

# Thermochemical Modelling in the BOFdePhos Project

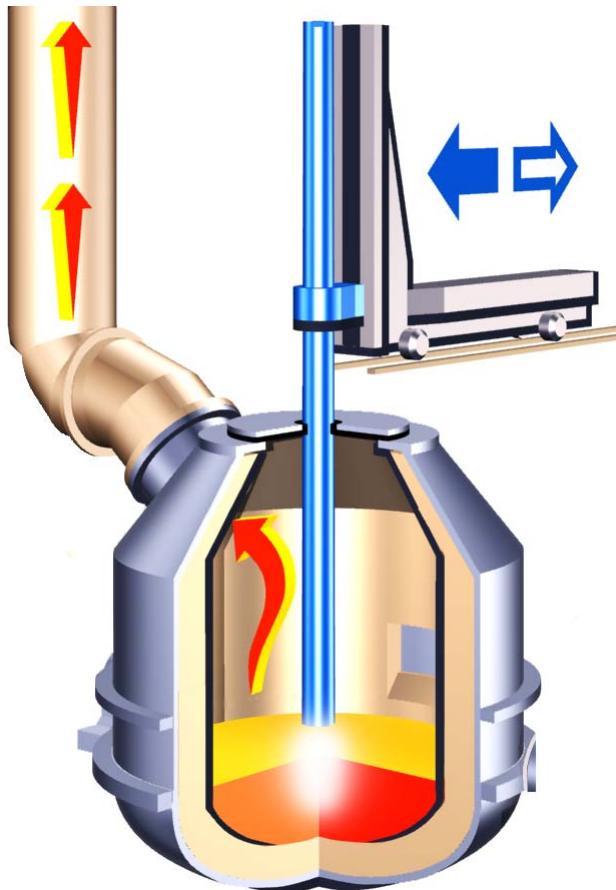
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<sup>1</sup>GTT-Technologies, <sup>2</sup>SMS-Demag

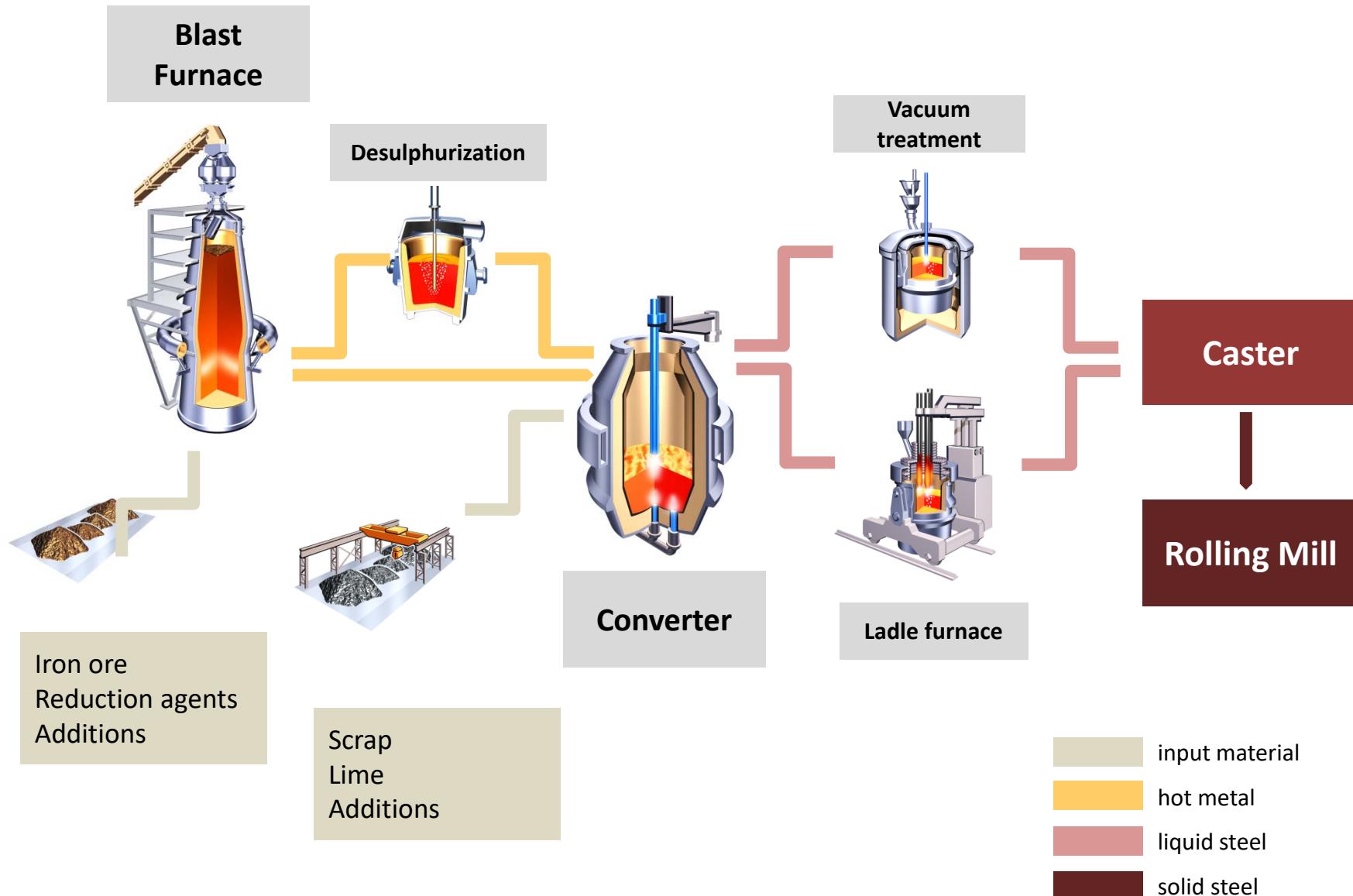
RCCM/GTT User Meeting, Tokyo 2016



# Titel



# Steel Production :The Oxygen Steelmaking route



# Introduction to BOF DePhos project

- BOF DePHOS: Dynamic on-line monitoring and end-point control of dephosphorisation in the BOF converter process
- Project period: 01.07.2014 – 31.12.2017
- Main Objective: Development of a comprehensive dynamic process models for the BOF process, including SimuSage based modelling
  - based on detailed studies of the thermodynamic and reaction kinetics fundamentals
  - determination of the end-point of the process with respect to phosphorus content and melt temperature with higher accuracy
  - to be used for online monitoring and process control
  - application of new sensors measuring the oxygen activity and height of the converter slag



# Project participants

- VDEh-Betriebsforschungsinstitut (BFI)  
Private-sector institute for applied research and development in steel technology
- Tata Steel UK (Tata) Steelmaking company involved with its BOF plants at Port Talbot and Ijmuiden
- SMS Siemag AG (SMS) Supplier for steelmaking and processing plants
- Gesellschaft für Technische Thermochemie und –physik mbH (GTT)  
Supply and consulting with respect to thermochemical databases and related software
- Kungliga Tekniska Hoegskolan (KTH) Technical university with wide activities in metallurgical and materials processes
- Minkon GmbH (Minkon) Supplier for sampling technology and measuring sensors for metallurgical processes



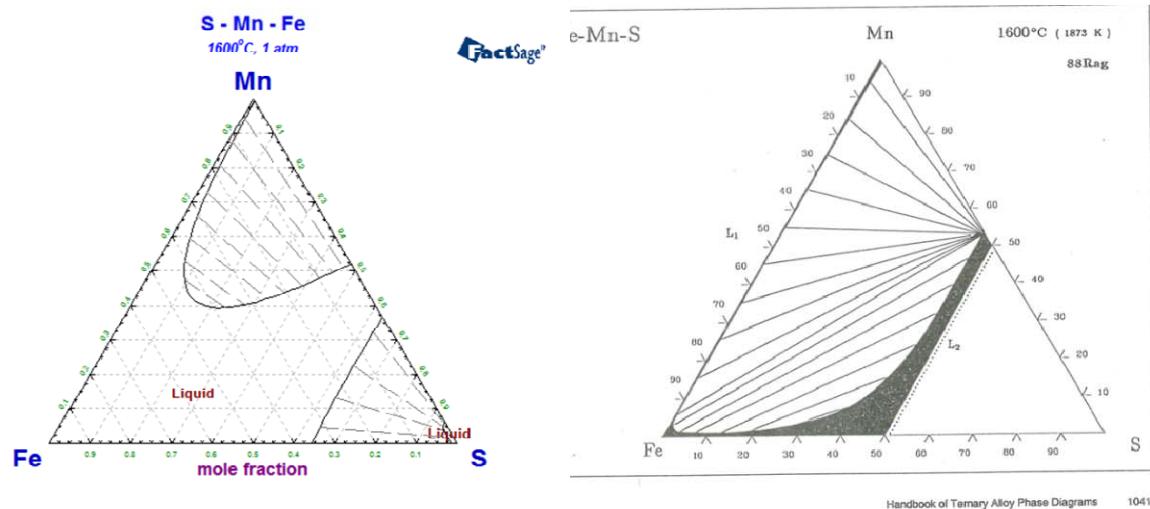
# GTT involvement in BOFdePhos

- Main activities of GTT are:
  - generation of a self-consistent thermodynamic database
  - generation of stand-alone process model based on interlinked local equilibria (with SMS)
  - integration of new thermodynamic database into process model (with SMS)
  - integration of third party kinetic models, especially CaO-dissolution, into process model (with SMS and KTH)
  - making available sub-models (to BFI and SMS)



