ANF
Métallurgie Fondamentale

PROCEDES D'ELABORATION

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22-25 octobre 2012

What is the meaning:

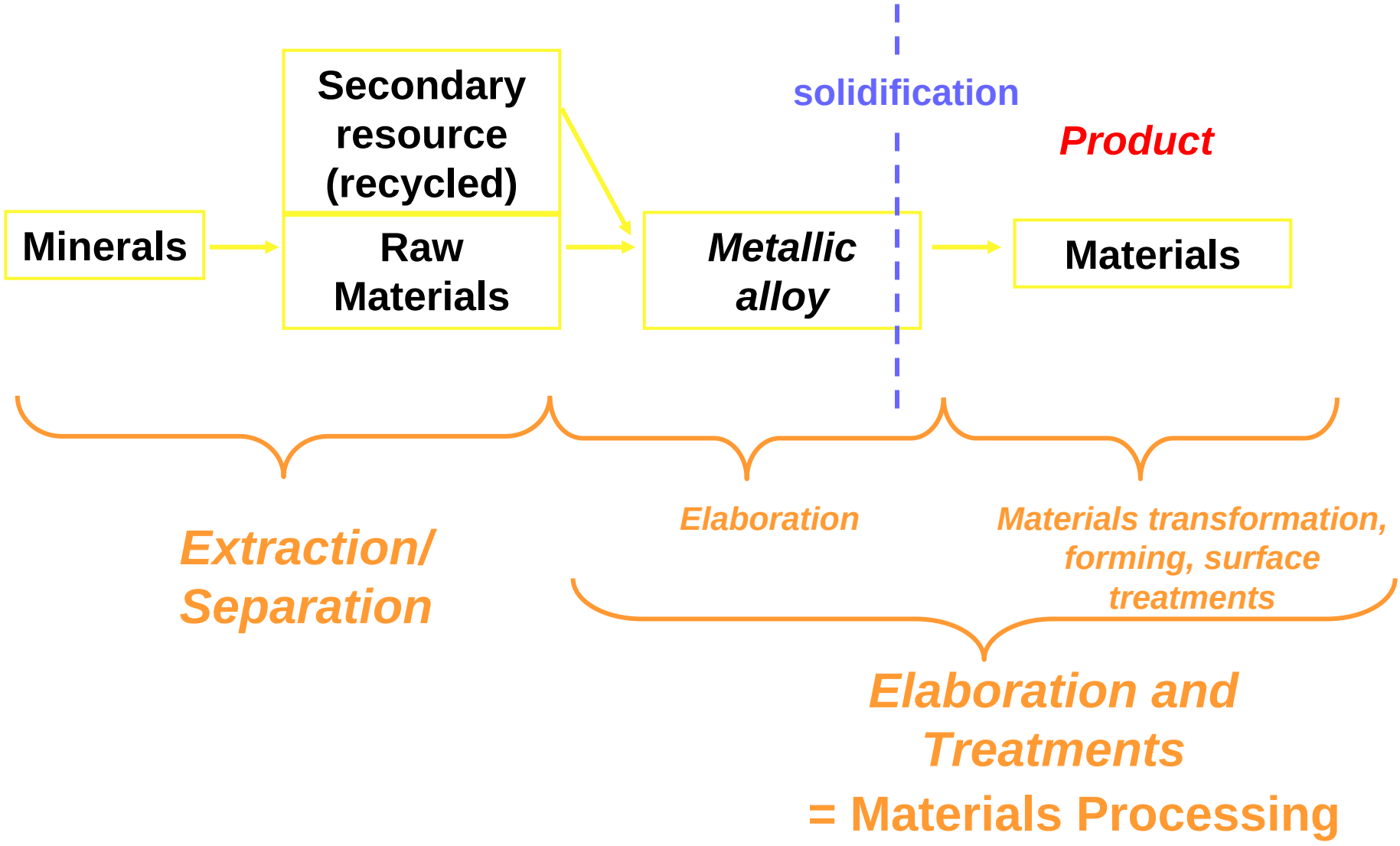
(***Procédés d'élaboration***)

Materials Processing?

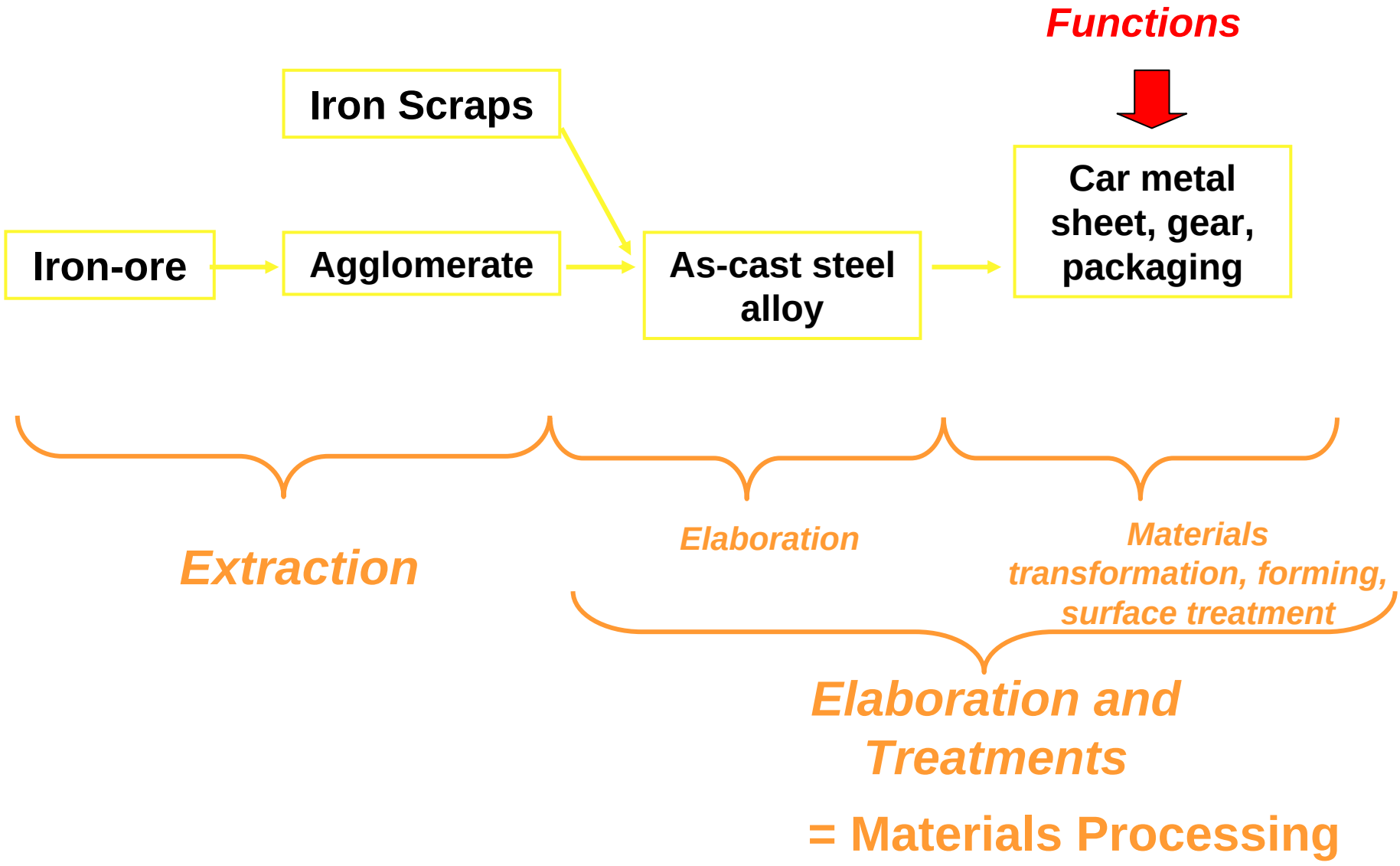
(***Génie des Procédés d'élaboration***)

Materials Process Engineering?

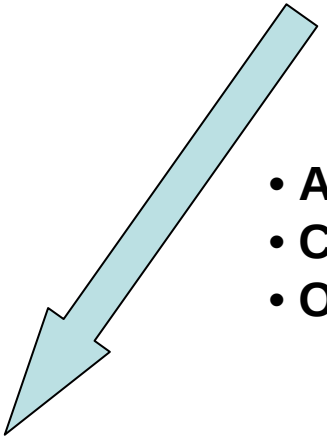
What is the *Materials Processing*?



What is the *Materials Processing*?



What is the *Materials Process Engineering*?



- **Analysis**
- **Control**
- **Optimization**

Car metal sheet, gear, packaging

Elaboration → **Composition Structure** → **Properties** → **Functions**

- **Analysis of the main physical phenomena**
- **Set up measurements and experimental studies**
- **Modeling (numerical)**
- **Simulation of the process and optimization of the operating parameters**

New challenges in 21st Century?

- **Improvement of Inclusion cleanliness and alloy purity**
- **Energy: efficiency and vector**
- **Environmental impact: assessment and reduction**
- **Waste stream (*Matières Premières Secondaires*):**
  - **Processing technologies for metals and minerals extraction from waste streams**
  - **Additional stress on the purification processes**

Summary

- **The main processing routes in metallurgy**
- **The main stages of the elaboration**
- **Materials Processing Fundamentals**
- **Illustrations: Modeling and simulation**
- **What about experiments?**

Main Processing Routes

- **Hydrometallurgy**
  - Low Energy cost
  - Small units
  - Recycling processes
  - No environmentally friendly
- **Pyrometallurgy**

Hydrometallurgy

Applications: Au, Zn, Co, Cr, Cu, Mn…

1st Stage: **Leaching: Dissolving the metals (as one of its salts)**

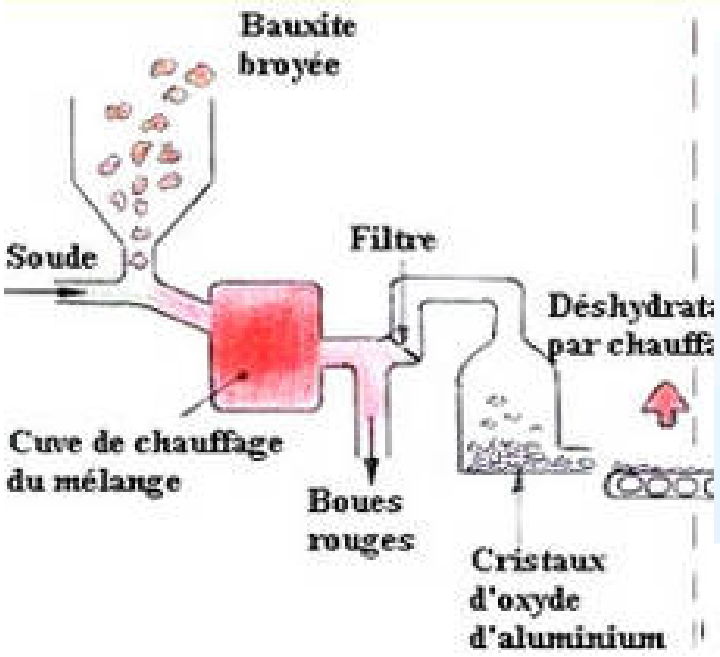
2nd Stage: **Purification: Separating the waste from the aqueous solution to an other phase by precipitation, crystallization, cementation**

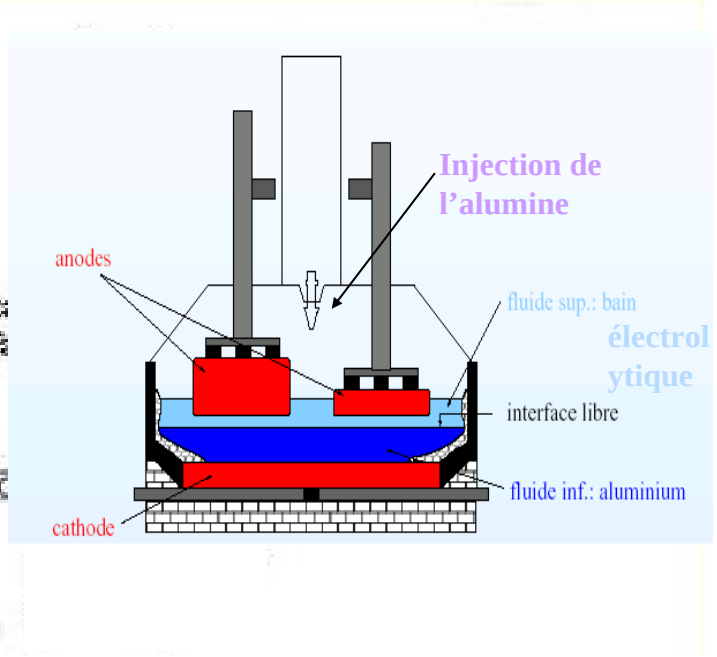
3nd Stage: **Elaboration of the solid metal: Electrolysis or solvent extraction**

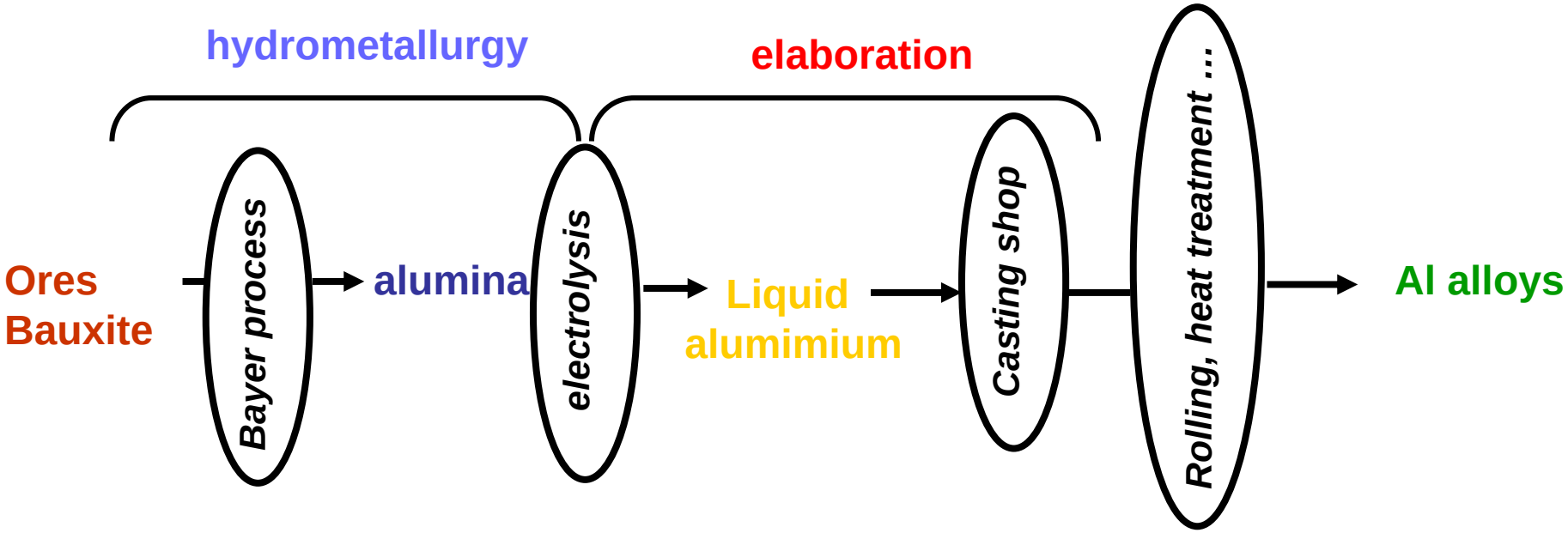
Fundamentals in hydrometallurgy:

