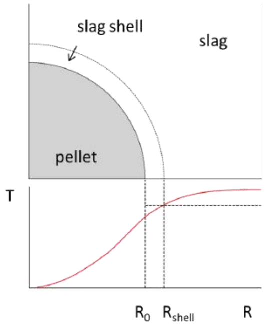
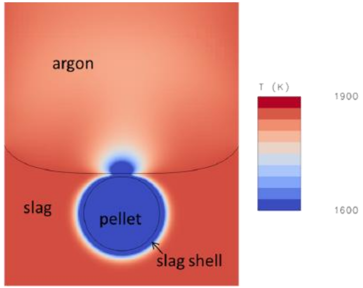
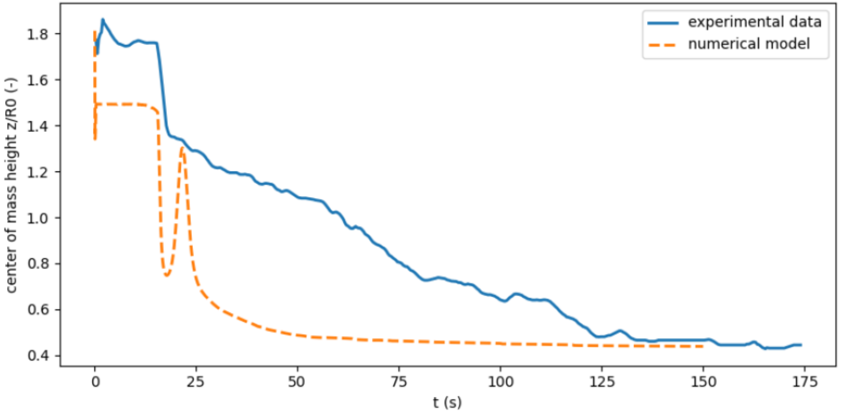
Melting of a DRI pellet in slag

- Industrial context:
  - Existing and new porous materials are under study: H-DRI, C-DRI, HBI with iron ore and alternative carbon → To provide iron source for new decarbonized steelmaking routes,
  - It is important to understand and predict the melting of these materials in slag and how the reactions play a role.
  - A comprehensive model will help to optimize the relevant particle properties and process parameters.









Simulations done in Basilisk ; a DNS code using dynamic adaptive mesh refinement following a quad/octree structure

J. Robin, S. Zaleski, E. Izard 2025

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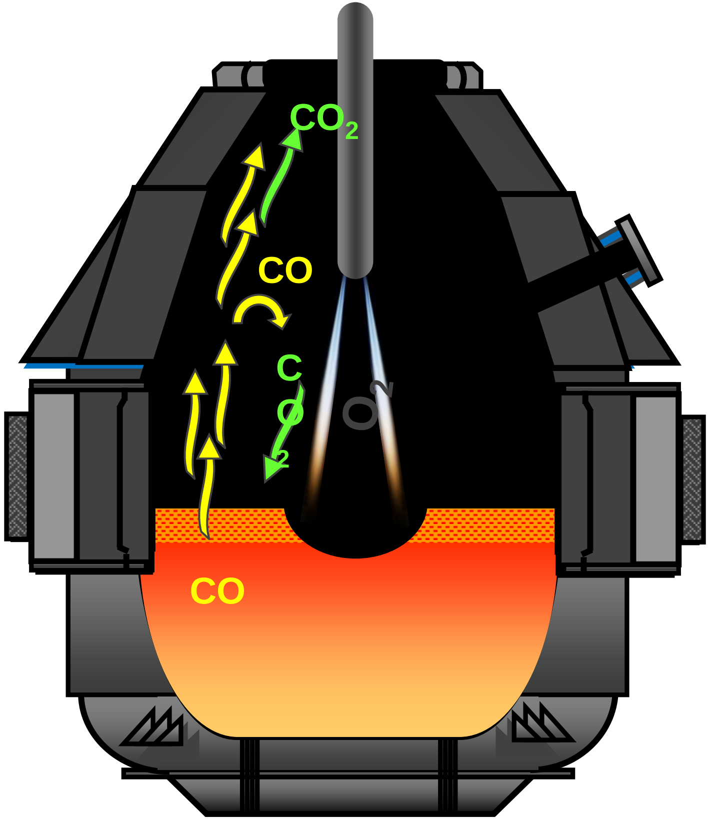
Modélisation multiphasique des réacteurs métallurgiques