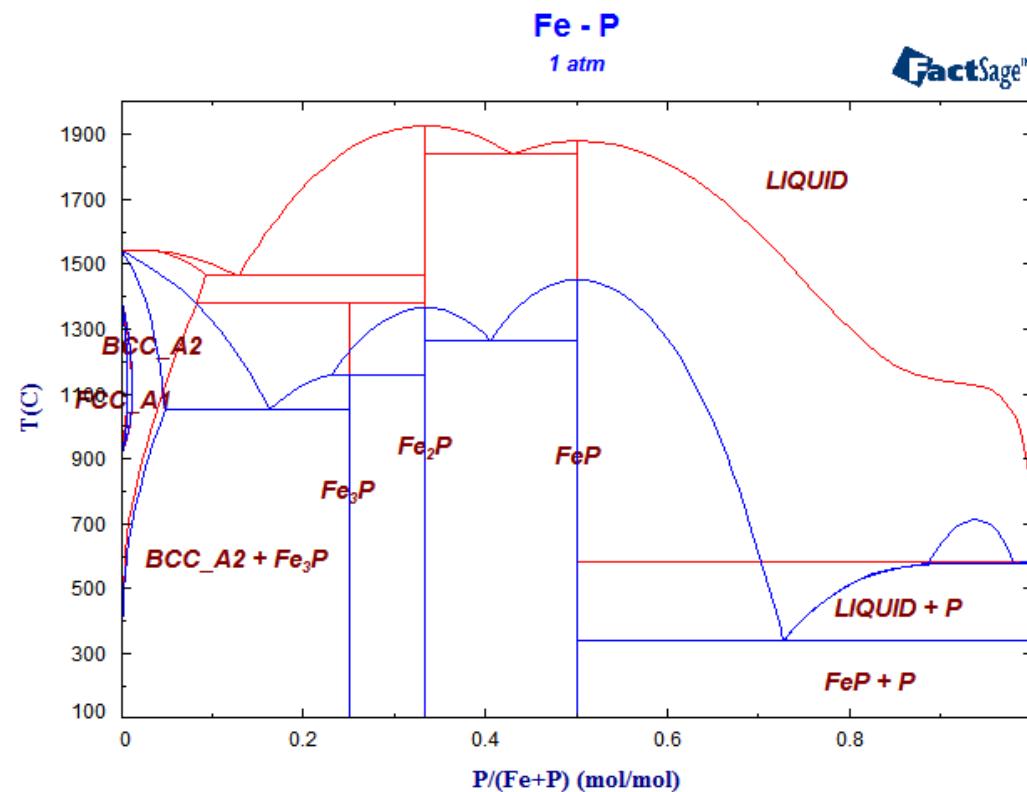
# Generation of a self-consistent thermodynamic database

## Data revision - Part 1



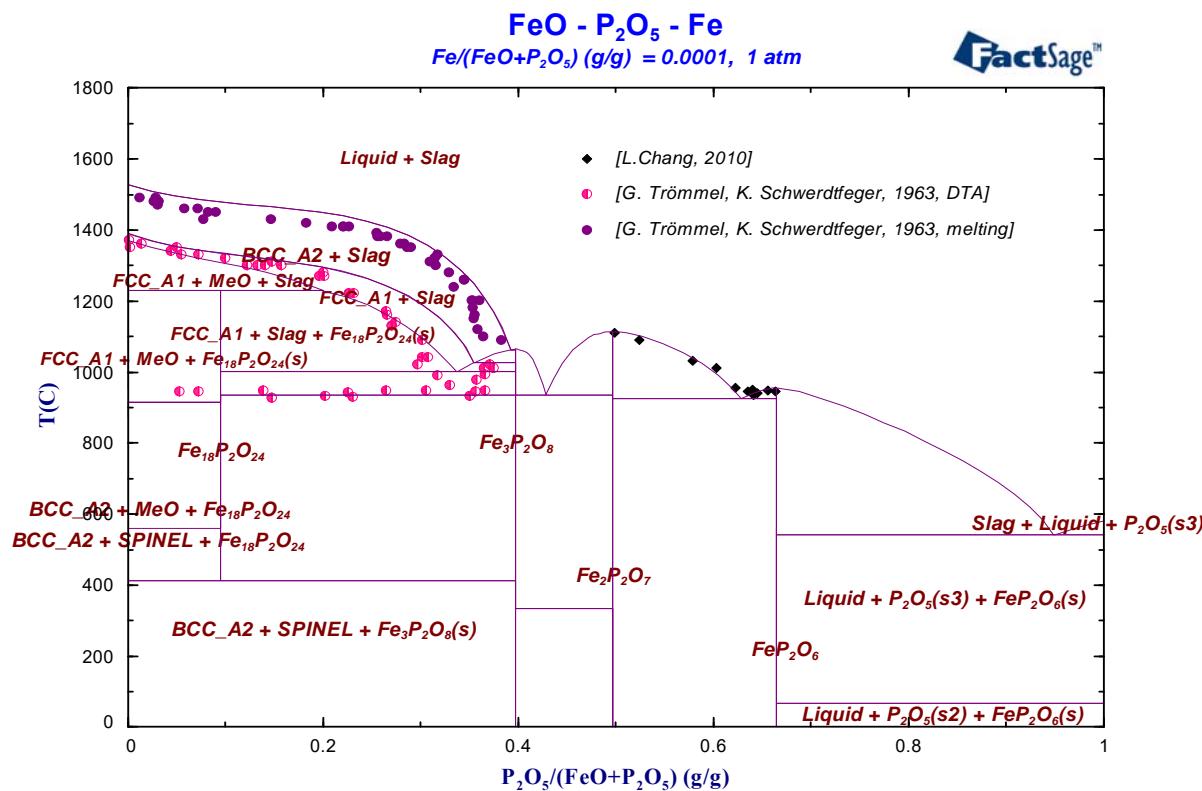
# Generation of a self-consistent thermodynamic database

## Data revision - Part 2



# Generation of a self-consistent thermodynamic database

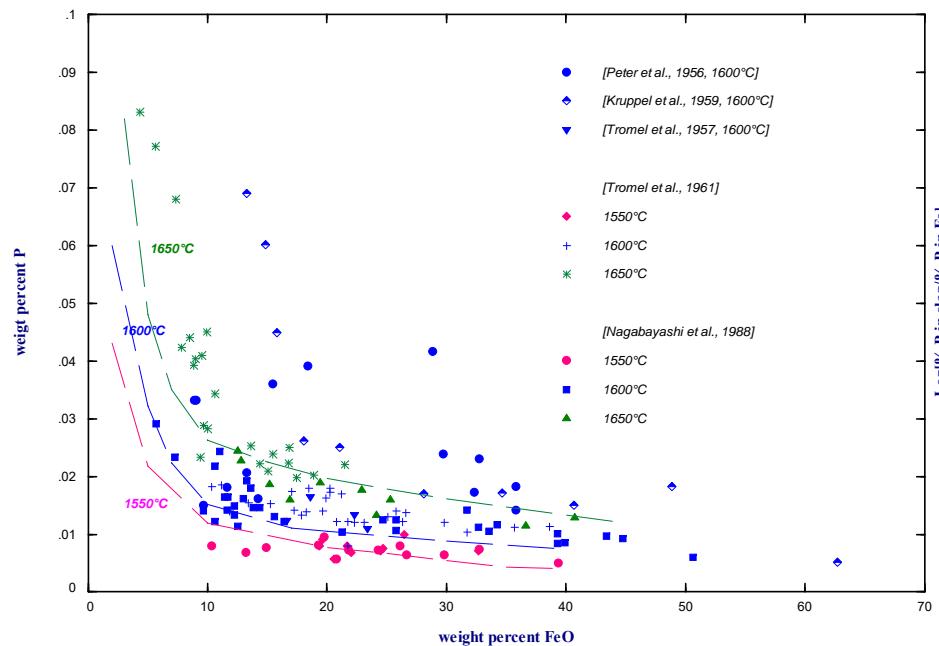
## Data revision - Part 2



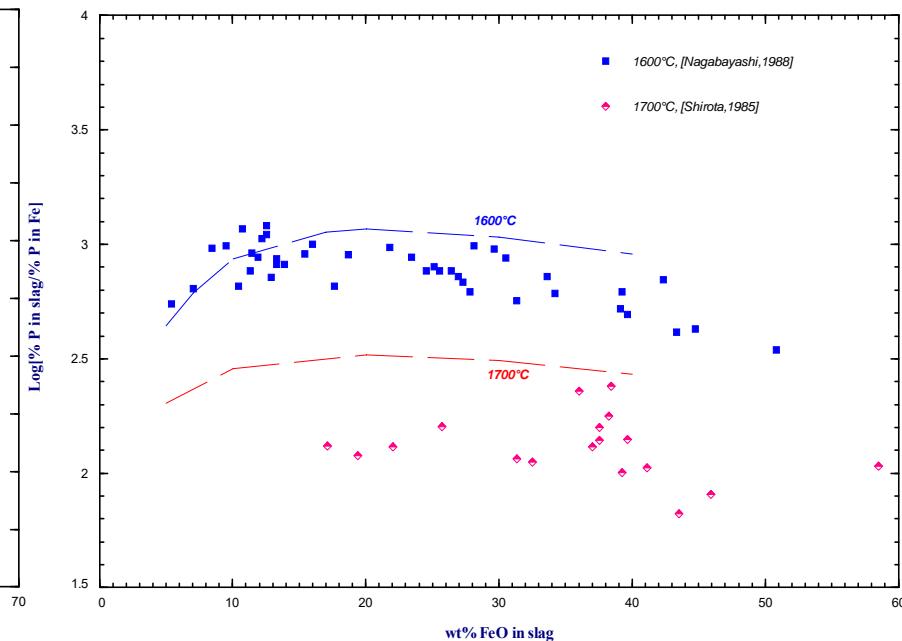
# Generation of a self-consistent thermodynamic database