Chemical, Electrochemical and Chemical Engineering

Production of primary aluminum

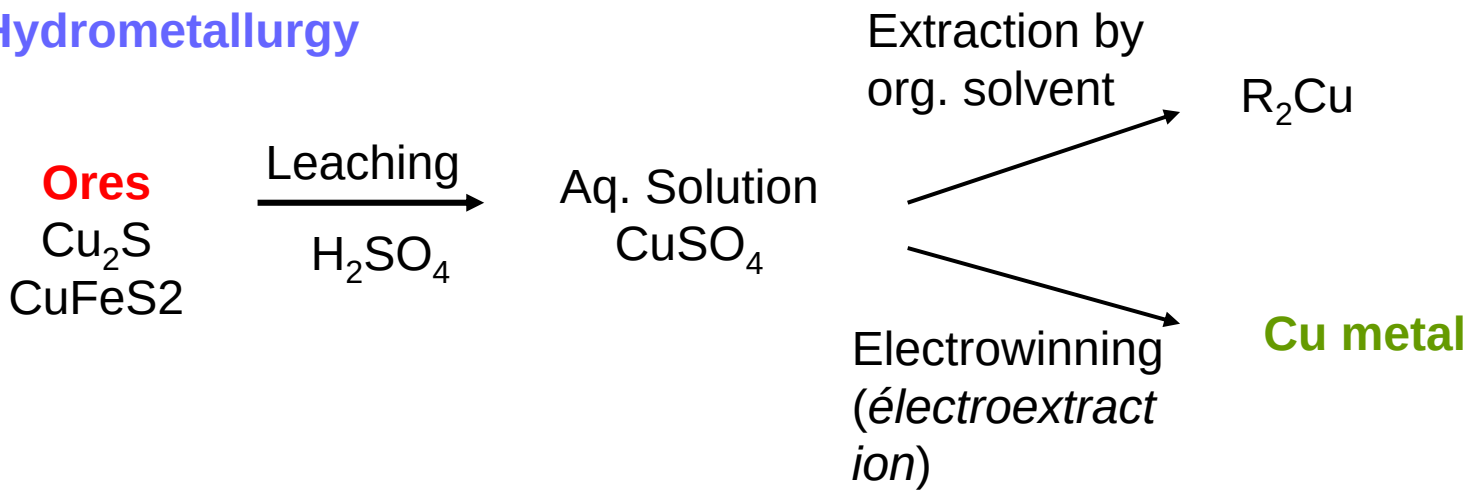




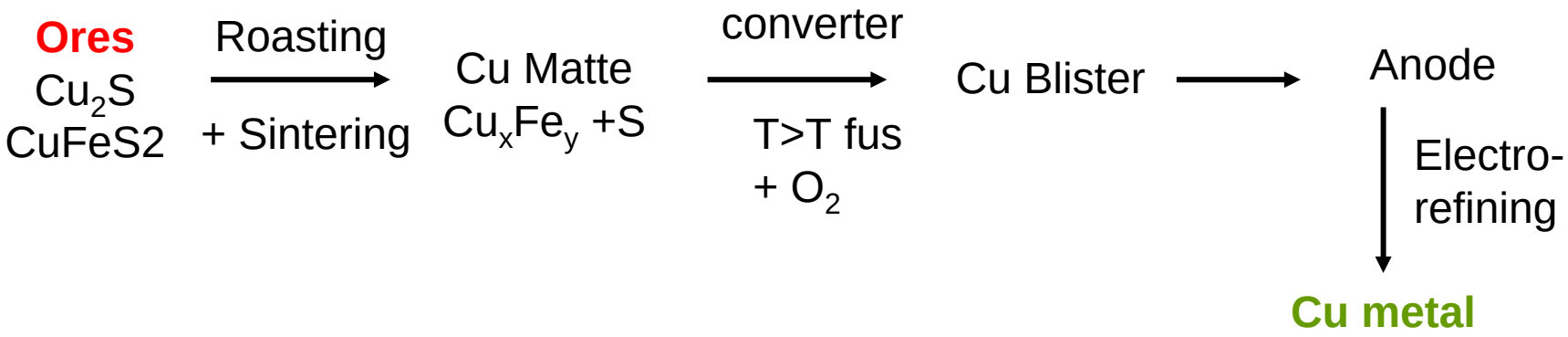


Production of primary Copper

Hydrometallurgy

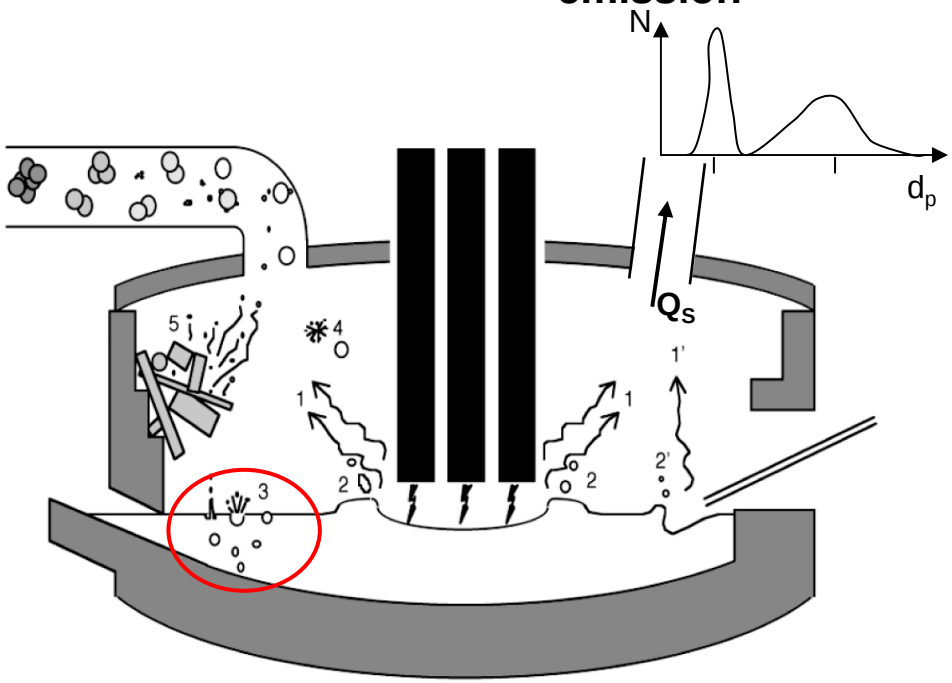


Pyrometallurgy



Zinc Recycling: Dust produced by the EAF (iron scarp remelting)

Dust emission **20 kg of dust/ t steel**



Zn	25 %
Pb	5 %
Salts	5 %
Cd	2 %

Leaching with NaOH, 90°C – 1h → Fe, Lime; Zn, Pb

Zn, Pb → Cementation (Zn powder) → Pb; Zn

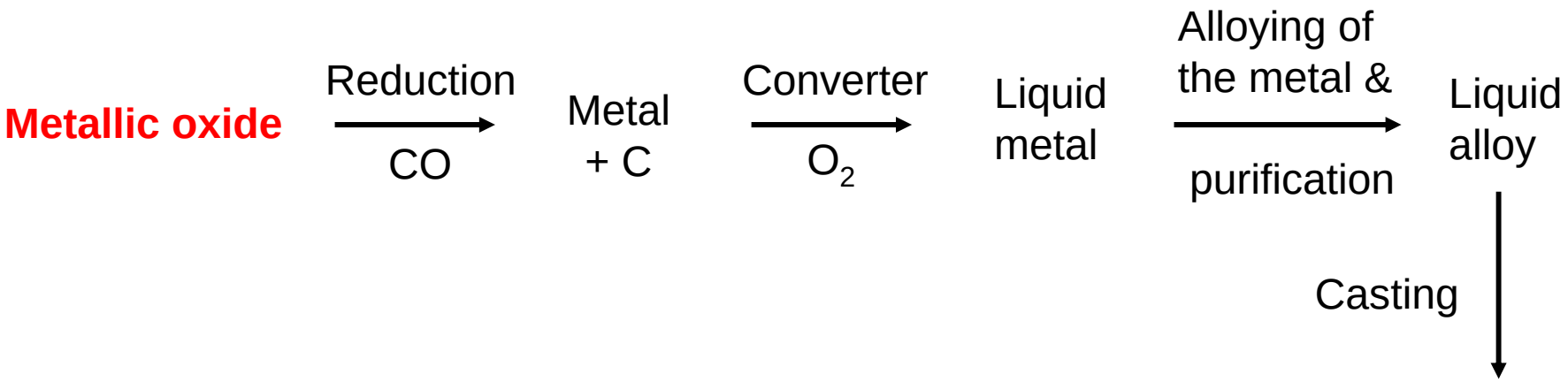
Zn → Elect → Zn metal

Main Processing Routes

- **Hydrometallurgy**
  - Low Energy cost
  - Small units
  - Recycling processes
  - No environmentally friendly
- **Pyrometallurgy**