Post combustion ratio:

$$\frac{\%CO_2}{\%CO+\%CO_2} \approx 8-11\%$$

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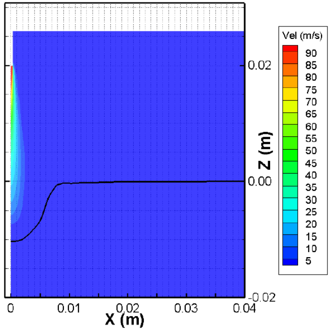
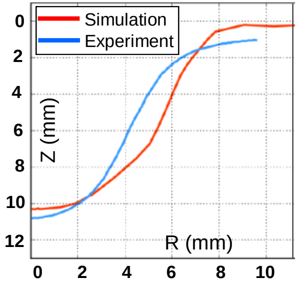
Modélisation multiphasique des réacteurs métallurgiques

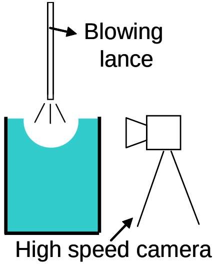
BOF Hydrodynamic model

Interaction between the supersonic jet and the free surface to predict cavity shape and depth

Source: Y. Doh et al 2008



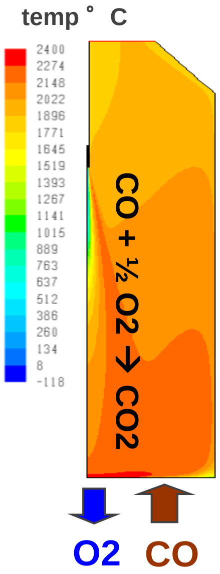


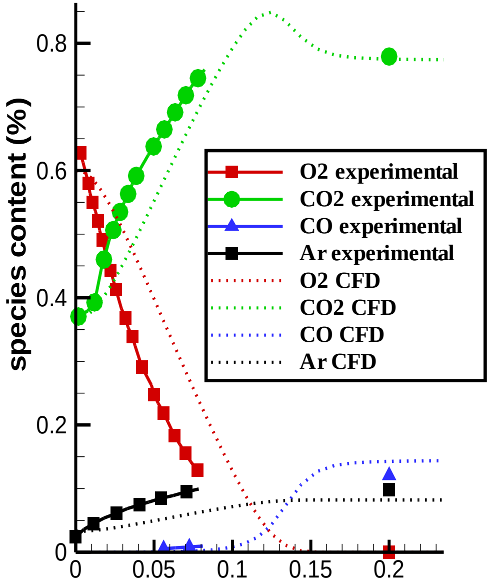


Top space model

Aerodynamics, post-combustion and heat transfer in top space

Simulation of the 6 ton pilot





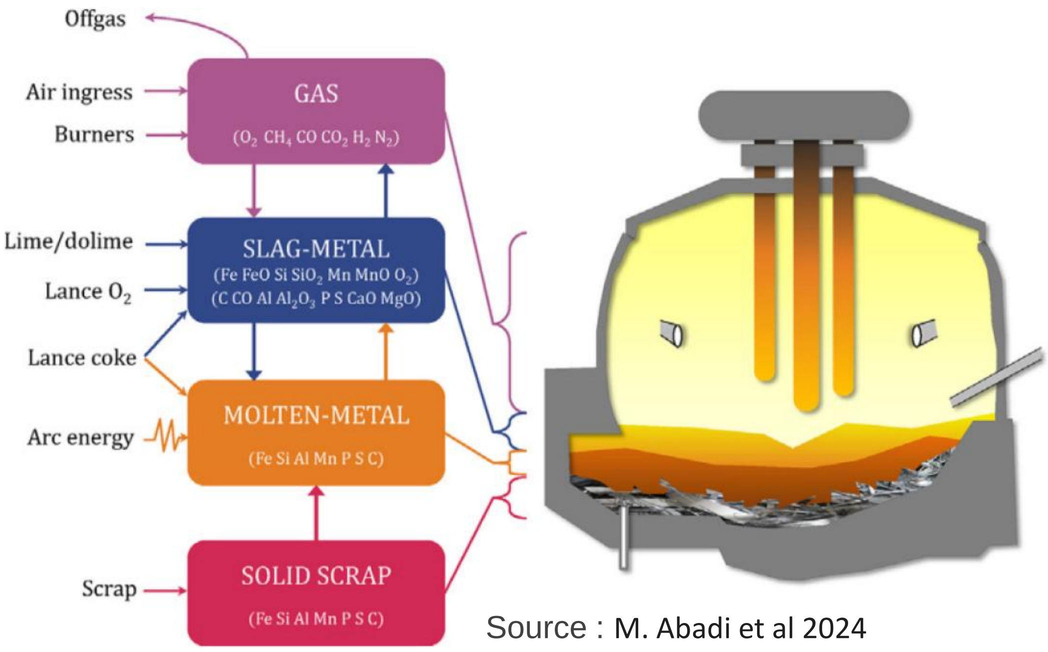
Species mole fraction along a radial direction (z = 1.5 m)