## Data revision - Part 2

Relationship between [%P] in liquid Fe and (FeO) in slag

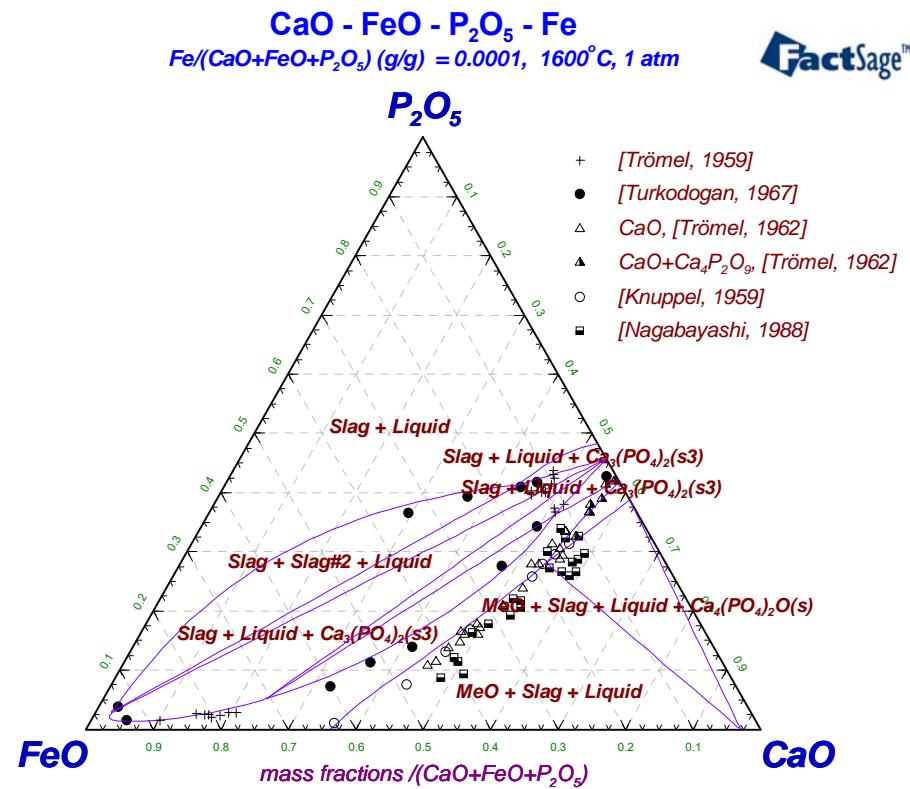


The  $L_p$  between molten iron and the slag along the CaO saturation.



# Generation of a self-consistent thermodynamic database

## Data revision - Part 2

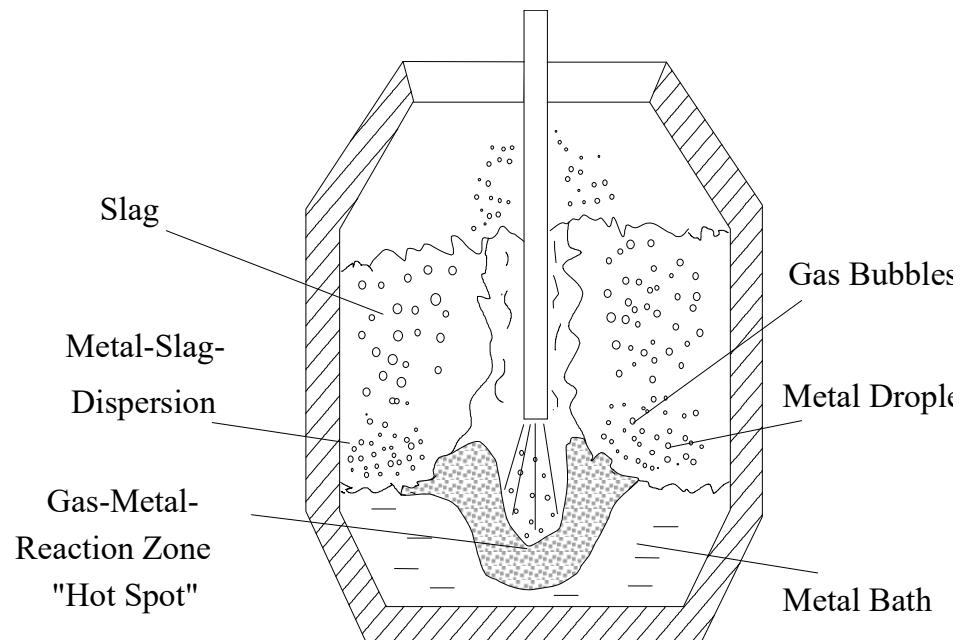
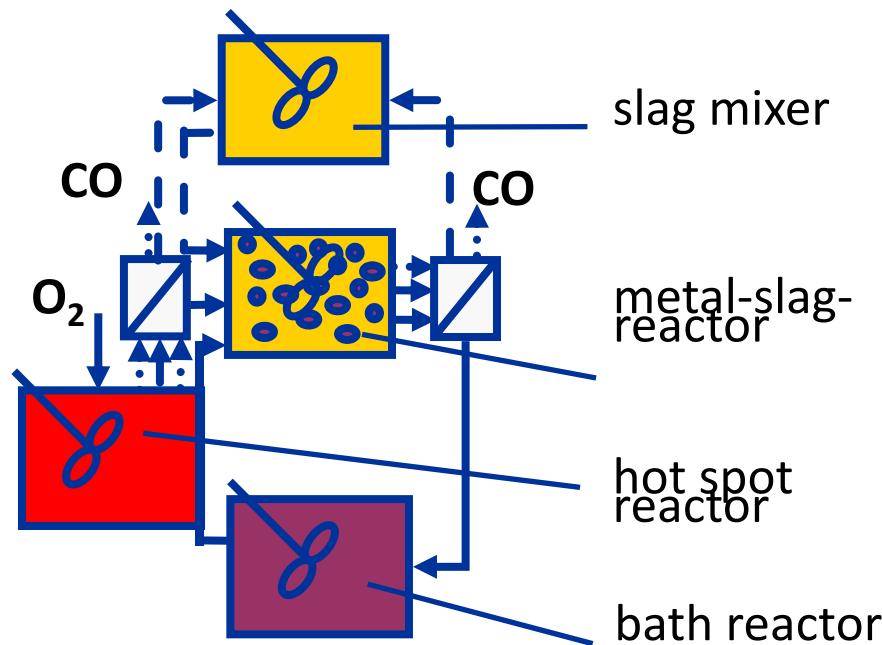


# Generation of stand-alone process model

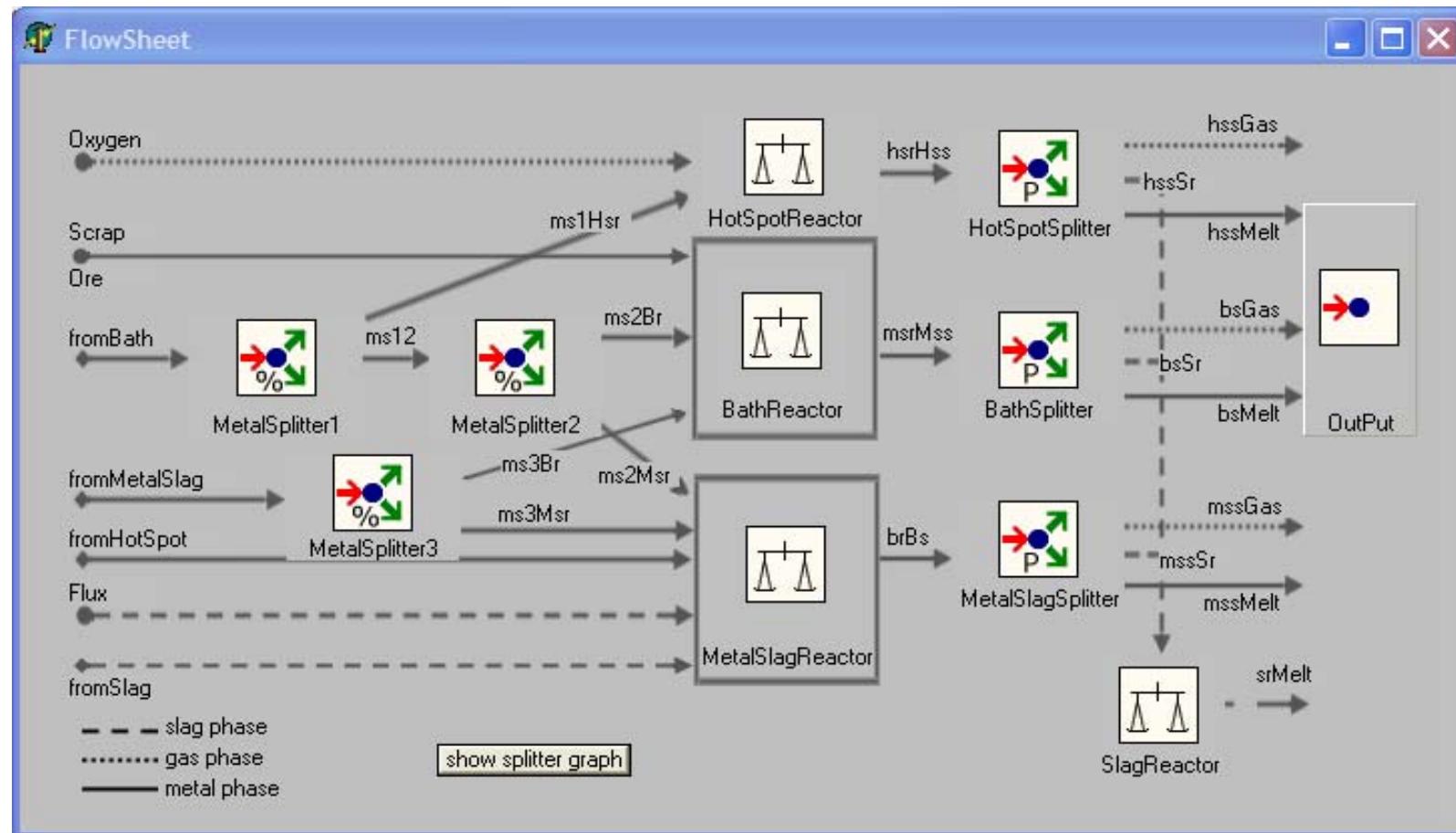
- Original Model: Traebert model
- New LD-Sage Model
  - Flowsheet
  - Preliminary results
  - The liquid slag issue
  - Reconsider the Traebert Model
  - Model redesigned
  - Aspect of simulating with SimuSage