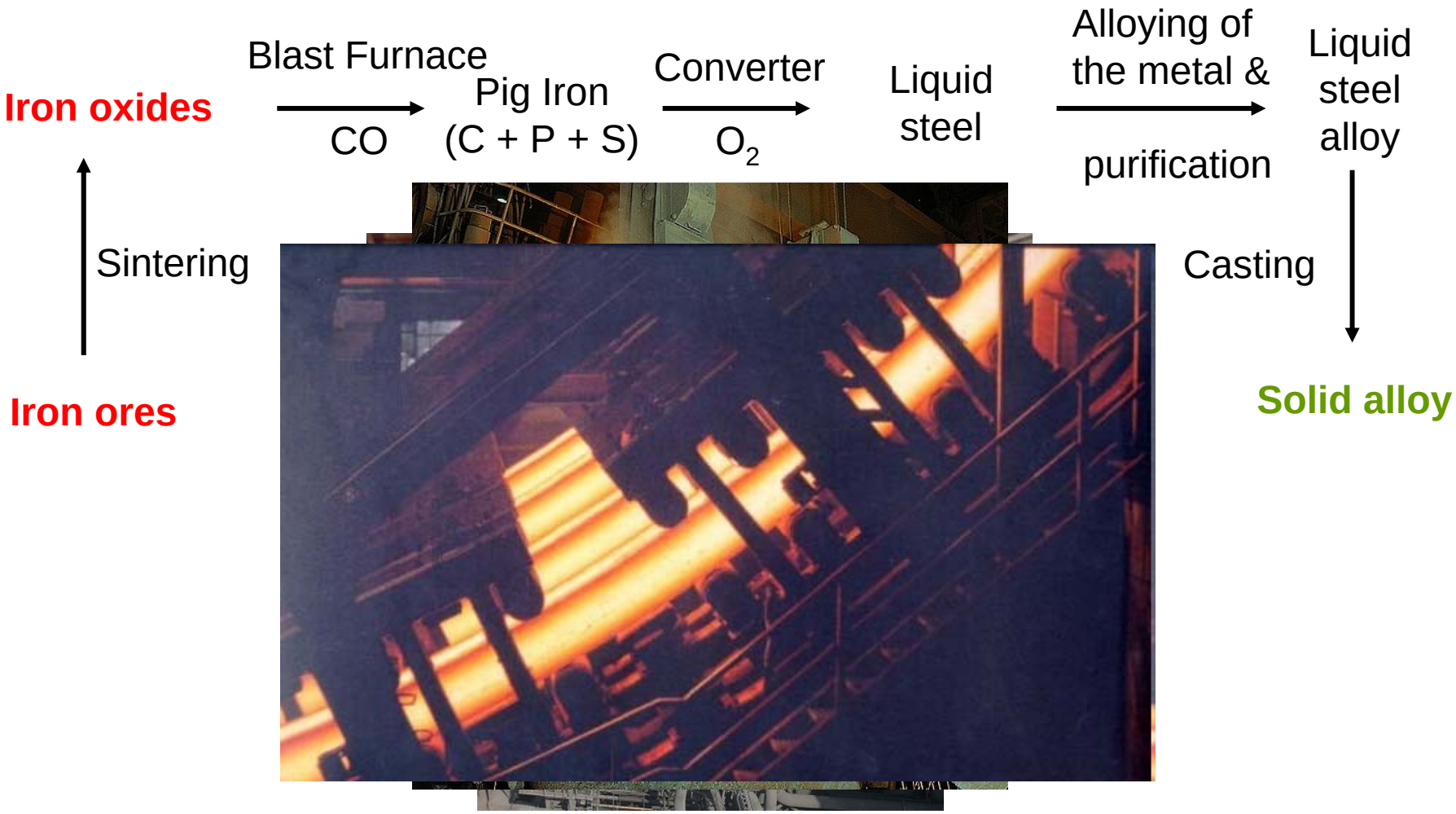
Pyrometallurgy

The main stages

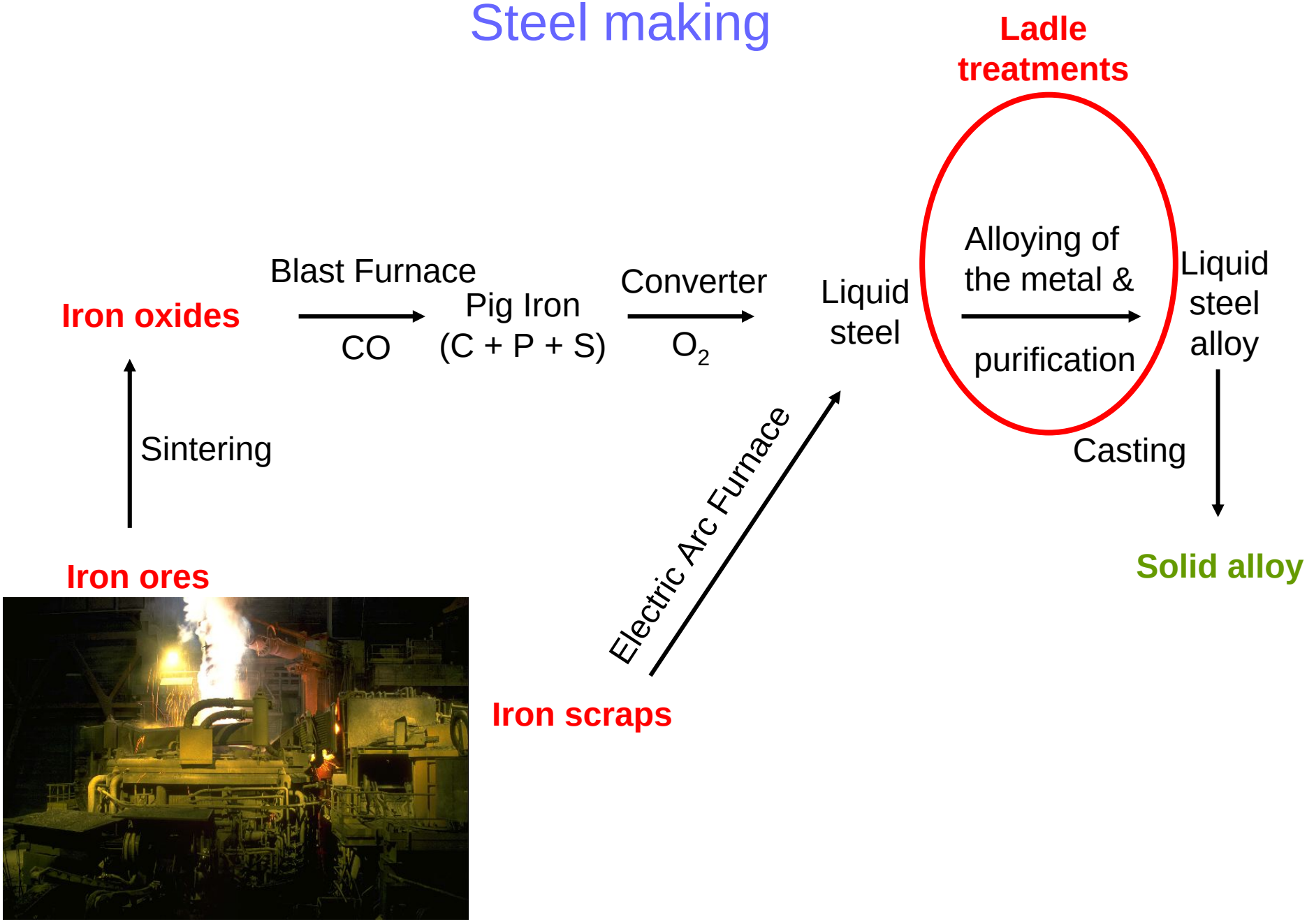


- **Steel making**
- **Aluminium making**
- **Titanium making**

Steel making



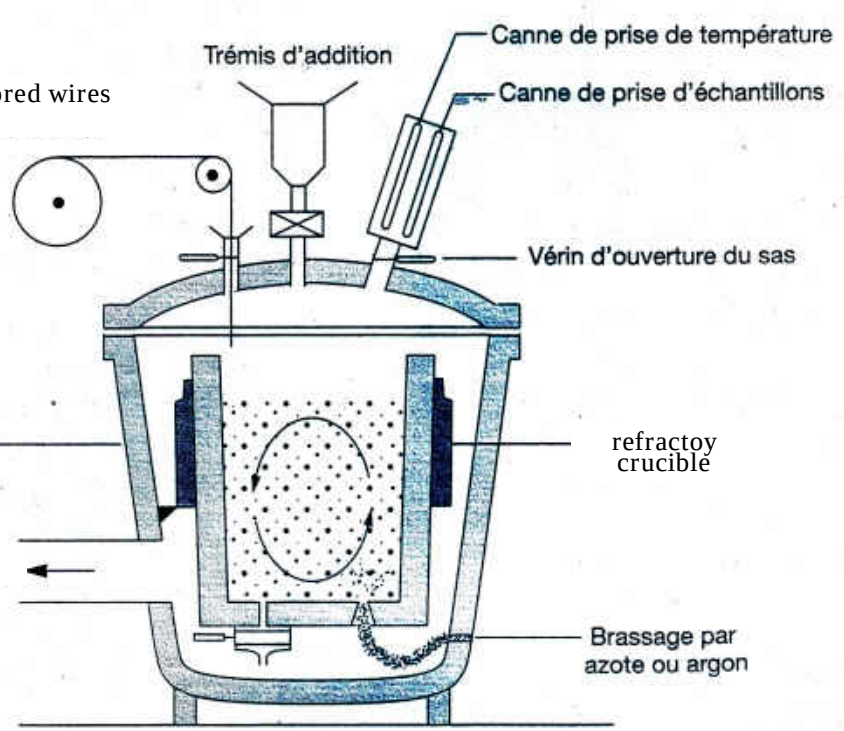
Steel making



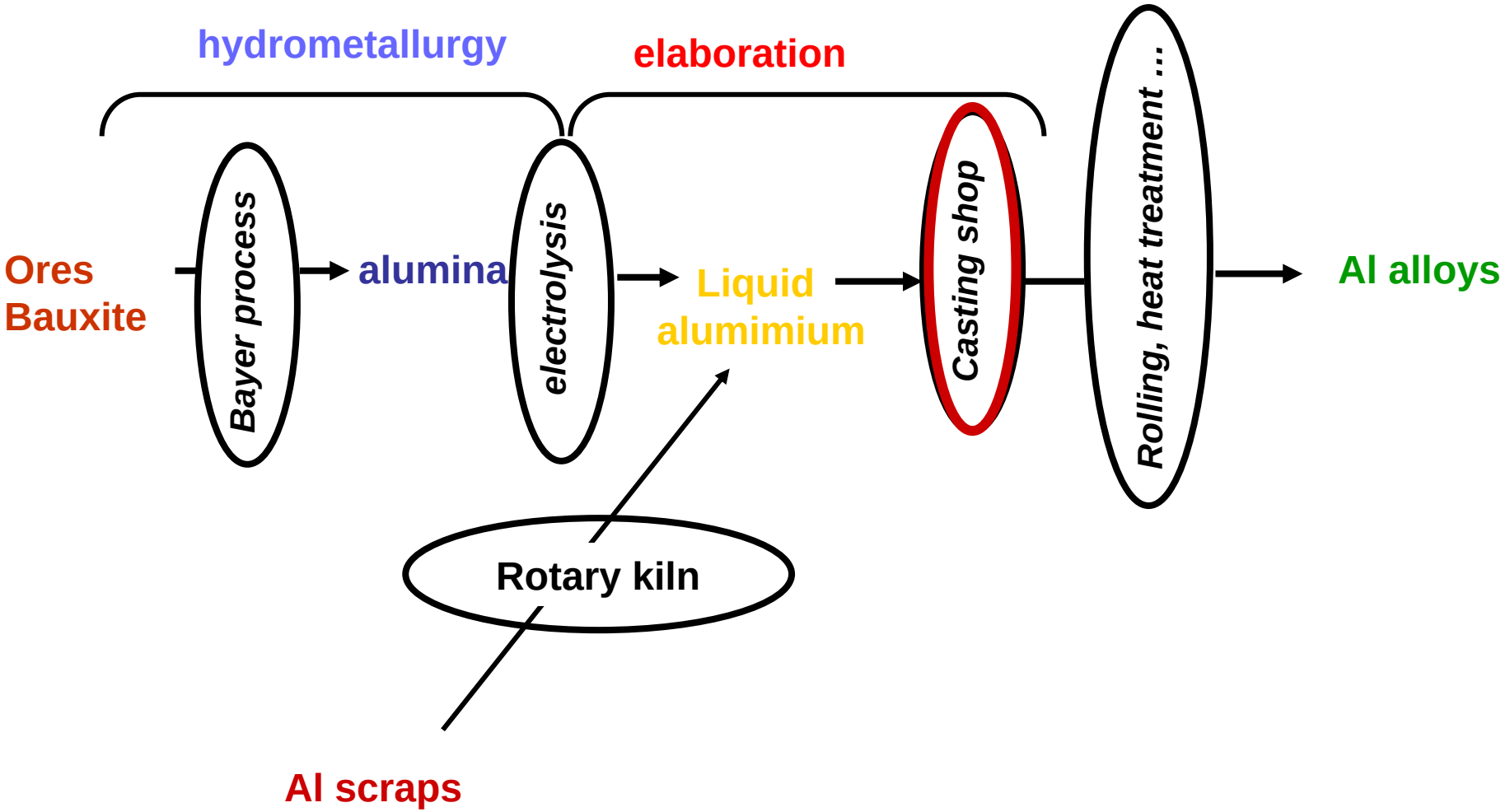
Refining of liquid steel

Gas-stirring ladle

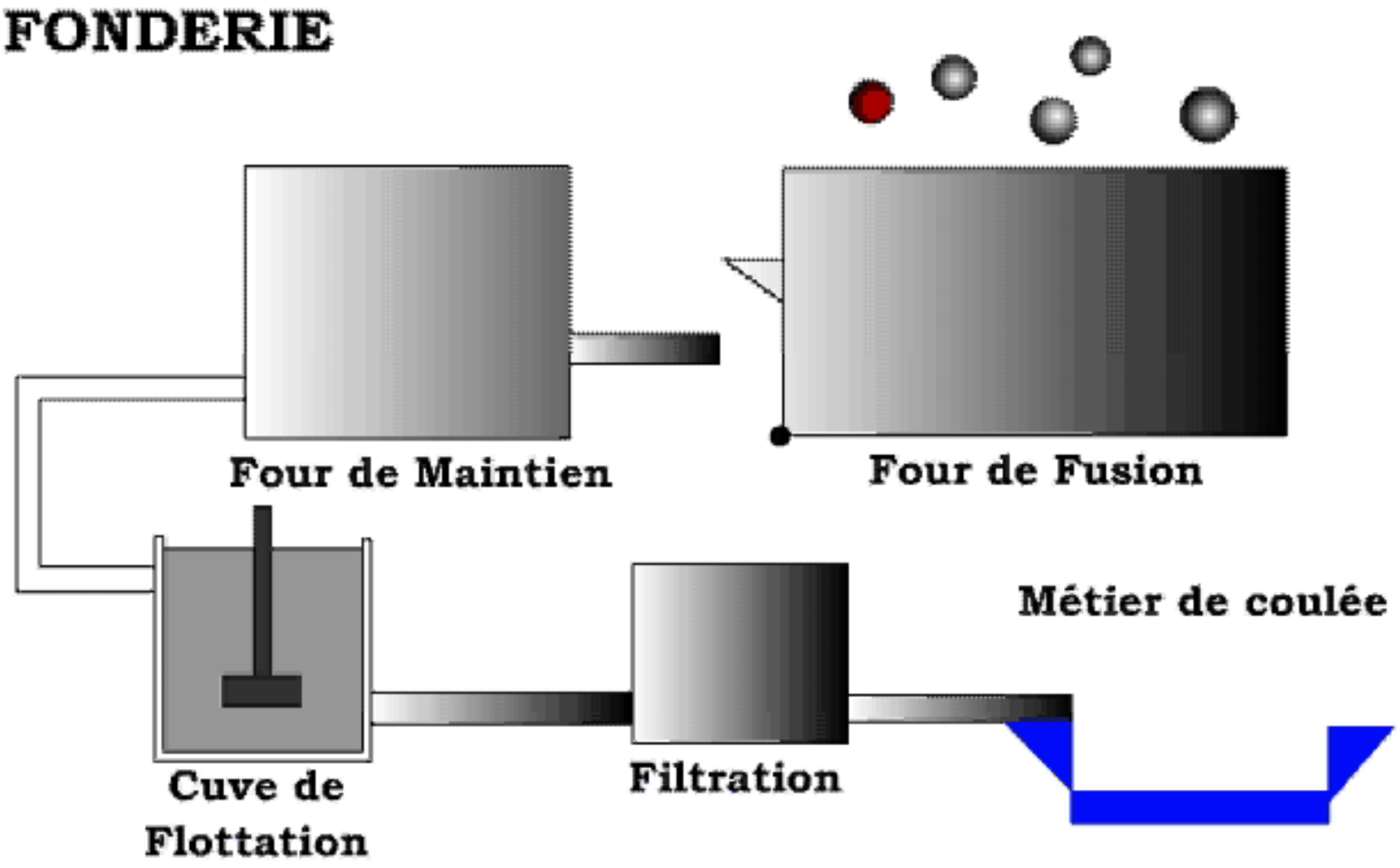
Stages
Degassing
Final Additions Ca, Al …
Inclusion separation