Source: G. Ghazal 2012

Future work
Modelling Liquid metal stirring in EAF (Electric Arc Furnace)

- EAF plays major role in the decarbonization, and recycling scraps is an integral part of the circular economy

- Two main challenges related to the design and operations of these new EAF
  - Higher capacities and possible difficulties to homogenize the melt
  - Additional power required for DRI melting



Source : M. Abadi et al 2024

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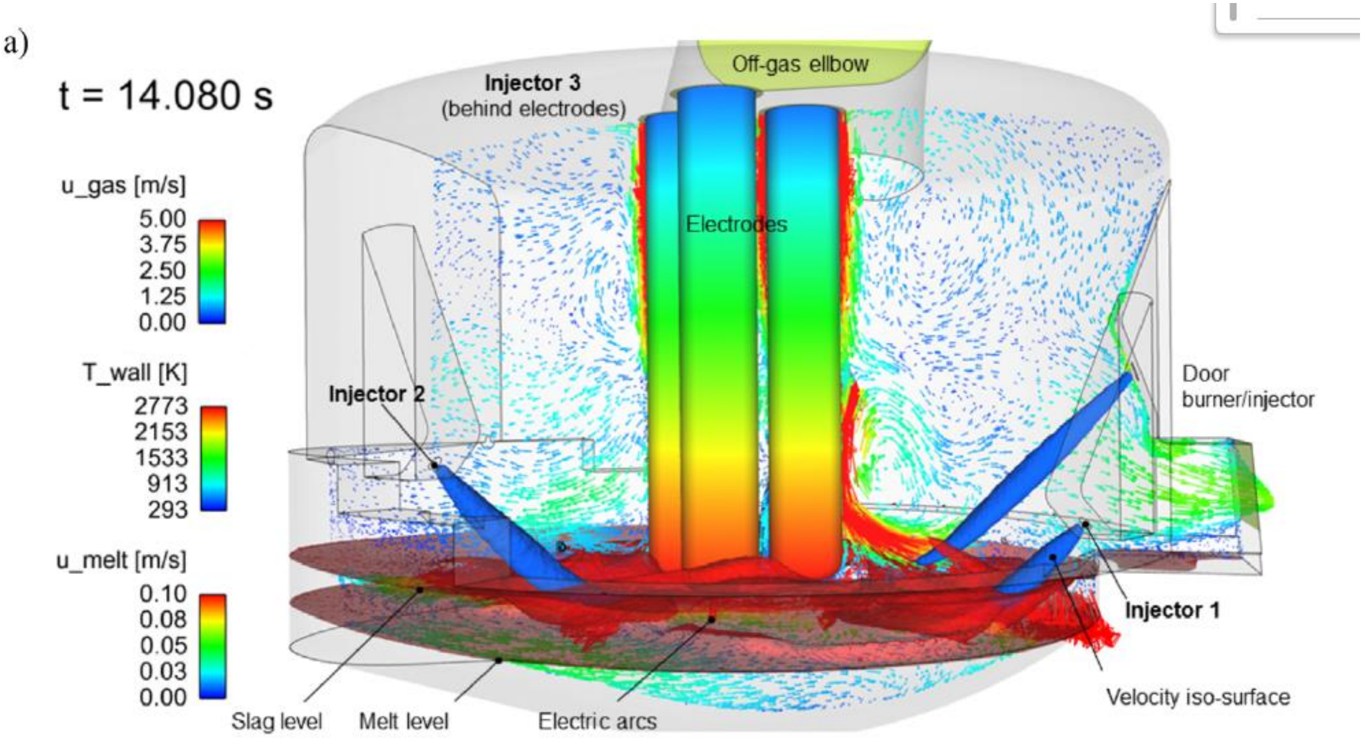
Future work
Modelling Liquid metal stirring in EAF (Electric Arc Furnace)