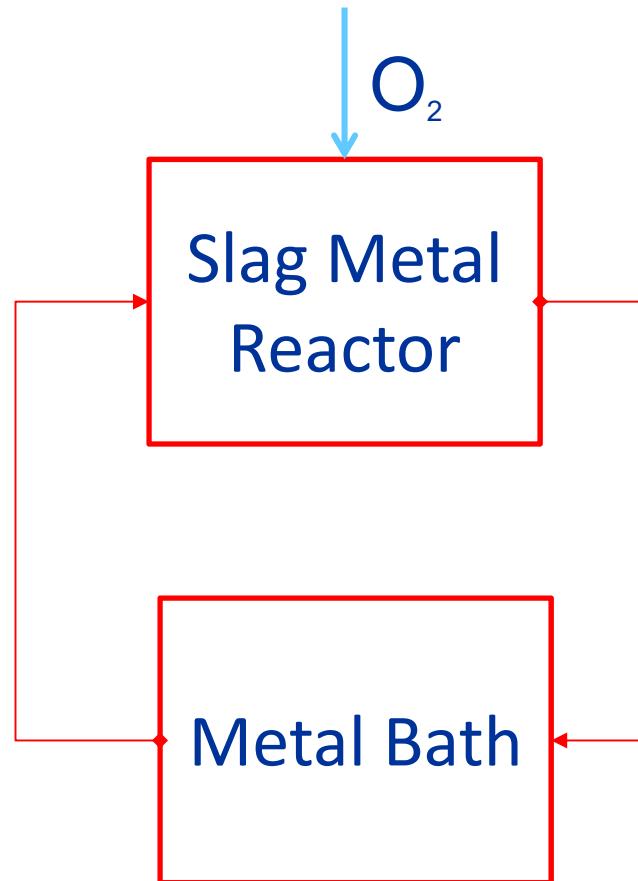
# Original Model: Traebert Model (1999)



# Flowsheet of the Traebert Model

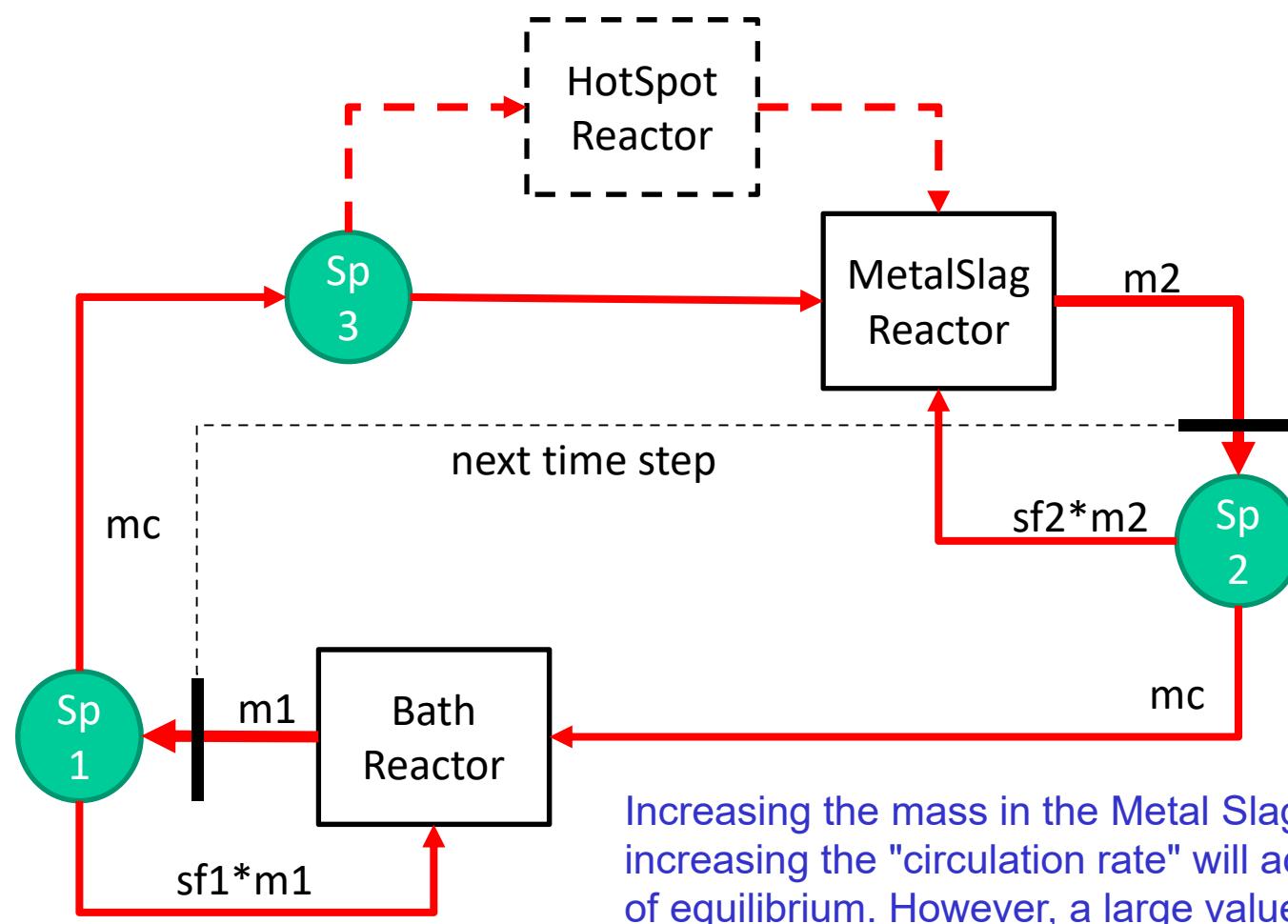


# First new LD-Sage concept (2015)



# New Pattern of Metal Circulation\*:

\*the contribution of scrap dissolution to  $m_1$  is not shown



In this :

$$sf1 = 1 - \frac{mc}{m1}$$

$$sf2 = 1 - \frac{mc}{m2}$$

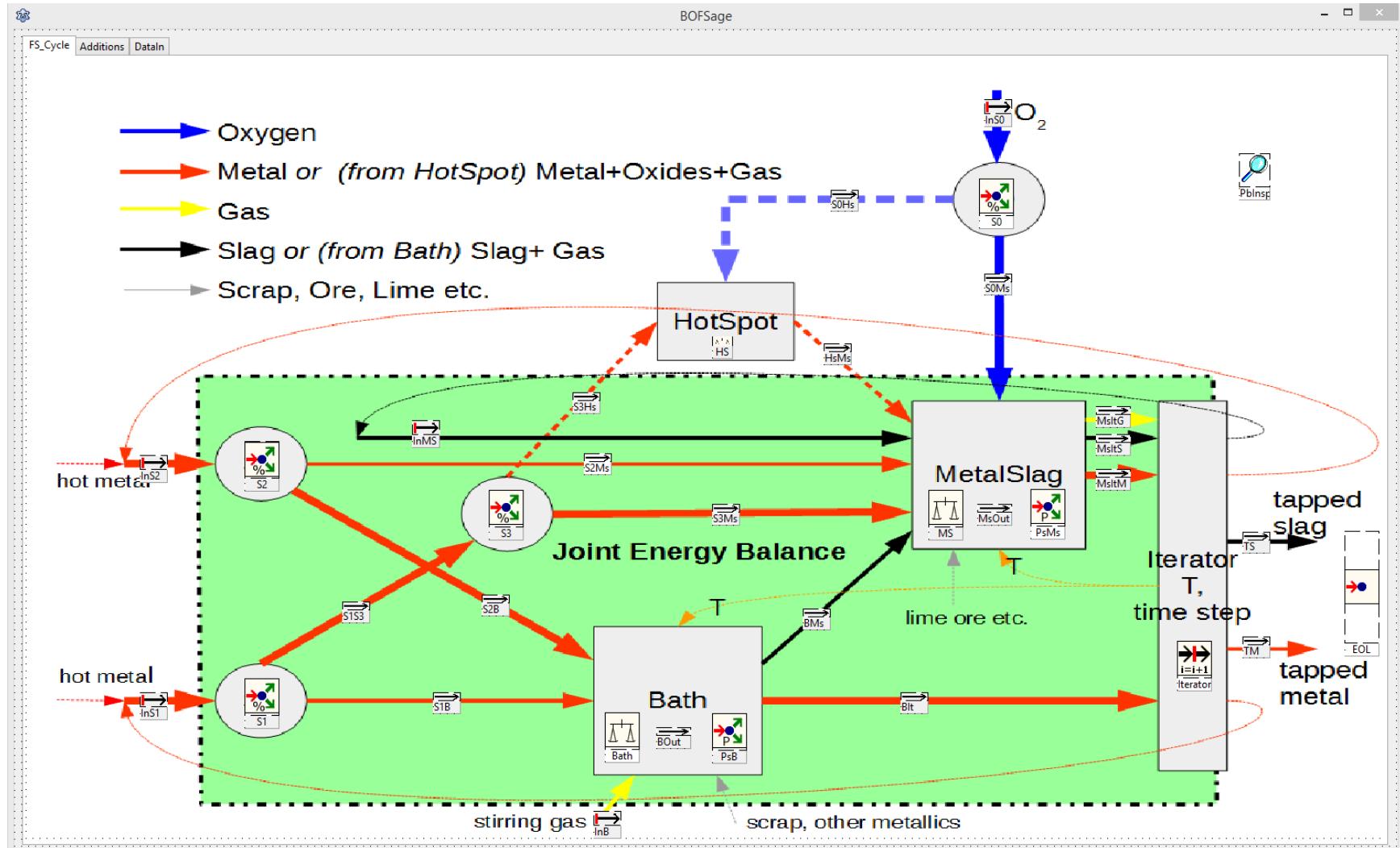
$mc$  = circulation rate\*  $\Delta t$   
 $\Delta t$  = iteration time step

Since  $mc$  cannot exceed  $m_1$  or  $m_2$   
high circulation rates will require small  $\Delta t$ .

Increasing the mass in the Metal Slag Reactor  $m_2$  as well as increasing the "circulation rate" will accelerate the achievement of equilibrium. However, a large value for  $m_2$  will mean that the process is close to equilibrium right from the beginning.