Aluminum making



Aluminum casting shop

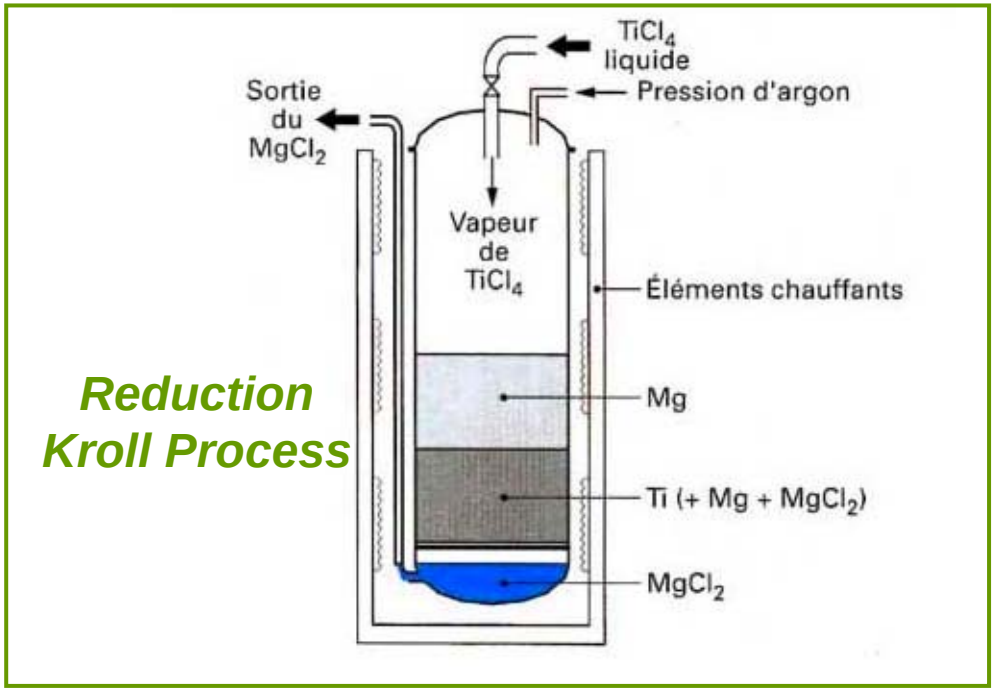


Titanium making

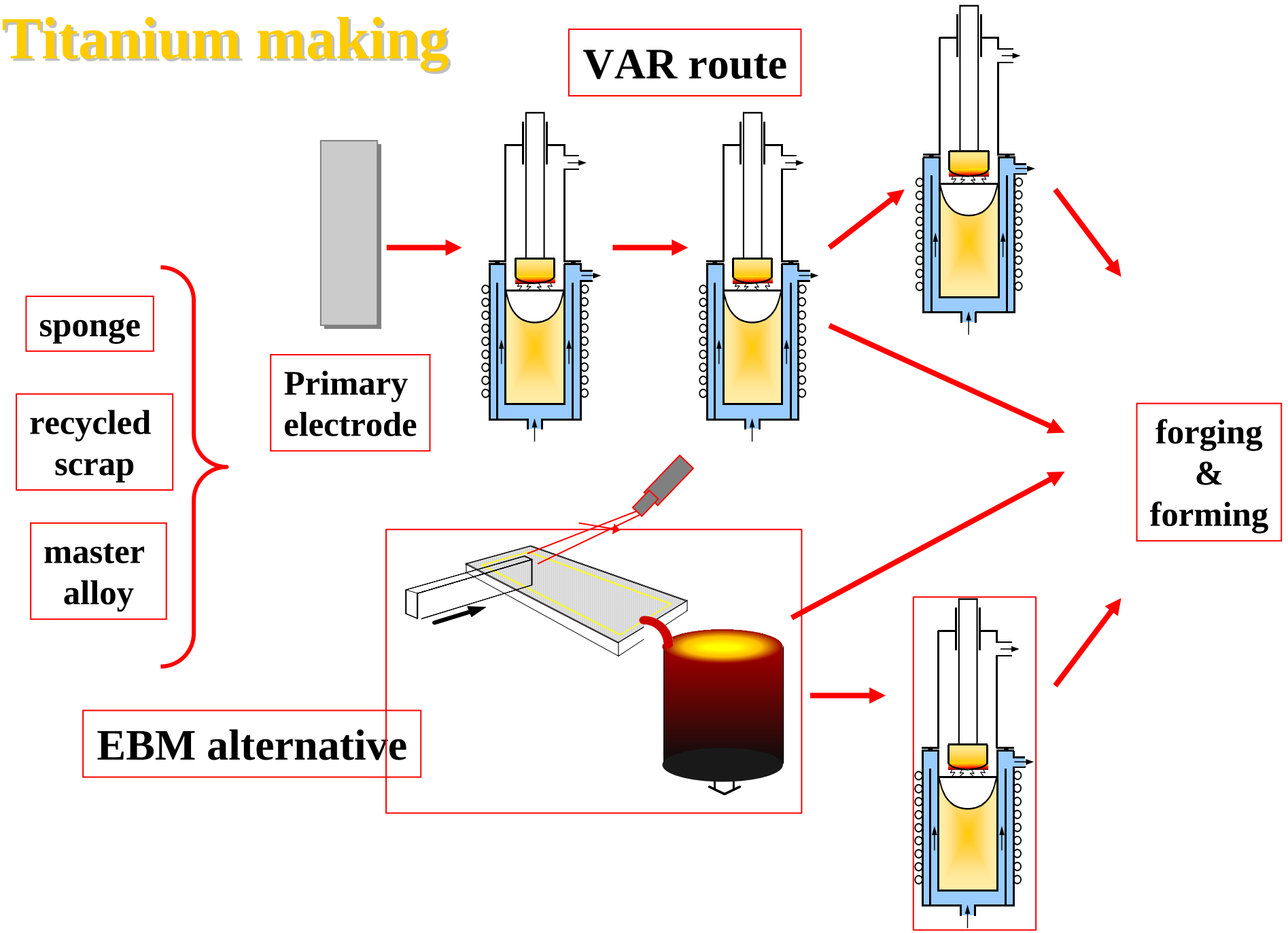
Metallic oxide TiO_2 → Carbochloration ($Cl_2 + C$) → $TiCl_4$ → Reduction (Mg) → Ti sponge → Alloying of the metal & purification → Liquid alloy → Casting → **Solid alloy**

pyrometallurgy

Reduction Kroll Process



Titanium making



Materials Processing Fundamentals

Chemical Engineering History

Unit Operations

WW2

Chemical Engineering 'Science'
AIChE (American Institute of Chemical Engineering)
MIT, IC

Process Design
Control System

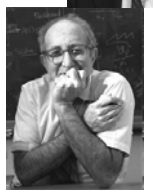
Transport Phenomena, R.B. Bird, 1960, Unified approach

Computer Science 1970

Application to Materials Engineering, J. Szekely

'*Voie Royale*'
J. Villermaux

Chemical Engineering Reactors, O. Levenspiel



1990

Materials Process Engineering (*Génie des Procédés d'Elaboration,* A. Vigne, D. Ablitzer)

Materials Processing Fundamentals

Process Engineering

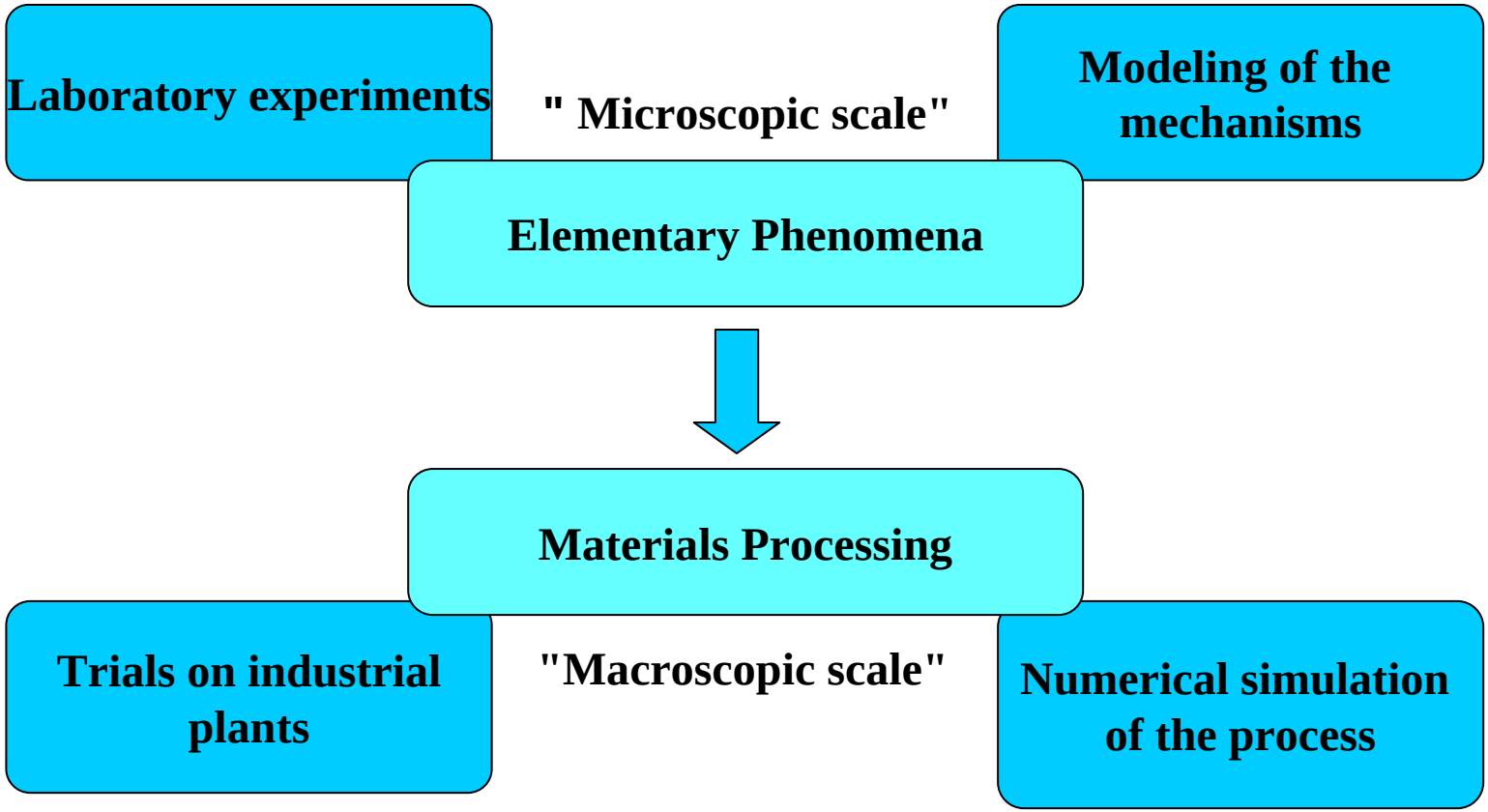
System Analysis

- Unit operation / Ideal reactor
- Chemical kinetics/Mass Transfers
- Thermodynamics
- System dynamic (unit control, automatic)

Mechanistic Analysis

- Fluid mechanic
- Thermal & thermochemistry
- Transport phenomena
- Chemical kinetics

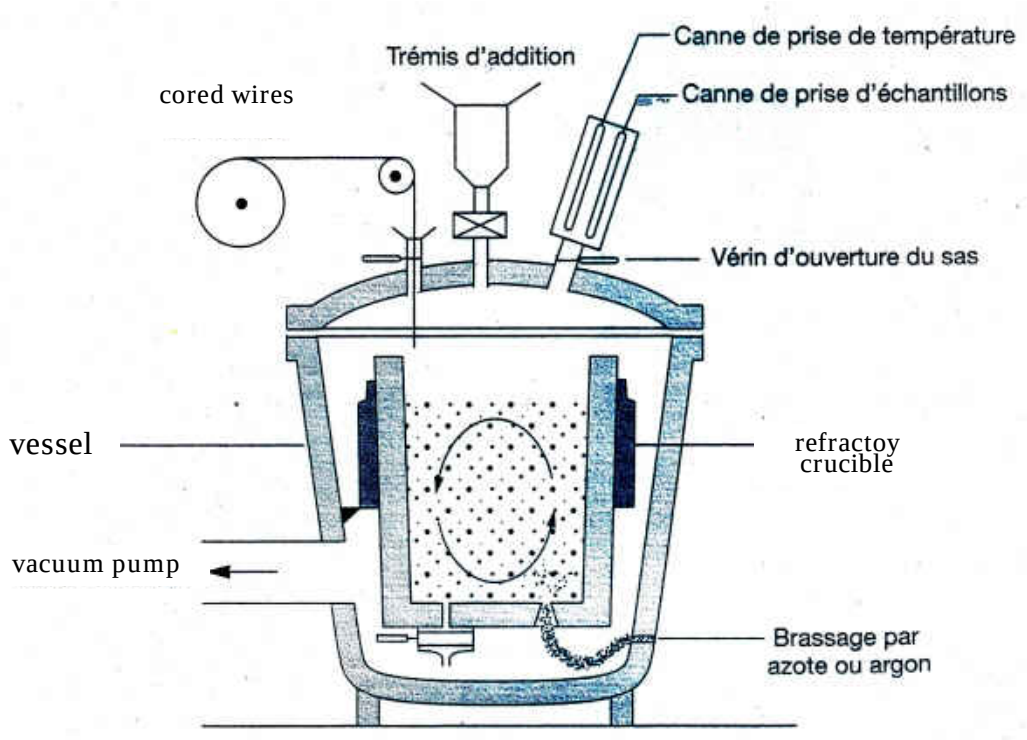
Research approach



Illustrations

1st Example: Refining of liquid steel

Gas-stirring ladle



1st Stage

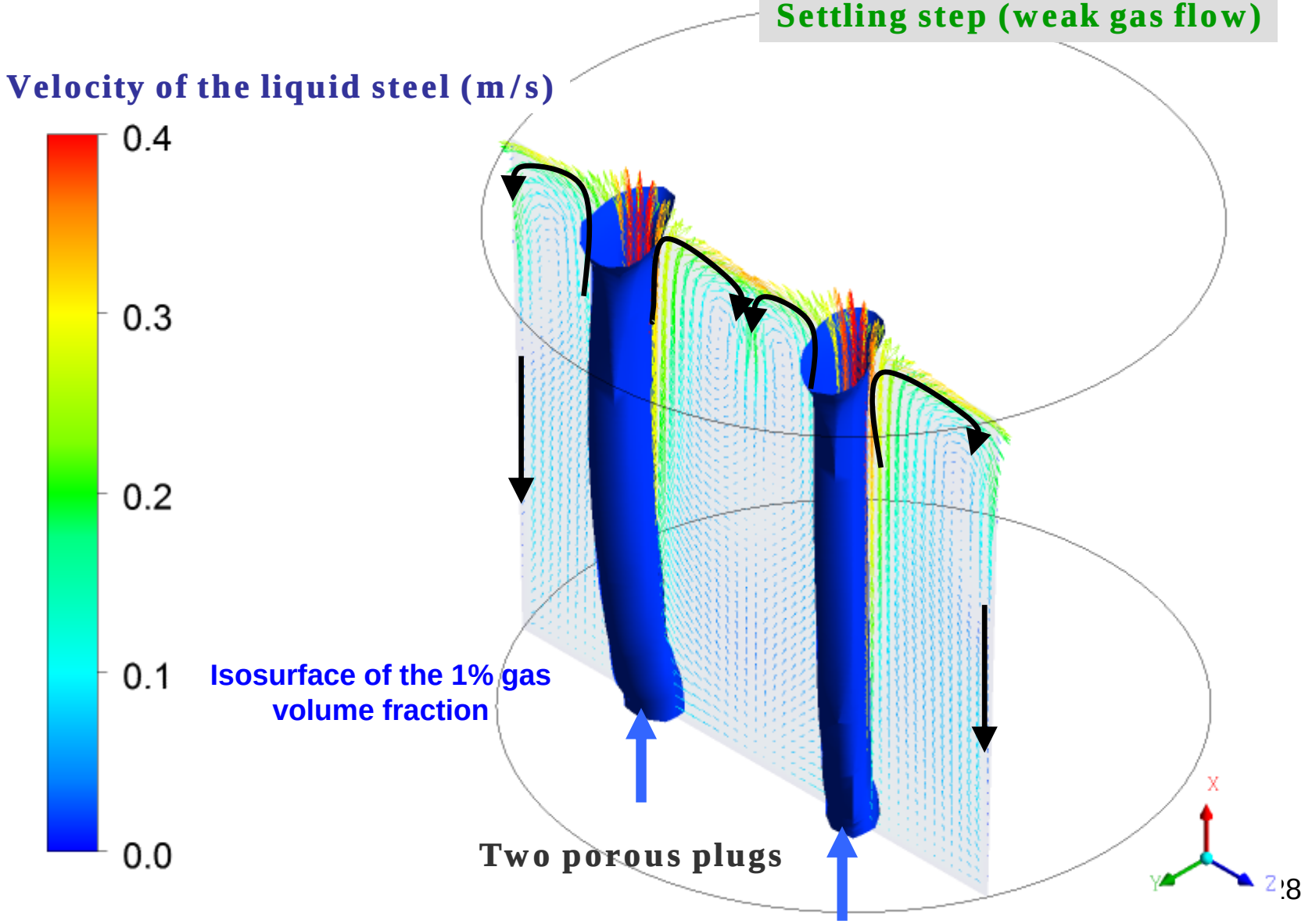
Modeling of Liquid/gas bubbles
Turbulent Fluid flow