H.-J. Odenthal et al 2017

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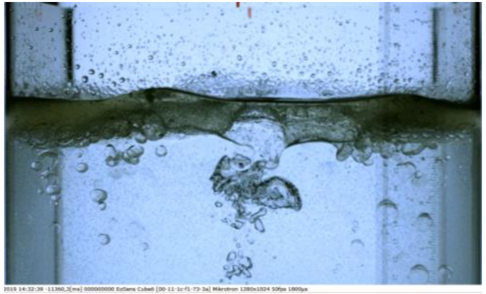
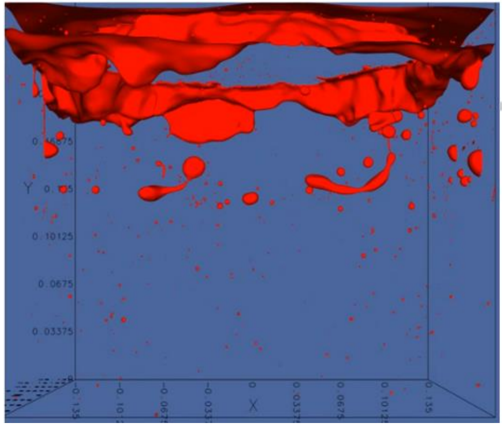
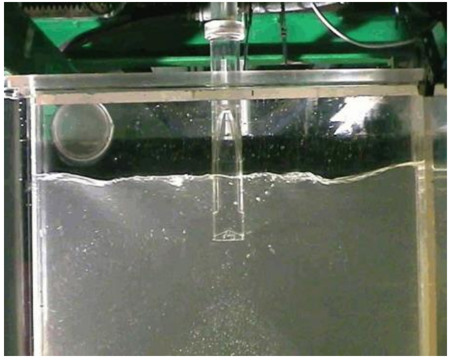
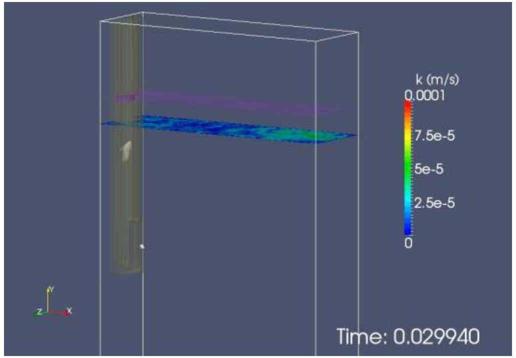
Liquid/Liquid mass transfer in liquid steel : A challenge for CFD

Desulfurization Process: Openeye in water/oil model and CFD simulation





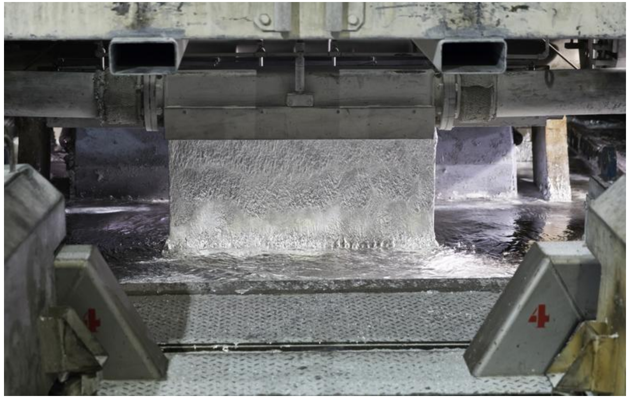




Continuous casting mold water model and CFD simulation

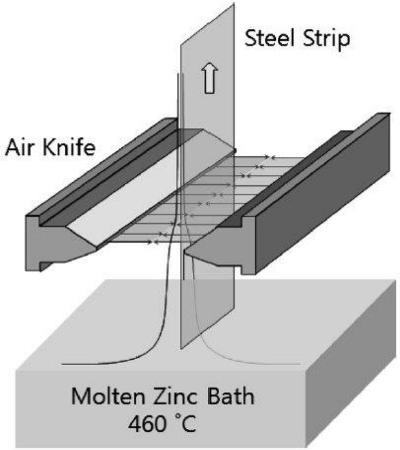
[1] L.D. De Oliveira Campos, Mass transfer coefficients across dynamic liquid steel/slag interface, PhD thesis, 2017
[2] N. Joubert, P. Gardin, S. Popinet, J. Maarek[1], S. Zaleski, Experimental and numerical modelling of mass transfer in a refining ladle, Metall. Res. Technol. 119 (2022)