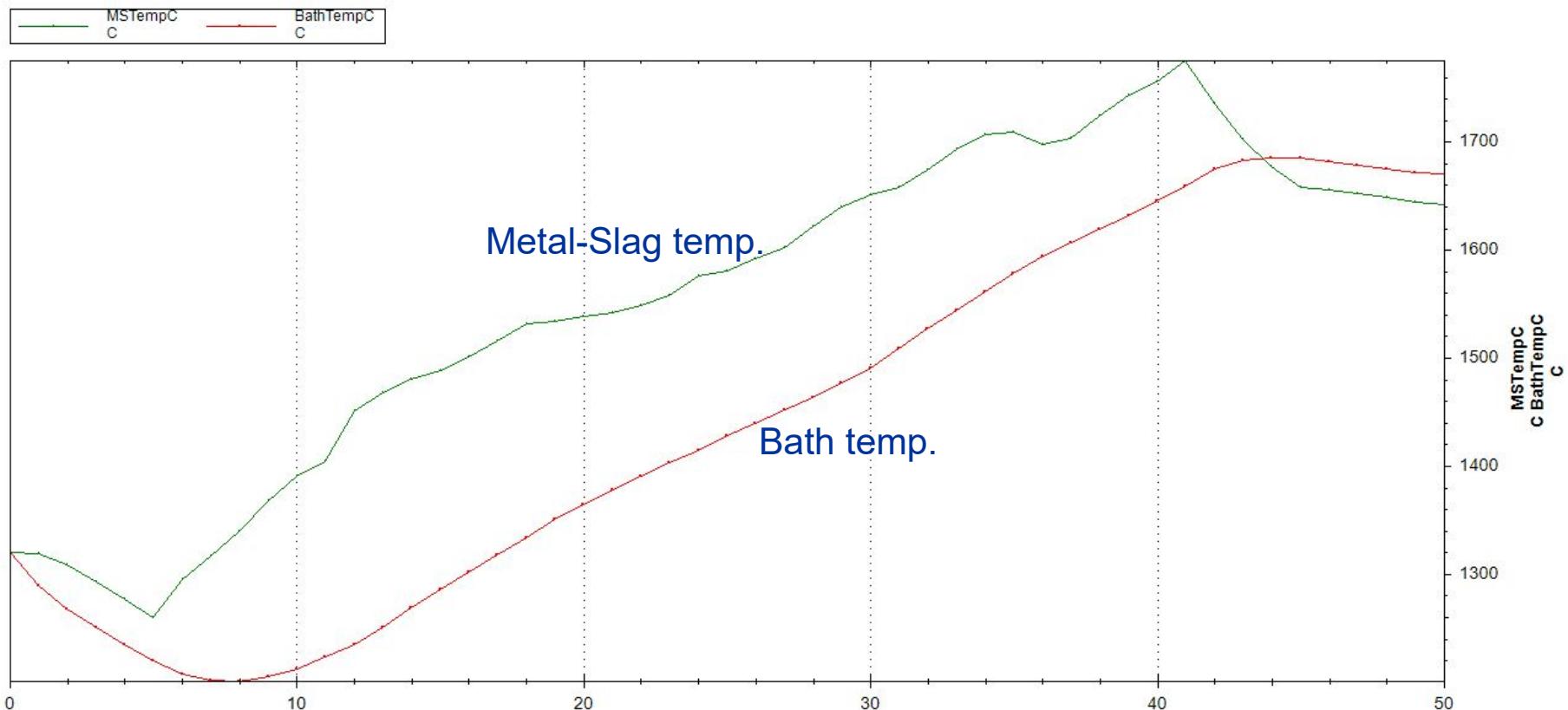


# Flowsheet of the new LD-Sage model



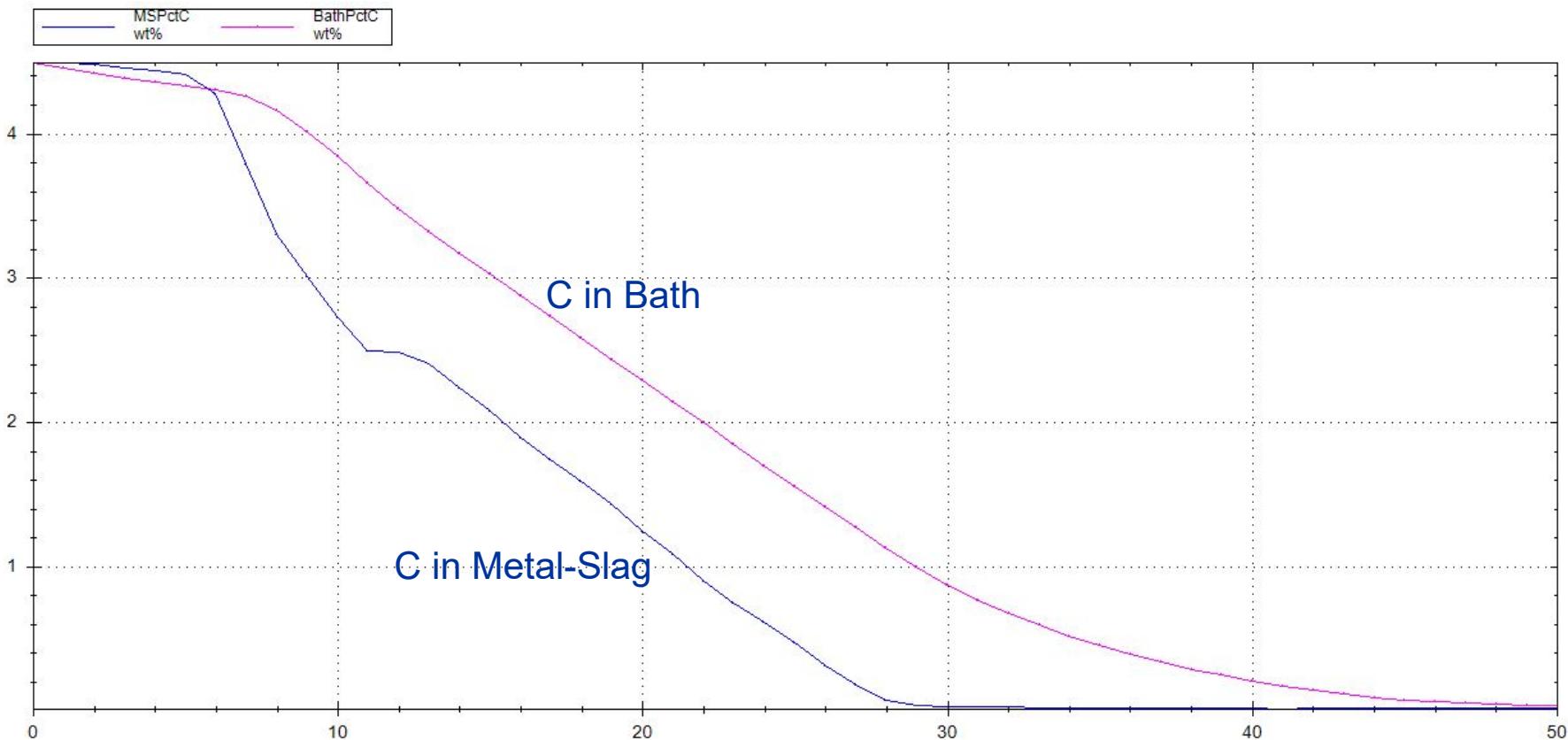
# Preliminary results of the first new LD-Sage model

## Temperatures in Model Cells vs time



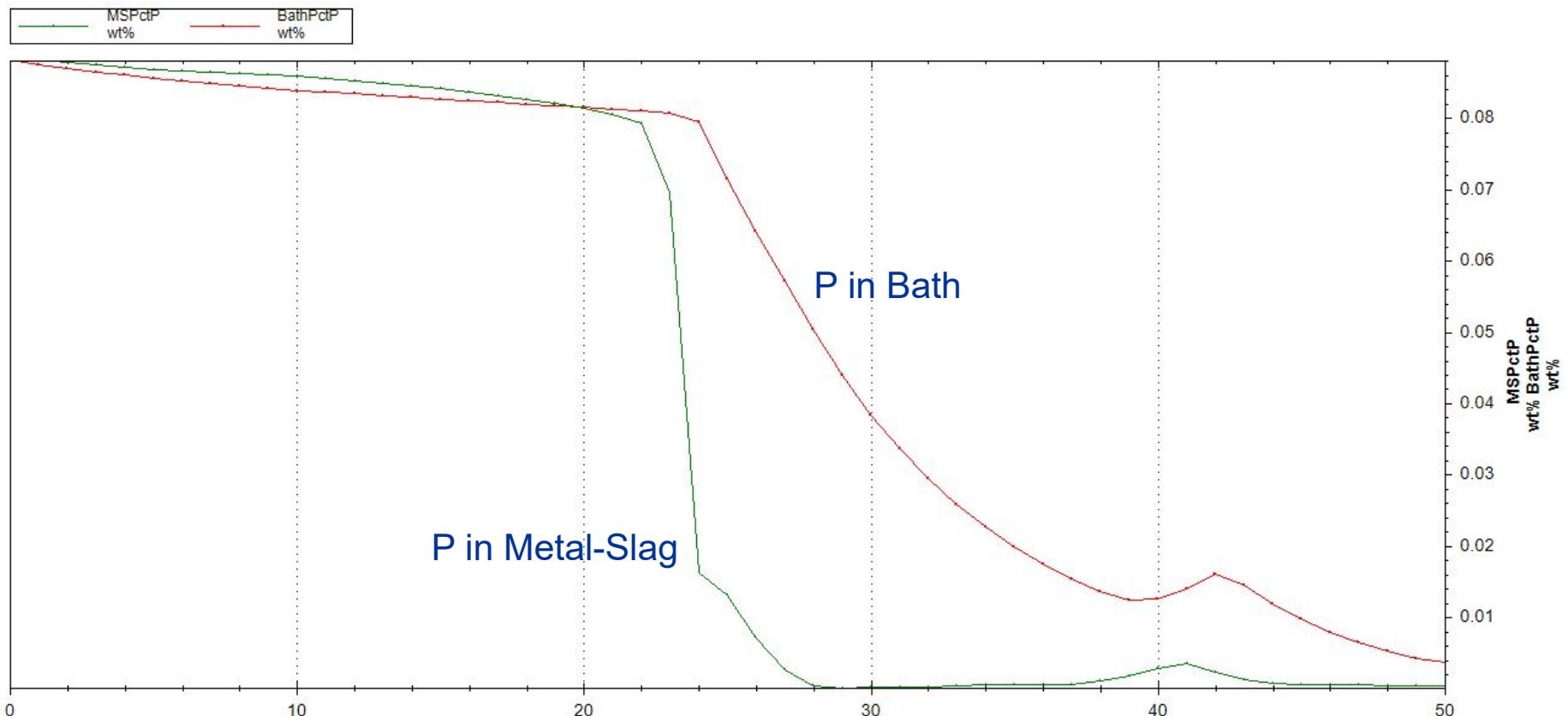
# Preliminary results from new LD-Sage model