2nd Stage

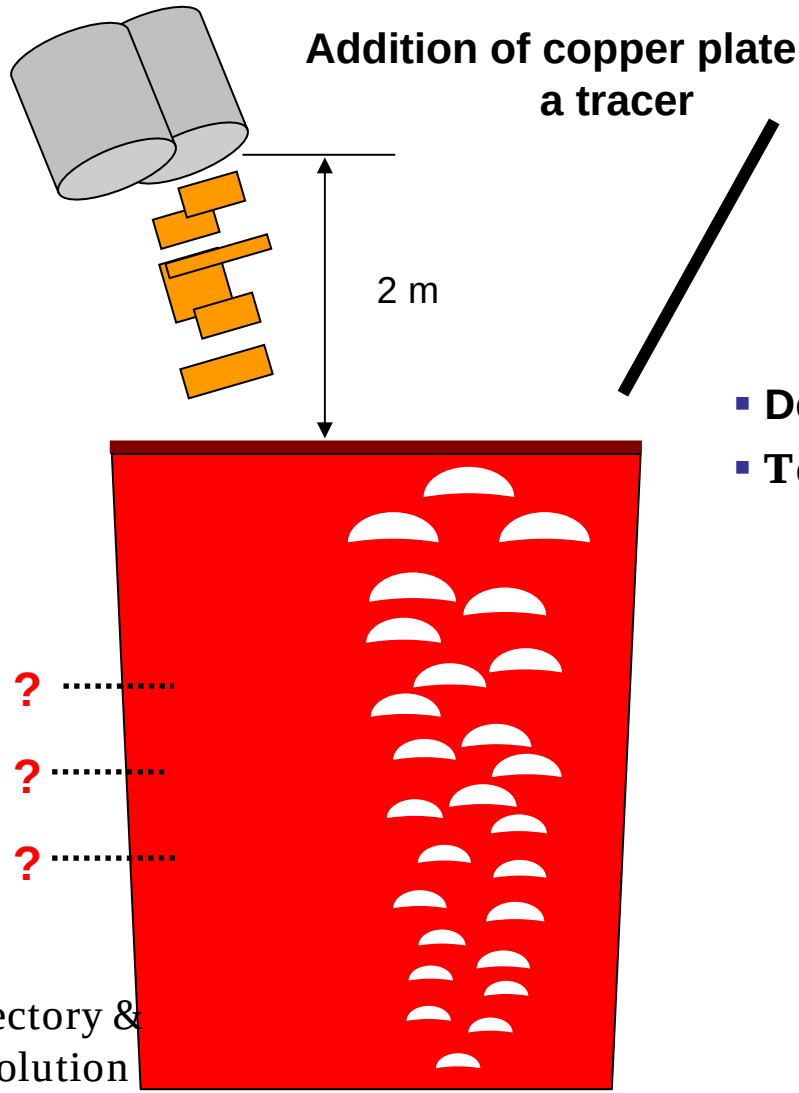
Modeling of inclusion behavior

Example of the hydrodynamics of an industrial ladle (60 t)

Settling step (weak gas flow)



Mixing time



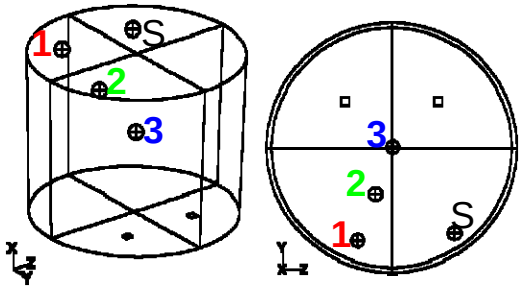
- Tracer : 60 kg of copper (0,1 wt%)
- Introduction duration : 3 s

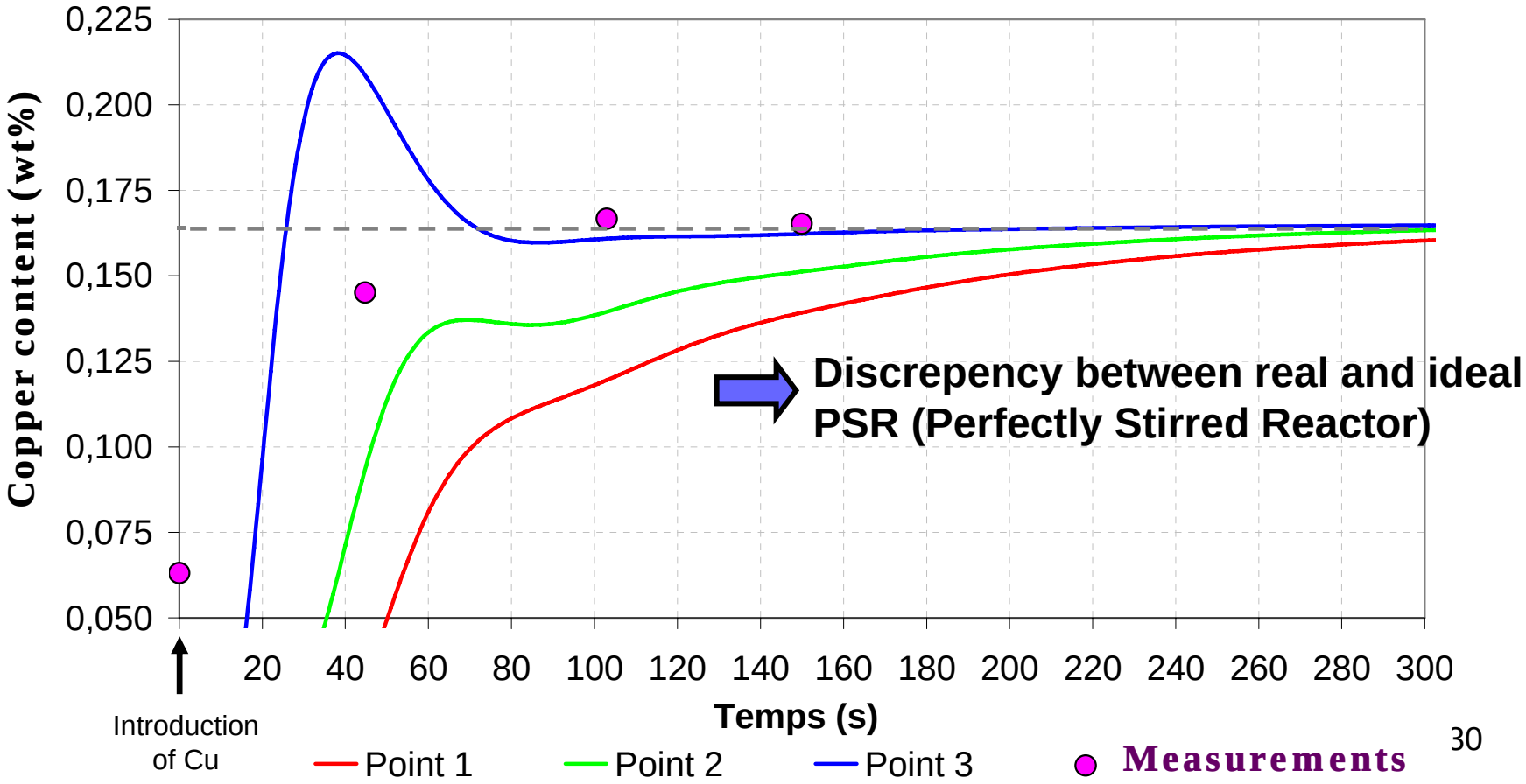
- Deep-sampling time interval: 50 s
- **Total time : 3 min**

trajectory & dissolution behaviour?

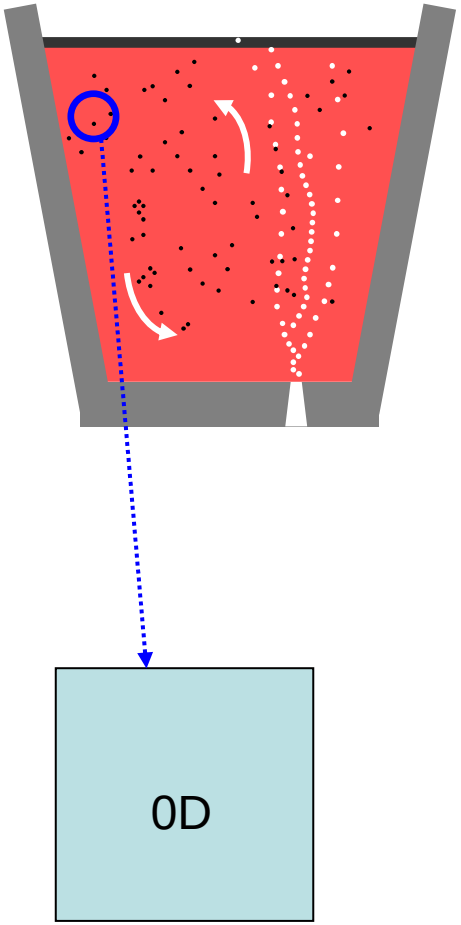
Mixing time

- **Initial tracer location: pts 1 to 3**
- **Location of the Sampling (pt S)**

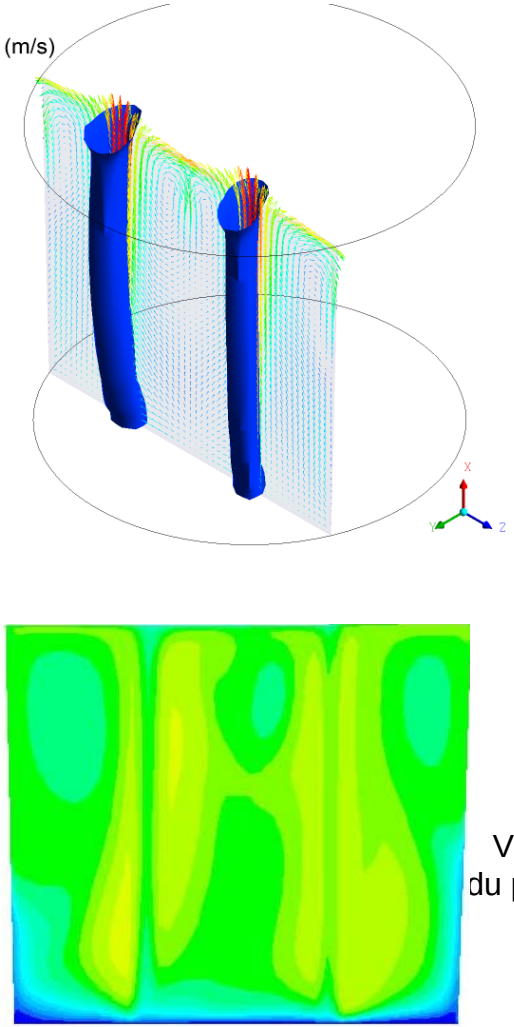




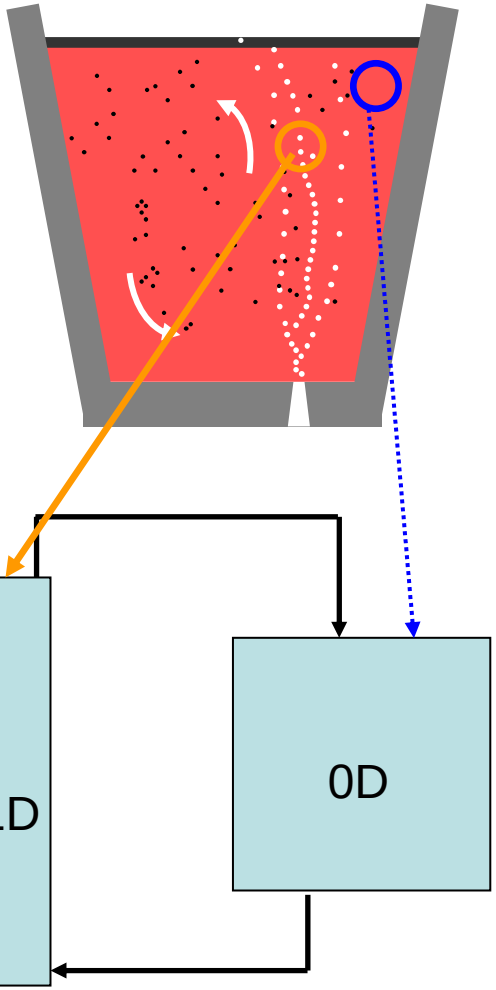
Inclusion behavior: Development of a 0D, 3D or 1D model