The wiping process

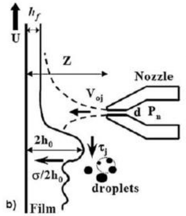


A high speed jet to control of the zinc layer thickness during the galvanisation process

Process issues: Non-uniform coating, edge overcoating, zinc running, splashing



Source: H. G. Yoon et al 2009



- Strip speed : ~ 1-2 m/s
- Air jet speed : ~100-200 m/s
- Film thickness of natural dragout : ~200 μm
- Film thickness with air jet: ~10-50 μm

Numerical Challenges

- 3D Multiphase flow modeling
- High Reynolds and turbulent flow
- Extreme time and spatial scale variations
- No current commercial code is able to simulate this problem in an acceptable computation time

M. Anderhuber, C. Gaultier, T. Coupez et al

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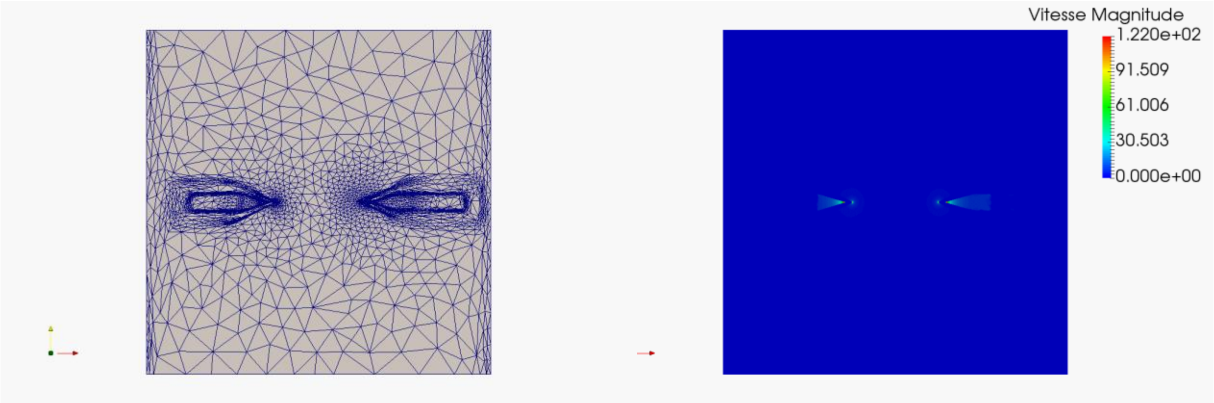
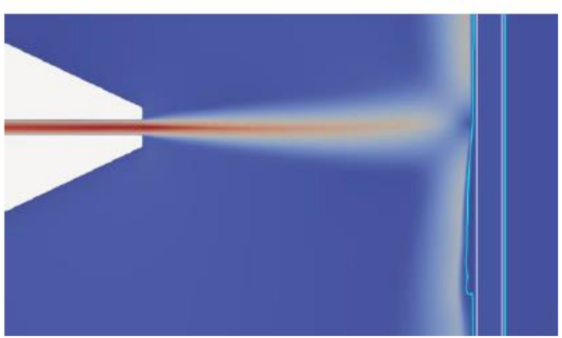
Wiping model : Anisotropic mesh adaptation



T. Coupez. 2011. *'Metric construction by length distribution tensor and edge based error for anisotropic adaptive meshing'*, Journal of Computational Physics, 230: 2391-405.



The 2D wiping case runs well and the film thickness is in the good order of magnitude

- Runbackflow is observed.
- Film thickness ~65 µm with wiping against 200 µm without it
- From experiments we expect a film thickness with wiping of about 43 µm