## Mass% C in Model Cells vs time

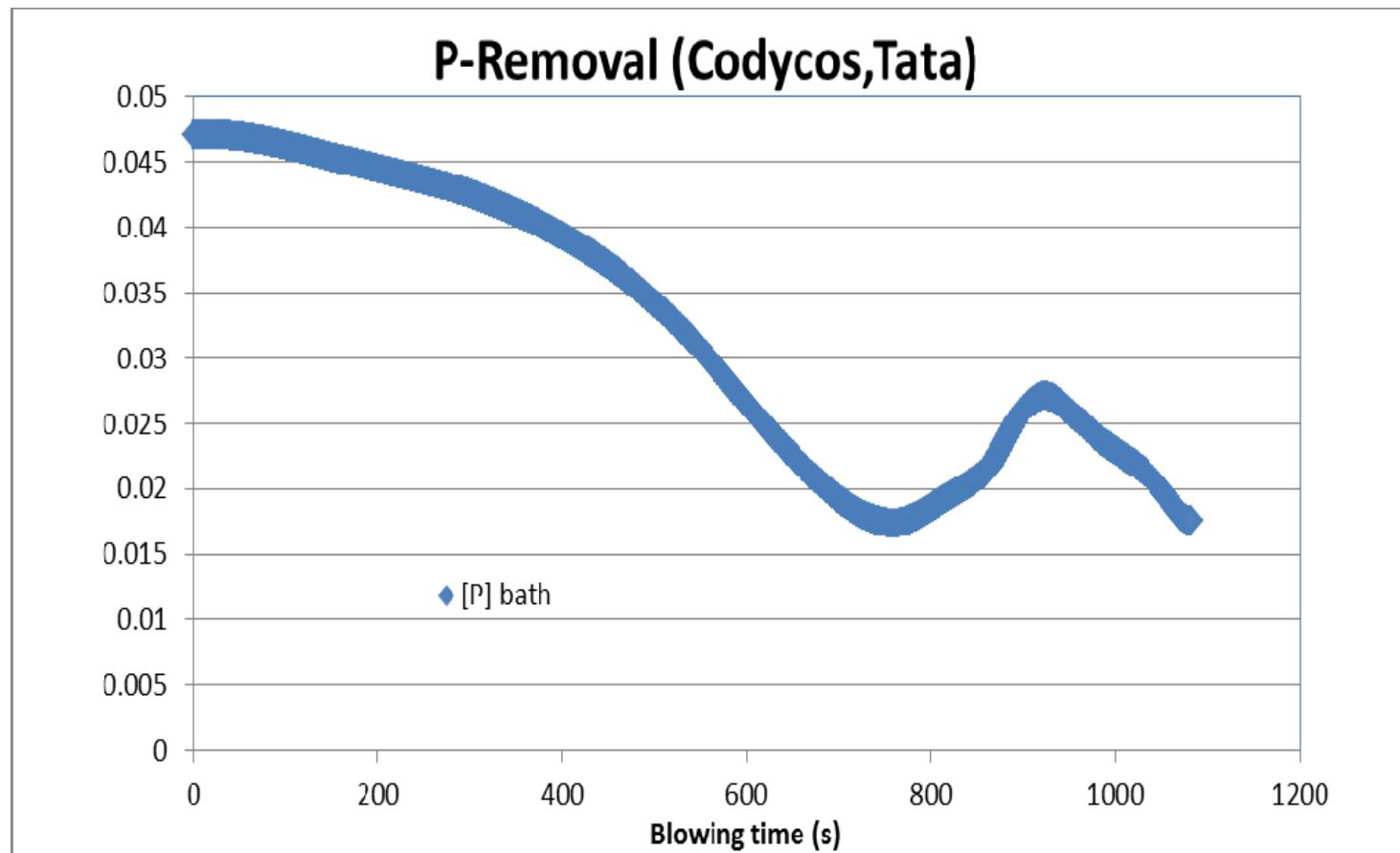


# Preliminary results from new LD-Sage model

## Mass% P in Model Cells vs time



## P-removal profile calculated by a project partner model (Tata, Codycos model)

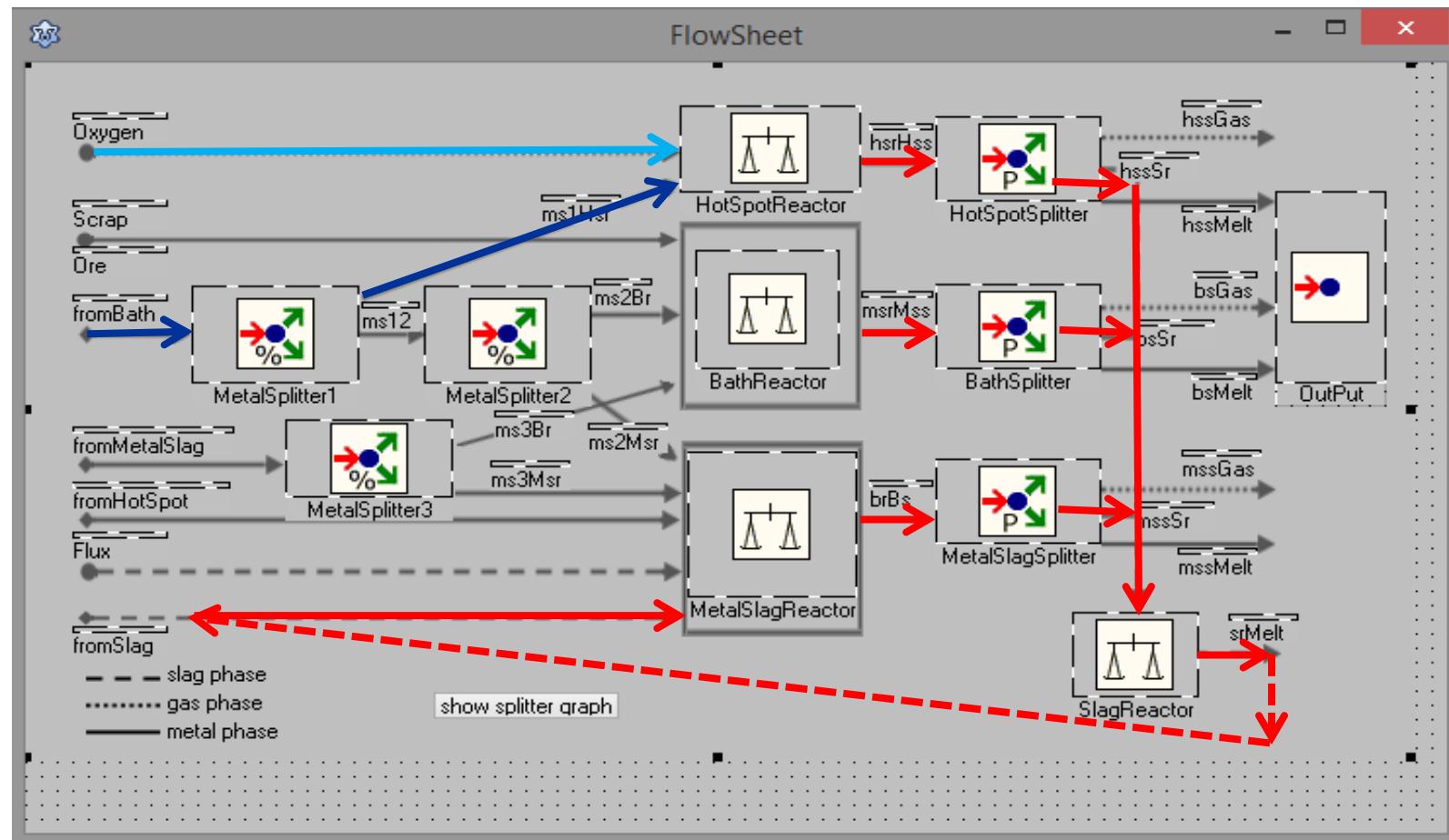


- KTH: Laboratory experiments on lime dissolution – what sort of slag are we to use?
  - 1<sup>st</sup> revelation: lime in a sea of slag is not the correct picture because initially there is an enormous amount of lime and very little slag
  - 2<sup>nd</sup> revelation: equilibrium calculations show that there is no liquid slag in contact with metal in the first half of the blow (this was found by other authors as well)
- The second point meant that we checked our database against literature and other data bases
  - => good agreement with literature (Phase diagrams)
  - => consistency of results with respect to equilibria between liquid metal, lime and oxygen: no slag formation

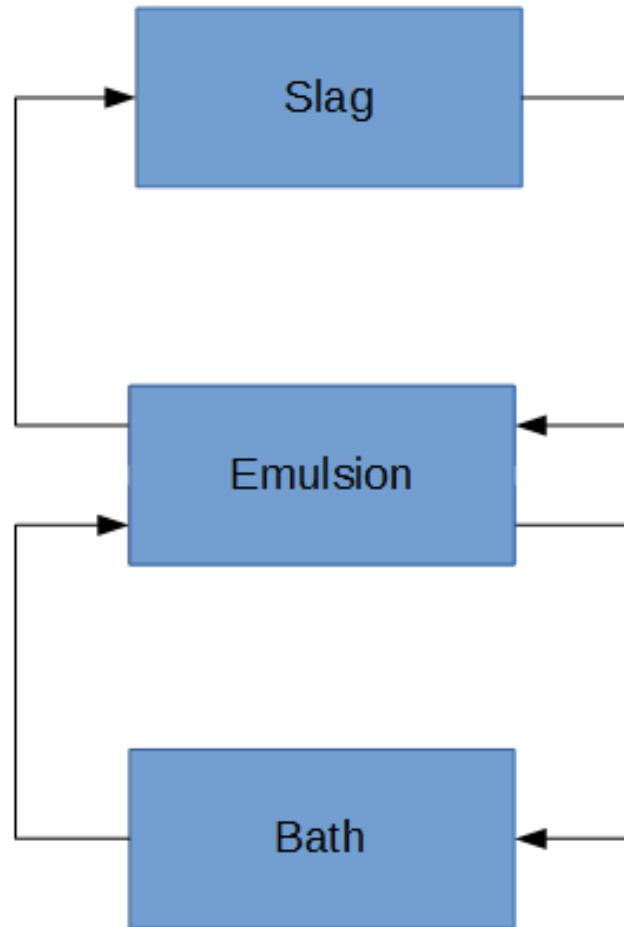
**Final conclusion: → Model needs to be redesigned**