Homogeneous ladle
0D



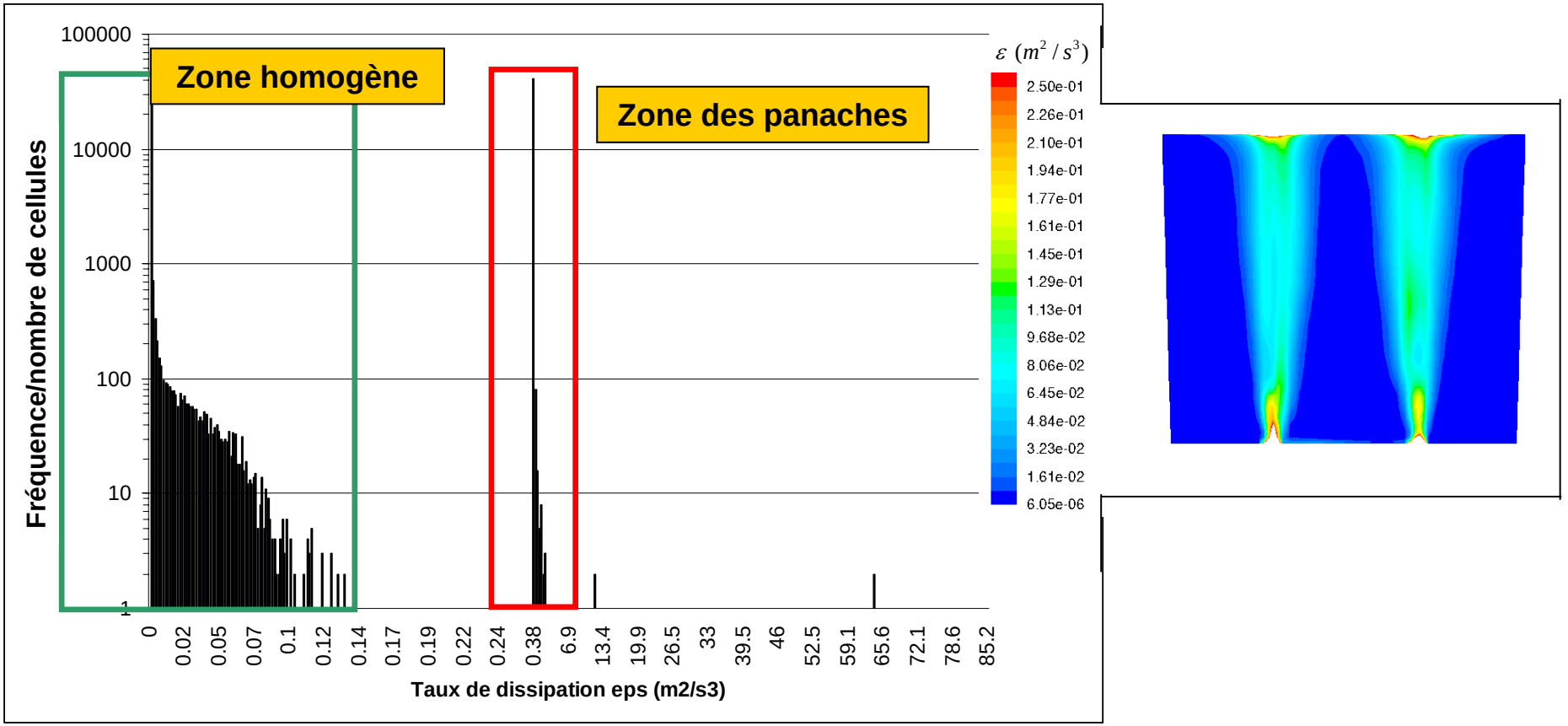
Heterogeneous ladle
3D



Coupling of 1D and 0D reactors

Averaging of the hydrodynamics properties

Two modes: bimodal distribution



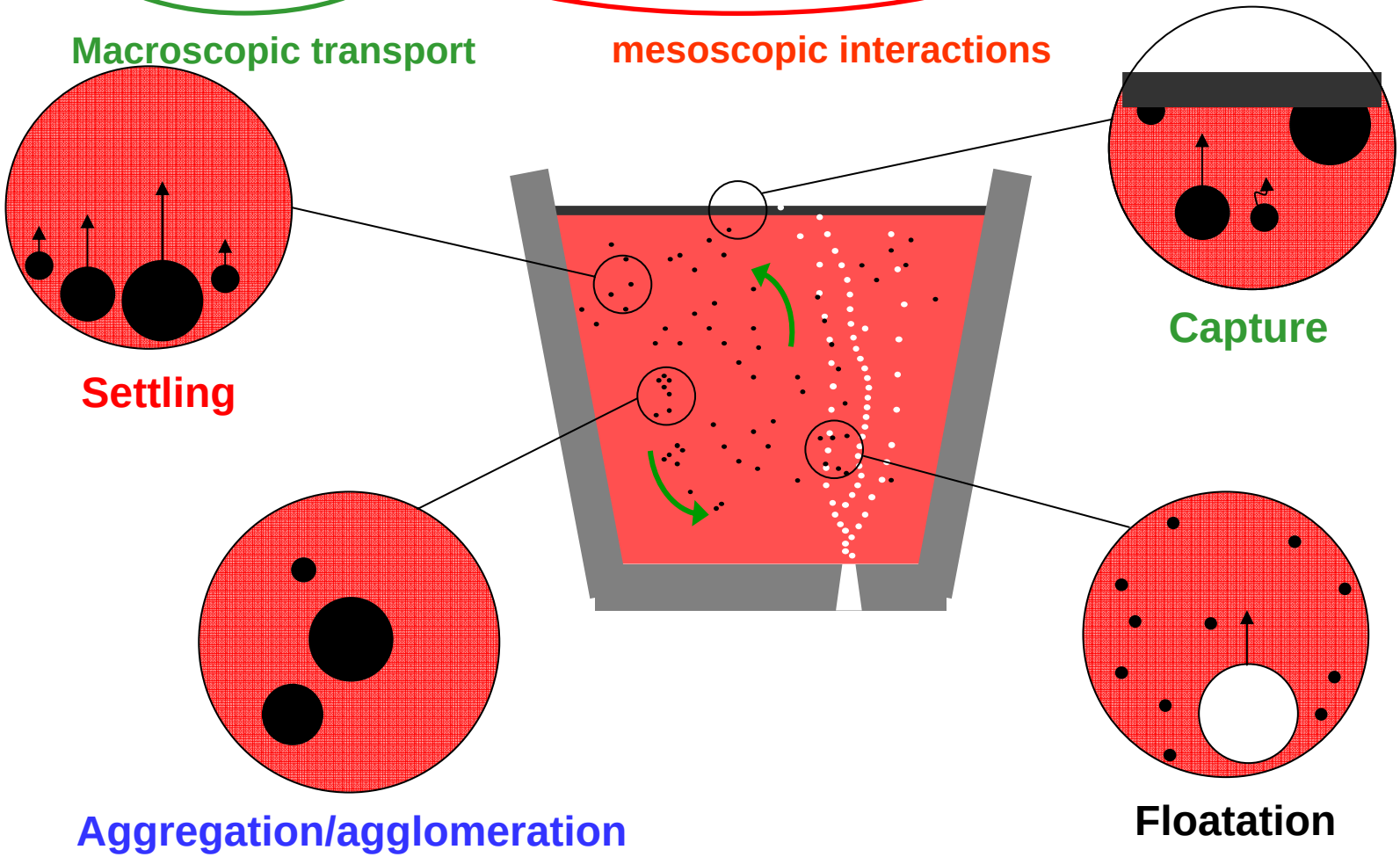
Modeling of the inclusion behavior

$$\frac{\partial \alpha_l N_i}{\partial t} + div(\alpha_l u_l N_i) = \alpha_l (B_i - D_i) - Z_{bi} - S_i$$

N_i *nb of inclusions of the i class / m³ of liquid*

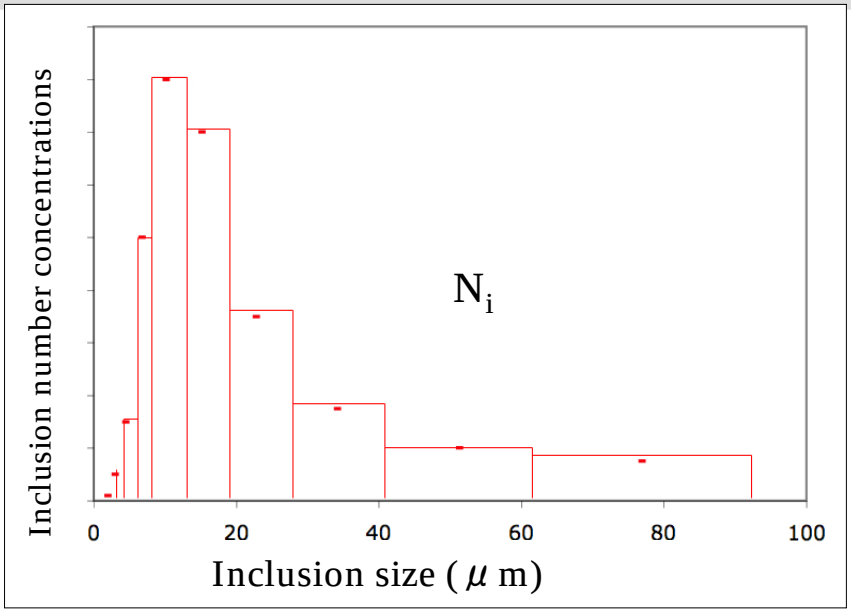
Macroscopic transport

mesoscopic interactions



Numerical Resolution

Discretization



N_i: number density
#part (size i) /m^3

Time splitting technique :

$$\forall \mathbf{i} \in [1, \mathbf{M}]$$

CFD (Fluent)

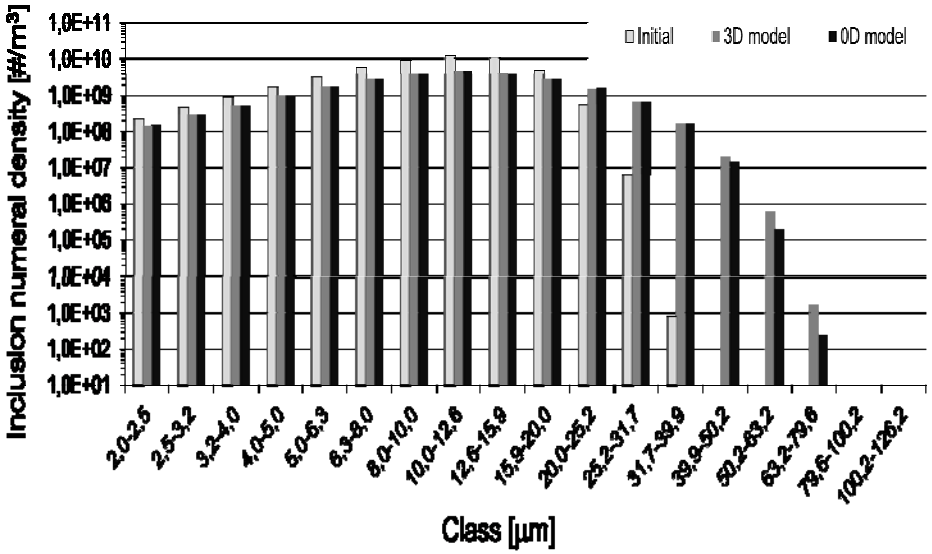
$$\frac{\partial \alpha_l \rho_l N_i}{\partial t} + div(\alpha_l \rho_l \boldsymbol{u}_l N_i) = 0$$ **OD** → Transport of scalars

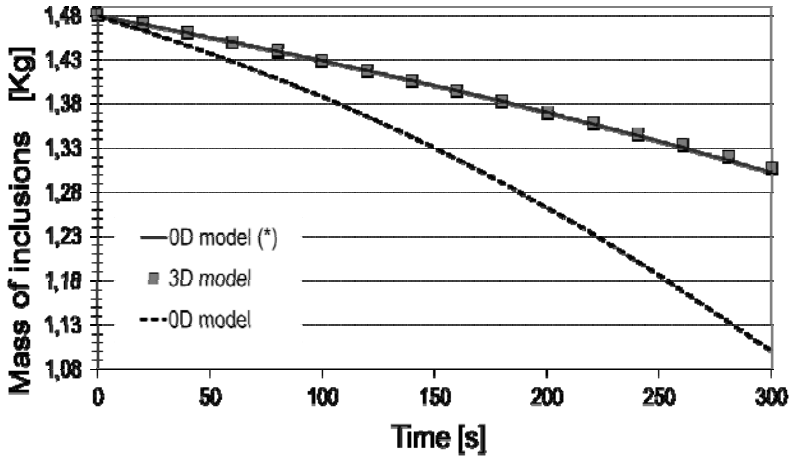
$$\frac{\partial \alpha_l N_i}{\partial t} = B_i - D_i - Z_{bi} - S_i$$ → Resolution of the PBE

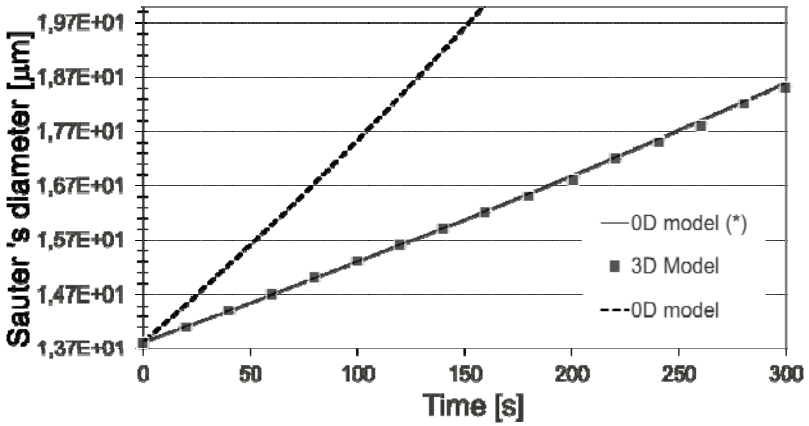
Method of Classes (UDF)

Method of Moments (QMOM)

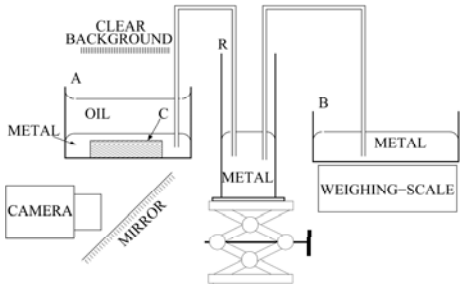
Fixed Pivot (Cell average - *Kumar, 2006*) → ***Bellot,Rimbert, AEM, 2011***

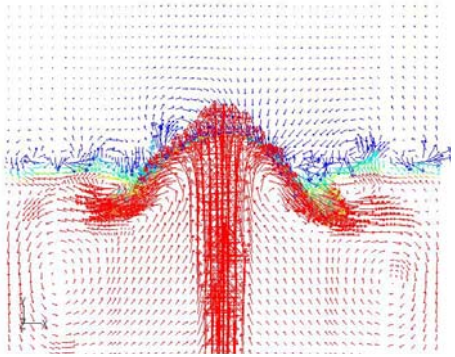

Inclusion numeral density [#/m³]
1,0E+11
1,0E+10
1,0E+09
1,0E+08
1,0E+07
1,0E+06
1,0E+05
1,0E+04
1,0E+03
1,0E+02
1,0E+01
Initial
3D model
0D model
2,0-2,5
2,5-3,2
3,2-4,0
4,0-5,0
5,0-6,3
6,3-8,0
8,0-10,0
10,0-12,6
12,6-15,9
15,9-20,0
20,0-25,2
25,2-31,7
31,7-39,9
39,9-50,2
50,2-63,2
63,2-79,6
79,6-100,2
100,2-126,2
Class [µm]


Mass of inclusions [Kg]
1,48
1,43
1,38
1,33
1,28
1,23
1,18
1,13
1,08
0D model (*)
3D model
0D model
0
50
100
150
200
250
300
Time [s]


Sauter 's diameter [µm]
1,97E+01
1,87E+01
1,77E+01
1,67E+01
1,57E+01
1,47E+01
1,37E+01
0D model (*)
3D Model
0D model
0
50
100
150
200
250
300
Time [s]

Research approach





Laboratory experiments

" Microscopic scale"

Modeling of the mechanisms

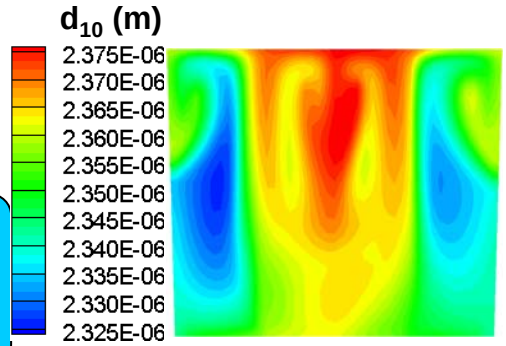
Elementary Phenomena

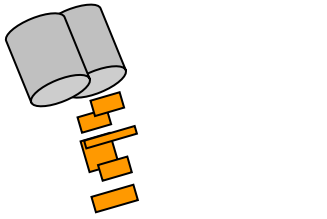
Materials Processing

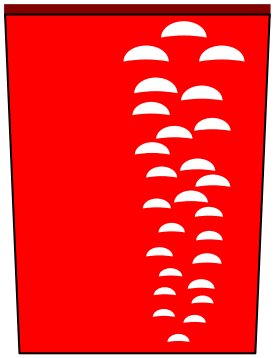
Trials on industrial plants

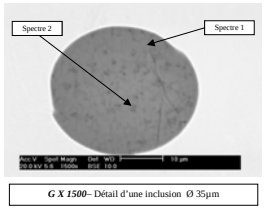
"Macroscopic scale"