M. Anderhuber, C. Gaultier, T. Coupez et al

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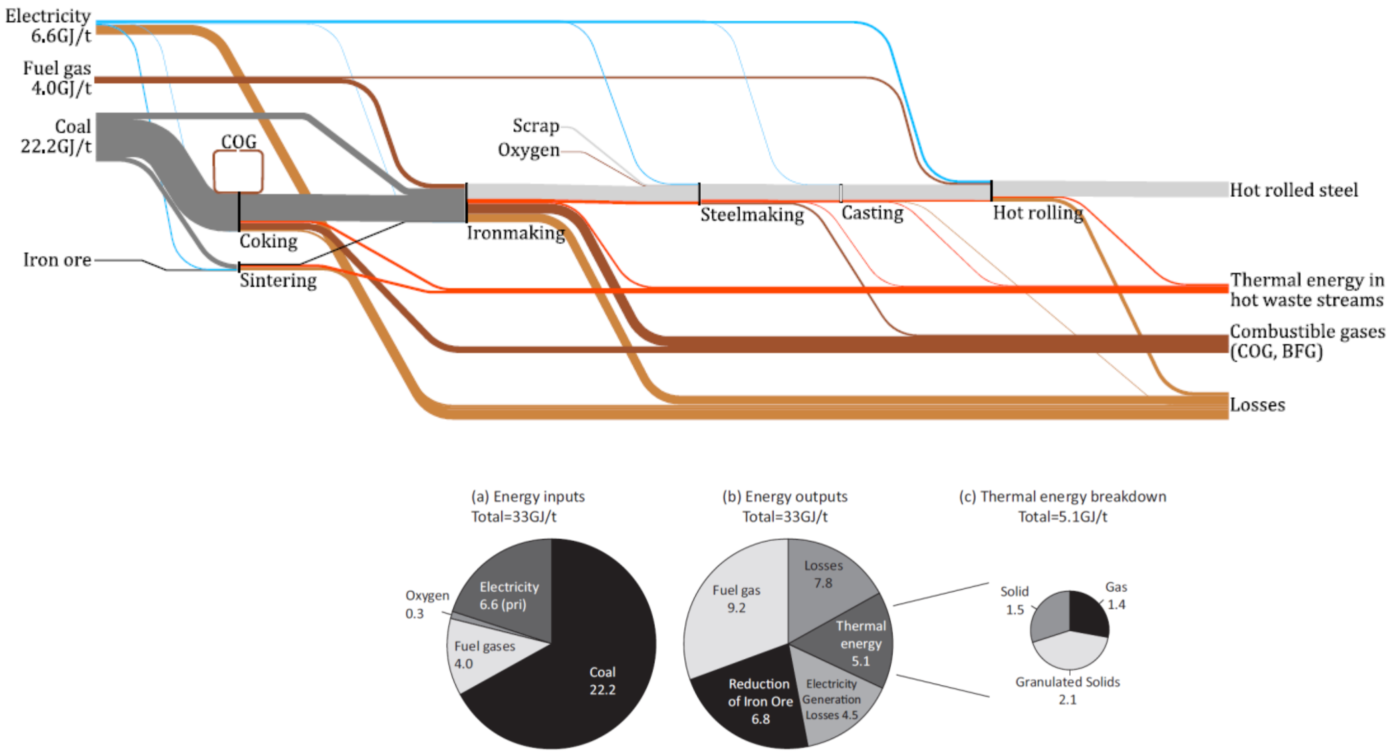
Source : McBrien et al 2016 (DOI)

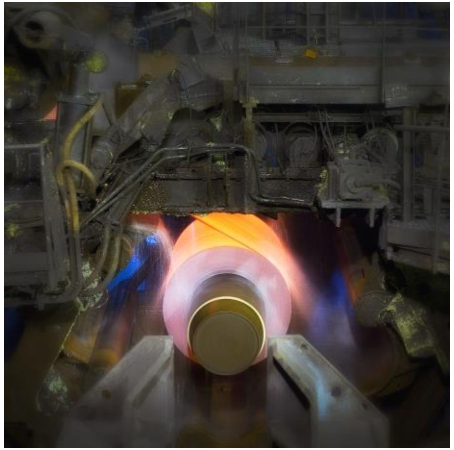
Potential for energy savings



Potential for energy savings

What is needed ?

- An integrated network of heat recovery
- Approaches which can improve heat transfer in ‘granular solids’ (coal, coke, ore, sinter, slags)
- Heat recovery opportunities from solid metal products



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Take away

- Some key figures :
  - Almost 2 billion tones of steels are produced yearly. This volume is expected to increase in the next 50 years.
  - 1 ton of steel requires 18.7 GJ of energy inputs and emits 1808 kg of CO_2.
- Decarbonising the steel industry involves major efforts and a fundamental shift in production methods. New processing routes are being investigated and breakthough technologies are emerging.
- A higher quality ore is essential for low carbon steelmaking. This comes in a context where premium-grade resources are being rapidly depleted, posing a significant challenge to the sustainability of future production routes.

→ High level research is therfore required for achieving net-zero targets without compromising material performance

- Some topics for the future ?
  - Multiscale modelling combining an accurate description of surface chemistry and CFD methods.
  - Machine Learning and hybrid models offer a potential to accelerate models and to improve them when industrial measurements are available
  - Energy storage in new generation heat exchangers

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