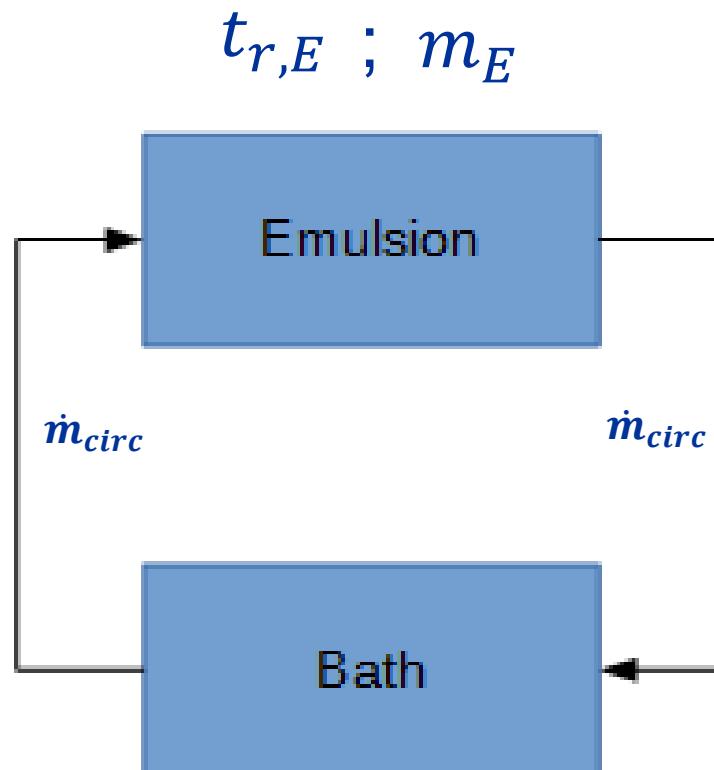
# Why did the Traebert Model show liquid slag?