Num. Sim. of the process

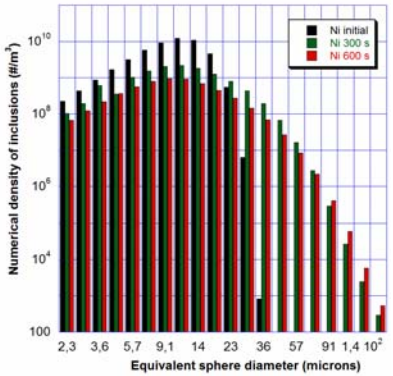






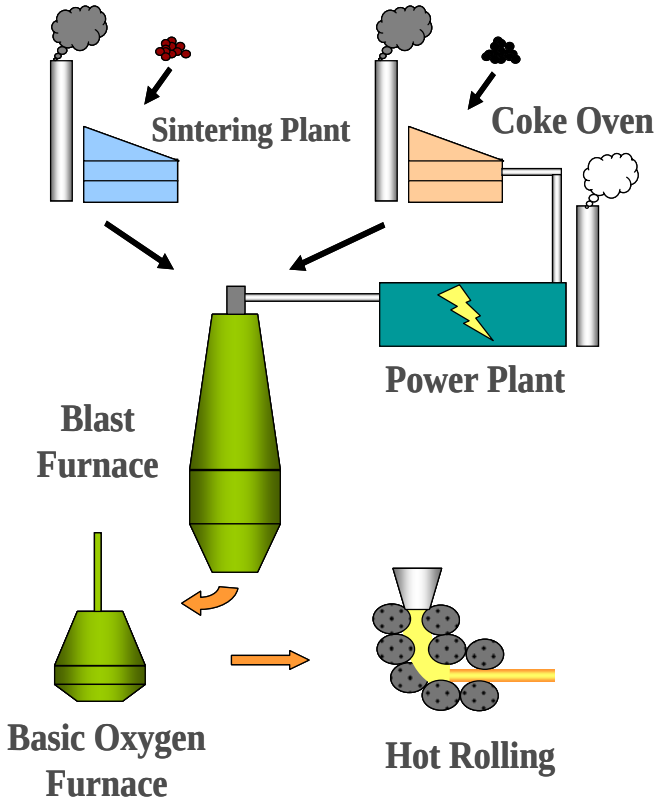


Dip sampling and inclusion counting



2nd Example: Environmental assessment using LCA

Life Cycle Analysis



Classical integrated Steelmill

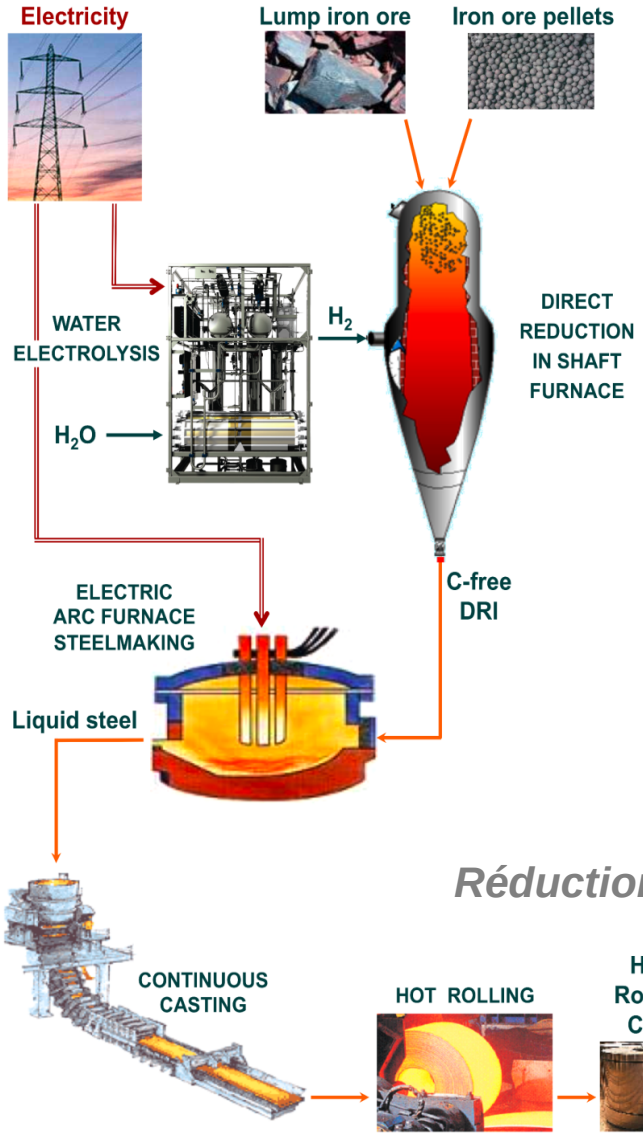
1 ton of hot rolled coiled

~

2 tons of CO_2 released in the atmosphere

2nd Example: Environmental assessment using LCA

Life Cycle Analysis



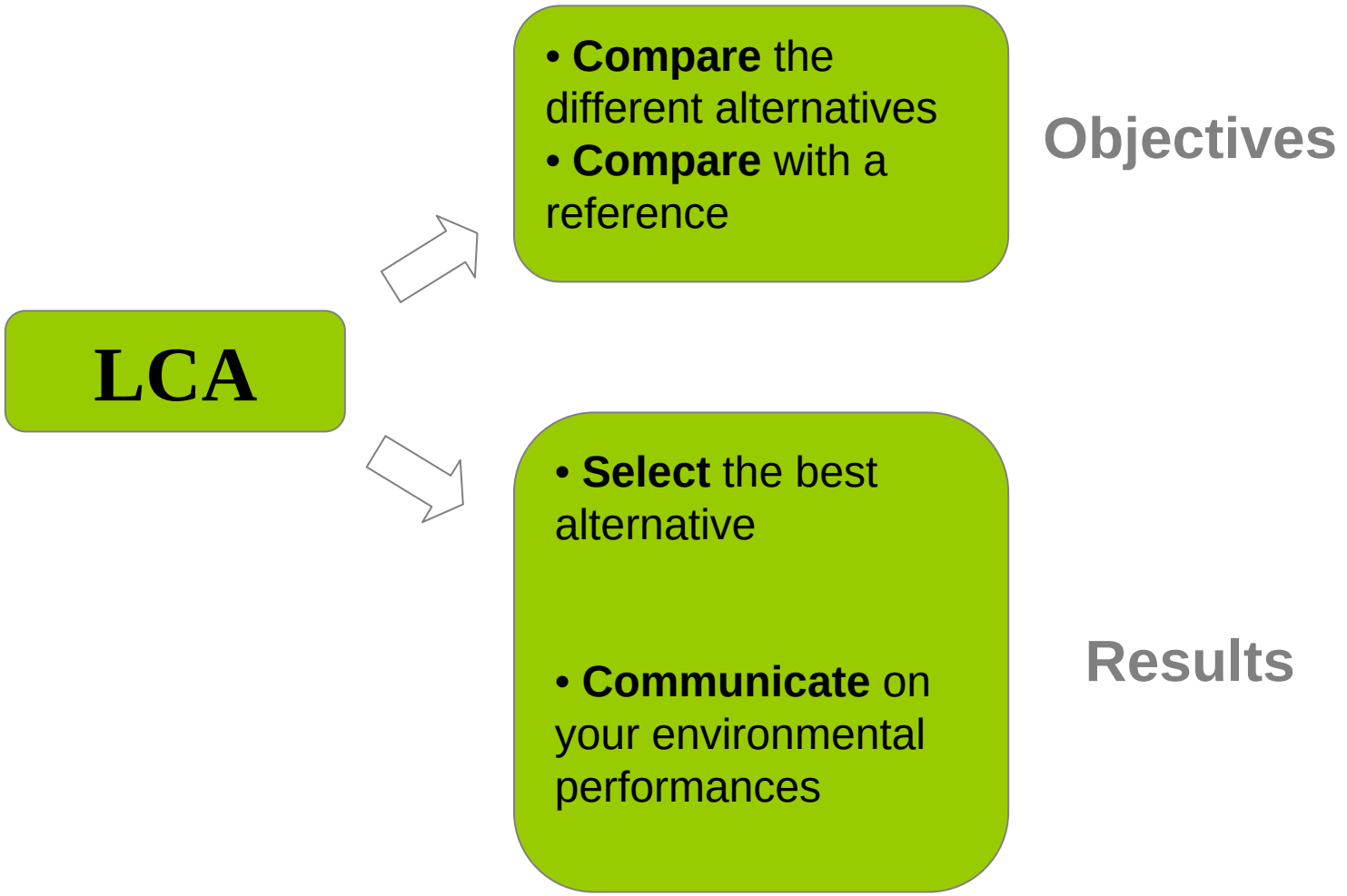
Réduction Directe à l'H_2

1 ton of hot rolled coiled

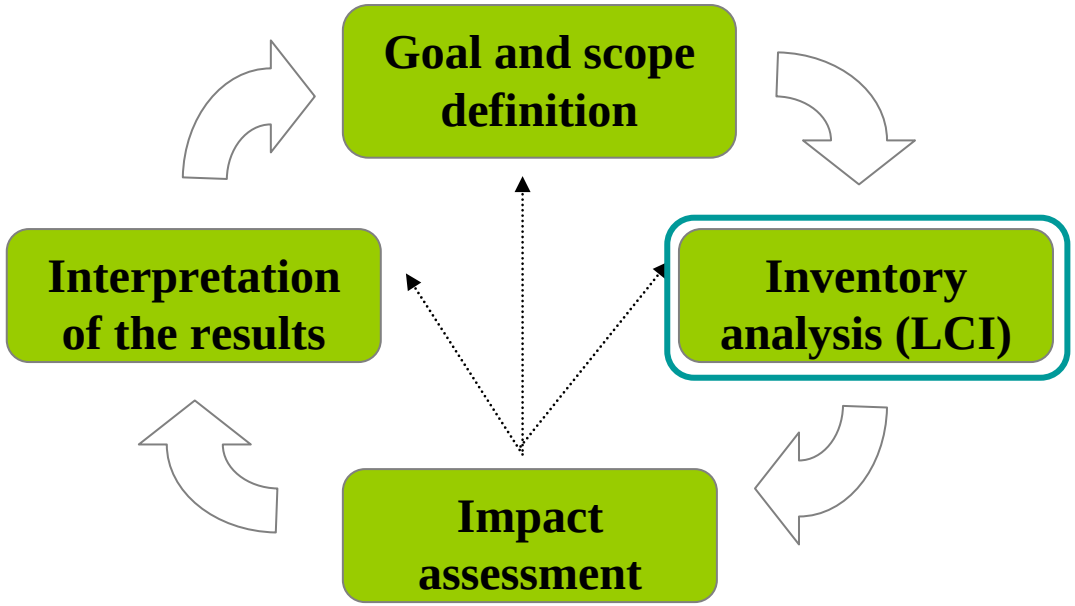
~

?? of CO_2 released in the atmosphere

Methodology

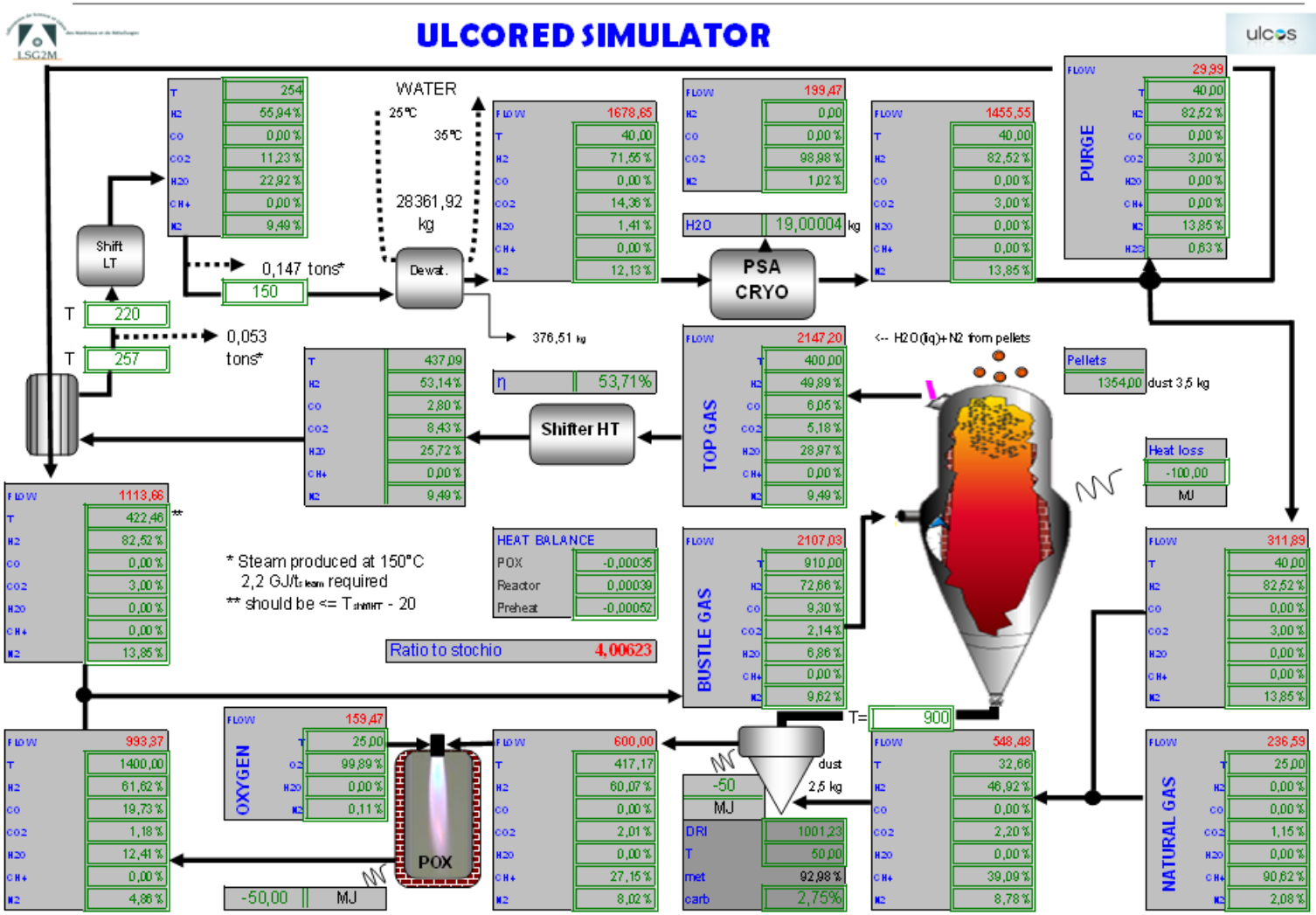


Methodology



- For processes that do not exist yet, no data are available
- We need to calculate those data