# LD-Sage model including a buffer of oxides and slags



# Simulating dynamic processes with SimuSage: residence time/circulation rate/ reactor size

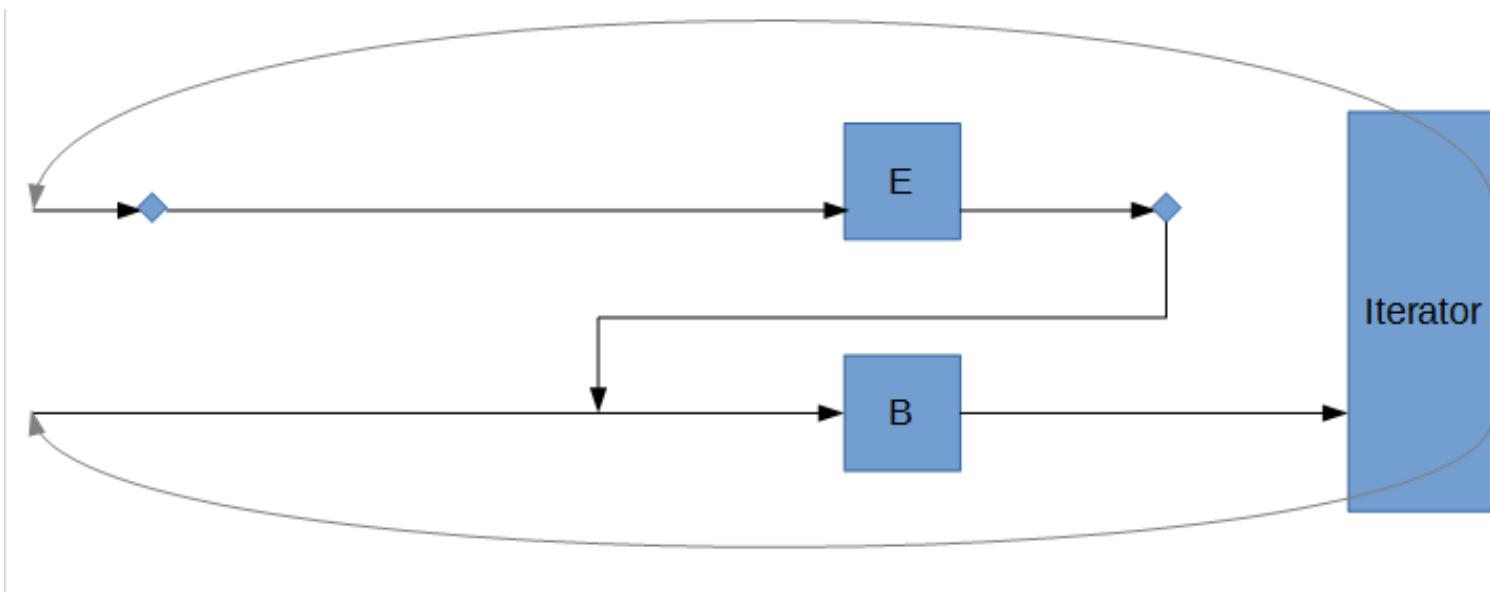


Reactor size

$$m_E = \dot{m}_{circ} * t_{r,E}$$

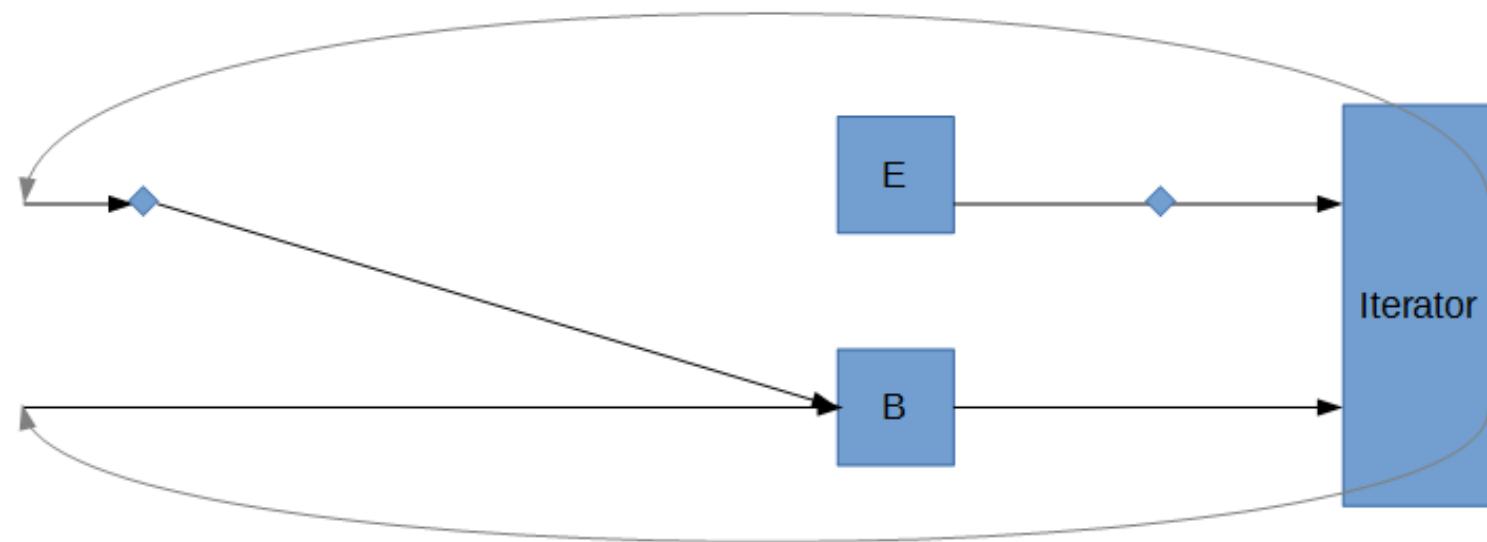
$$m_B = \dot{m}_{circ} * t_{r,B}$$

# Simulating dynamic processes with SimuSage: residence time and circulation rate



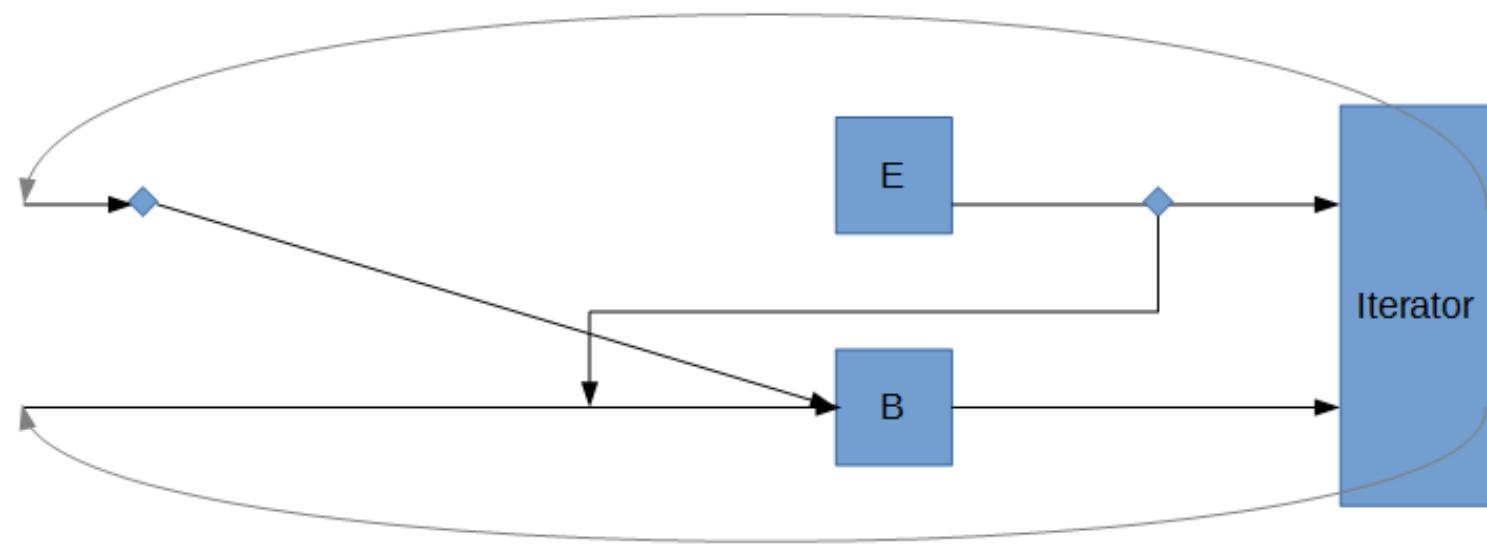
$$t_{r,E} = 0$$

# Simulating dynamic processes with SimuSage: residence time and circulation rate



$$t_{r,E} = t_{timestep}$$

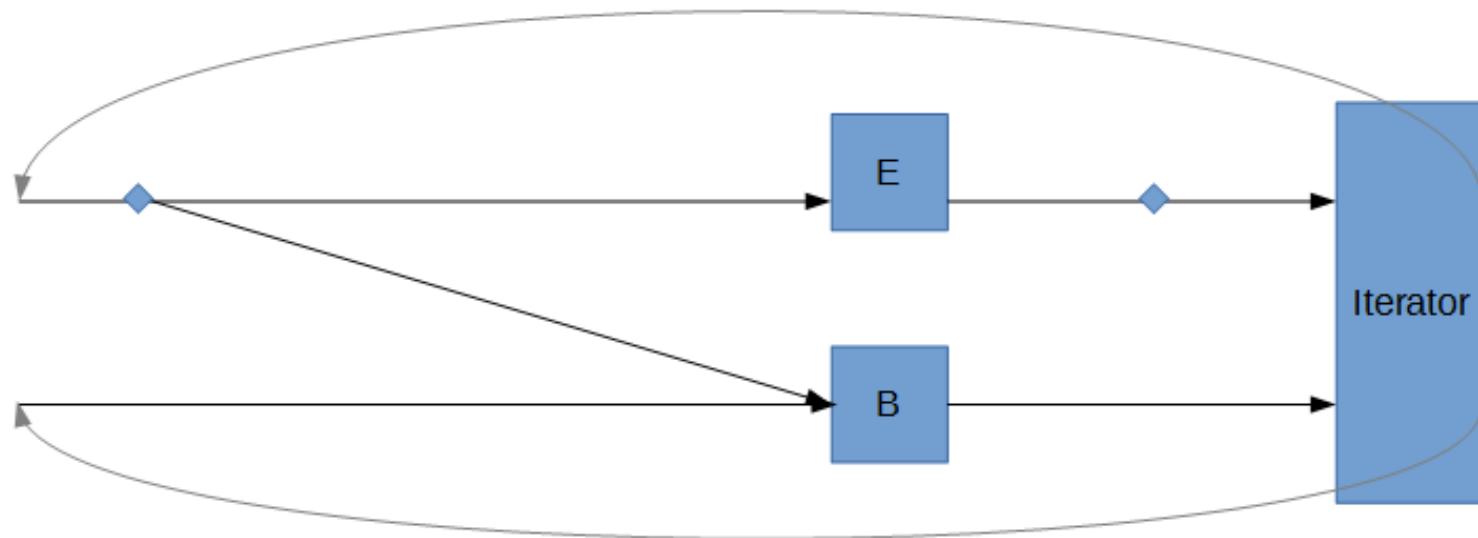
# Simulating dynamic processes with SimuSage: residence time and circulation rate



$$t_{r,E} < t_{\text{timestep}}$$

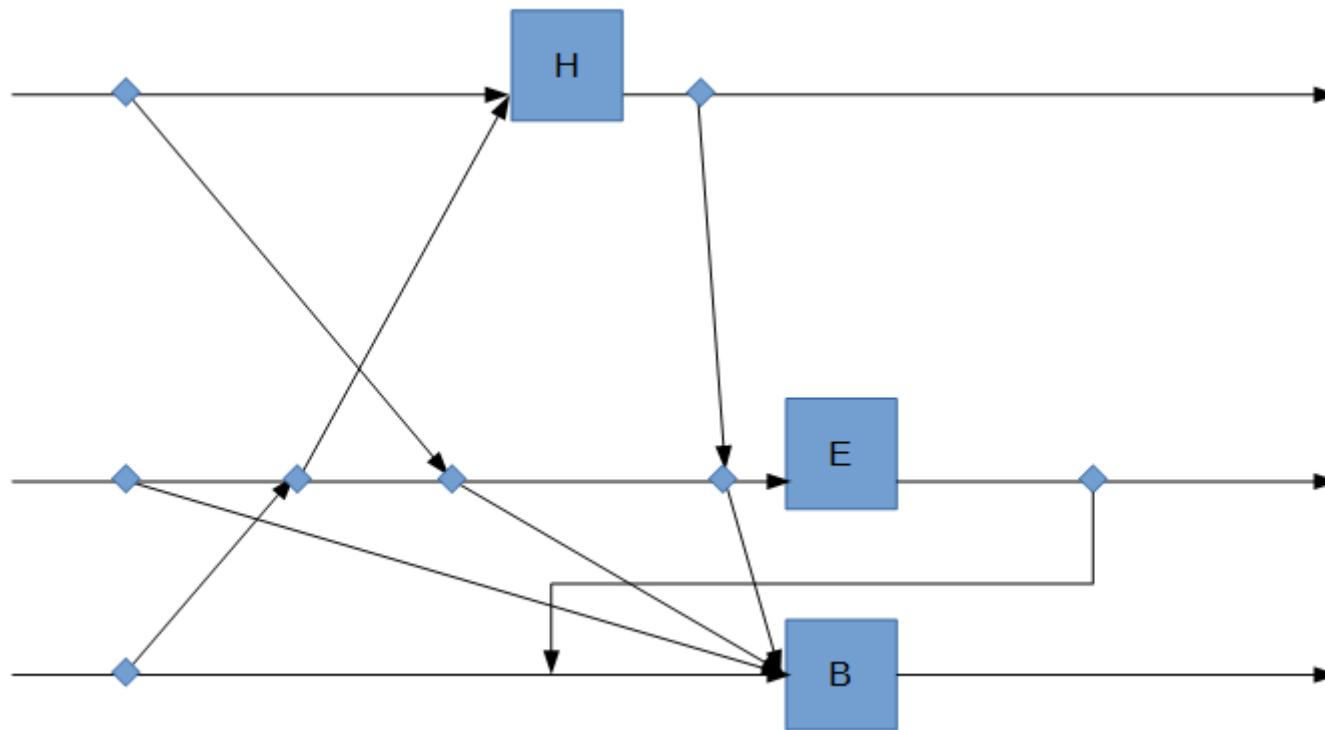


# Simulating dynamic processes with SimuSage: residence time and circulation rate



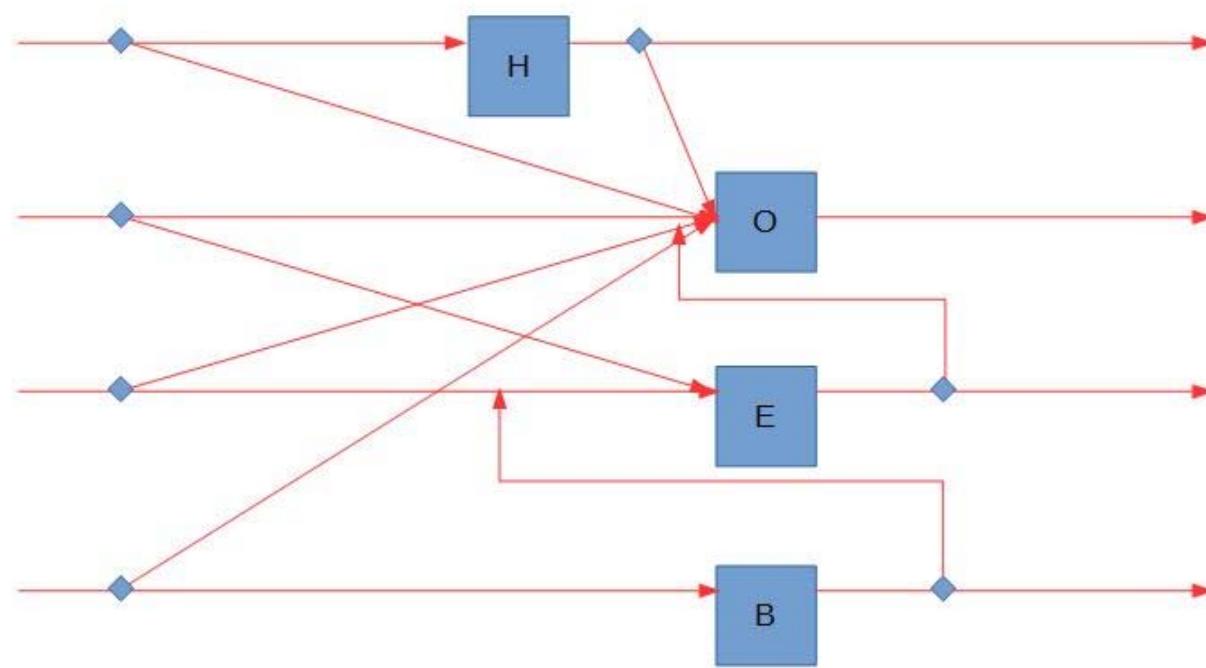
$$t_{r,E} > t_{timestep}$$

# Sketch of the new LD-Sage model Flowsheet - liqMetal



# Sketch of the new LD-Sage model

## Flowsheet - slag



We are looking forward to  
presenting the results of the  
new model next year !

Thank you for  
your attention !