ULCORED modelling

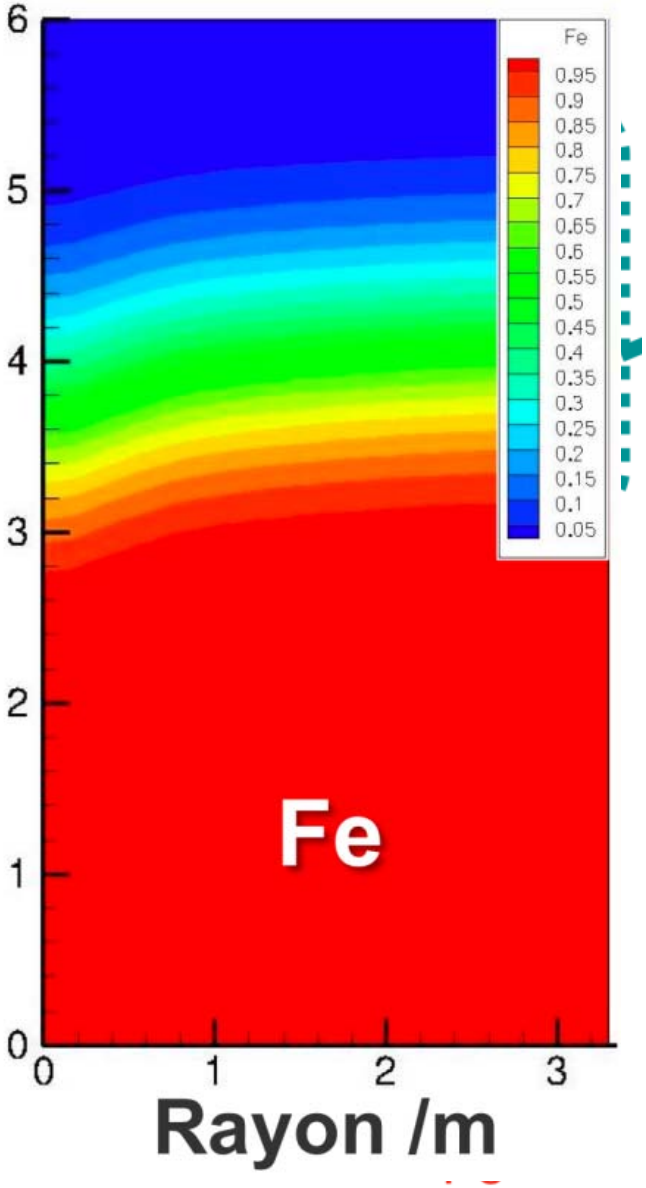


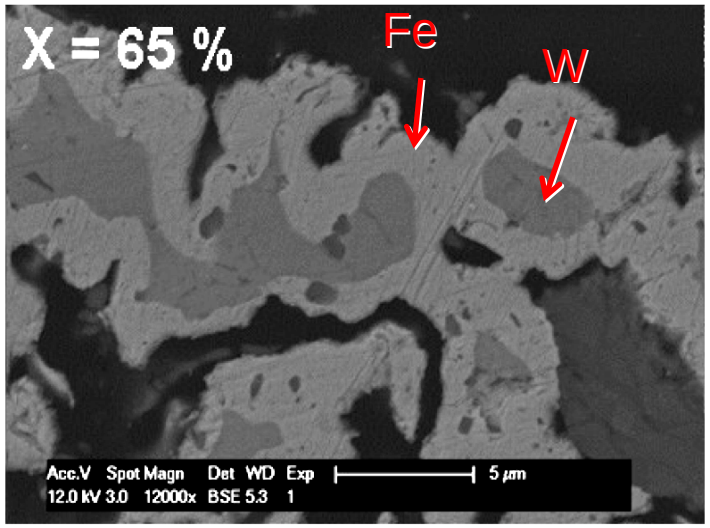
boulettes

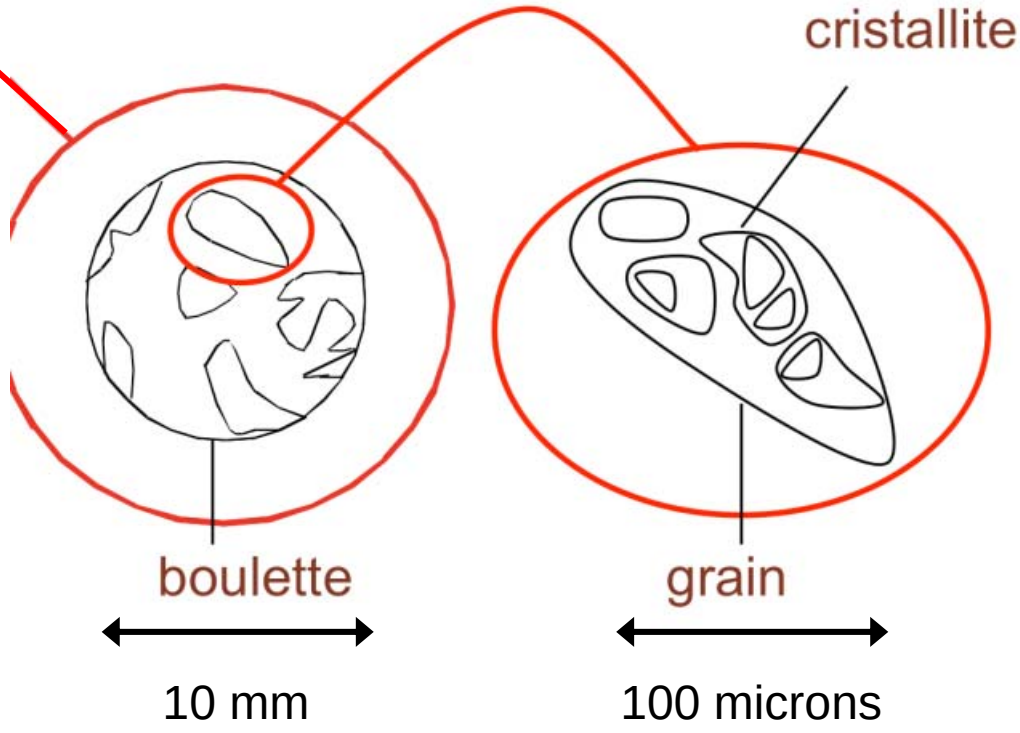
'CFD Modelling'

Fe_2O_3

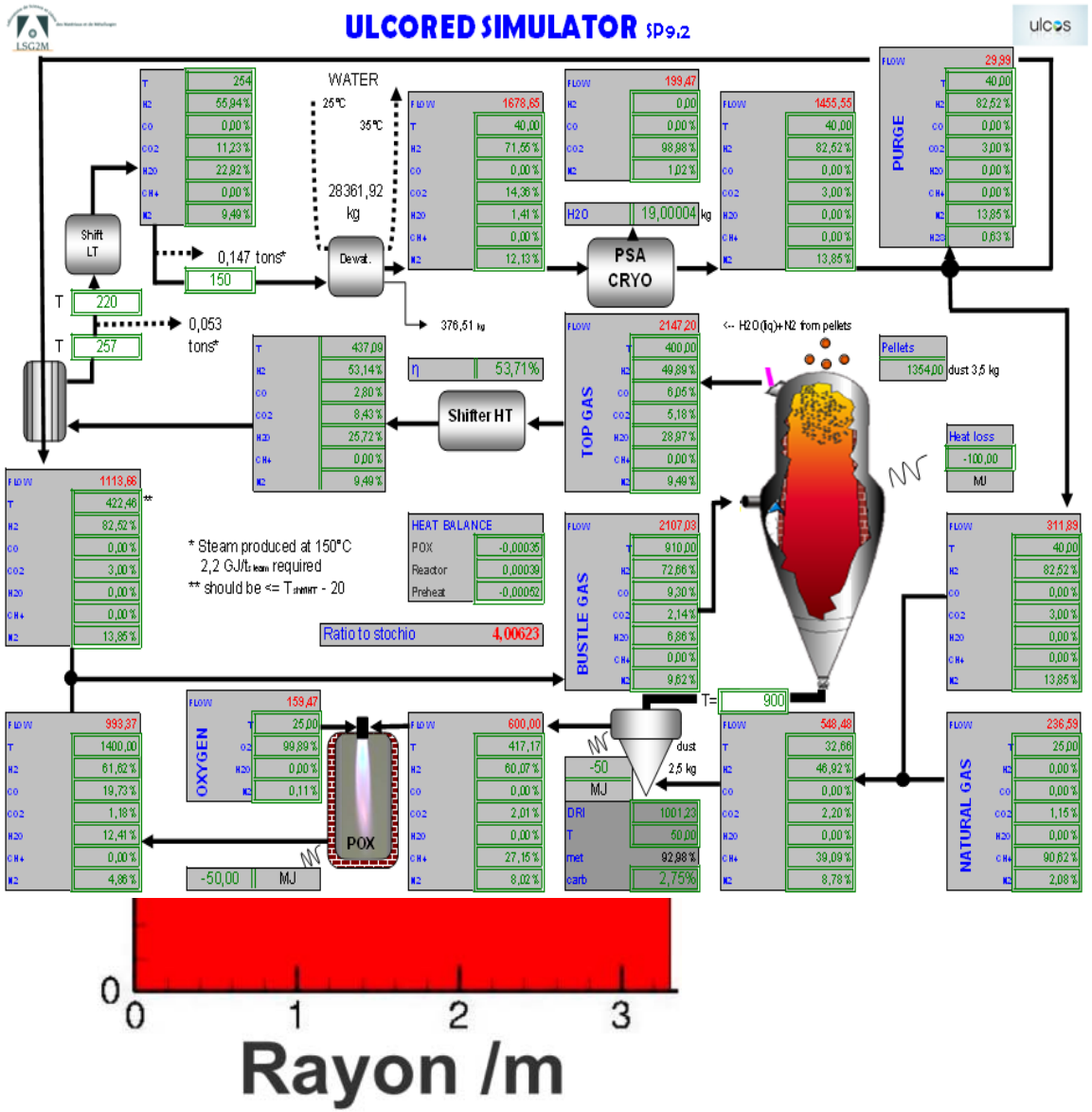
gaz de







‘CFD Modelling’



What about the experiments?

Experimental approach

- **High temperature**
- **Liquid reactivity**
- **How to see through opaque liquid materials?**

- **Numerical simulation**

Pyrometallurgy:

- Worcester Polytechnic Intitute, MA, USA (M. Makhlouf)
- Mac Gill University, Canada (R. Guthrie)
- University of British Columbia, BC, Canada (A. Mitchell)
- University of Illinois (Urbana Champaign), USA (B. Thomas)
- University of Birmingham, UK (M. Ward)
- University of Illmenau, Germany (C. Karcher)
- University of Leoben, Austria (S. Michelic)
- University of Sendaï, Japan (S. Tanigushi)
- …

Réseau National de Plateformes d'Elaboration d'alliages métalliques par passage à l'état liquide

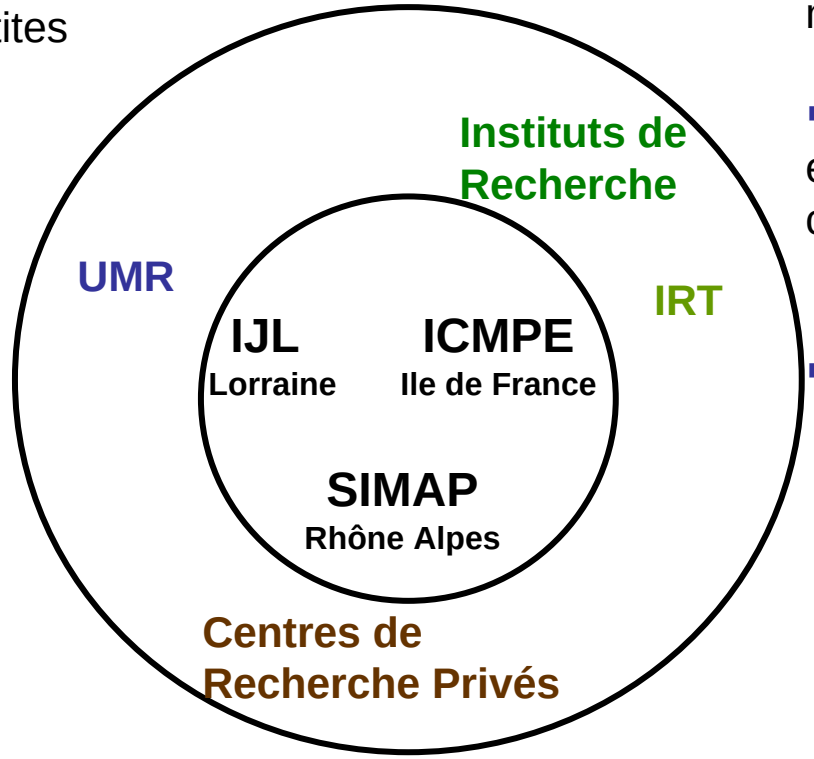
Le constat

Les points faibles:

- Difficultés pour maintenir les compétences techniques et scientifiques sur les procédés
- Un manque critique de petites expérimentations soignées

Les points forts:

- Equipements d'élaboration lourds de qualité
- Des spécialistes sont encore présents mais la pyramide d'âge est inquiétante



Les objectifs

- Développer des projets de recherche communs
- Coordonner l'usage et la maintenance
- Renforcer les savoir-faire et la transmission des compétences
- Assurer la visibilité

Among the future challenges

- **To make advances in the understanding and the control of the purification phenomena during liquid materials processing**

Multiphase & Multiscale modeling
Interface mass transfer
Thermochemistry

Experiments at the laboratory scale focused on a mechanism

- high energy beamline
- Confocal microscope
- …

- **To develop integrated analysis on a whole processing route so as to compare energy consumption and environmental impacts.**

Main References

(1) Some perspectives on the mathematical modelling of materials processing operations, Julian Szekely and Gerardo Trapaga 1994 *Modelling Simul. Mater. Sci. Eng.* **2** pp.809-828, doi:10.1088/0965-0393/2/4/002

(2) Transport Phenomena, R. Byron. Bird, Warren E. Stewart, Edwin N. Lightfoot, Wiley, New York, 2nd Edition, 2006

(3) Elaboration des matériaux et génie des procédés, Ecole d'été du CNRS, St Pierre d'Oléron, juin 2005, Publié sous la direction de Denis Ablitzer et Jean-Pierre Petitet