Process simulation of complex metallurgical Systems

Advanced Process Modelling Forum 2013

SIEMENS VAI

"Process simulation of complex metallurgical systems"

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APM Forum 2013

Contents

Portfolio

- Part of Siemens Industry Sector
- Technology, mechanical engineering, automation and electrical engineering for metallurgical plants in the areas of
  - New plants
  - Modernisation
  - Service

Mining

Blast furnaces

Smelting/Direct reduction

Steel plants

Mini mills

Continuous casting

Hot/Plate mills

Cold band

Long rolling

Metallurgical services

Electrics Automation

Ironmaking processes

- Business segment of business unit Siemens VAI Metals Technologies
- Competence for
  - Agglomeration, pelletising, sinter technologies
  - Conventional iron making
    - Blast furnace
  - Alternative iron making
    - Corex®
    - Finex®
    - Midrex®/DR
    - Finmet®

Ironmaking processes

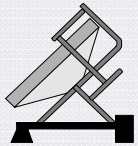
SIEMENS VAI

Raw Materials for ironmaking

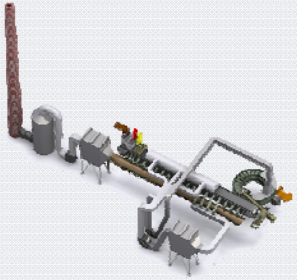
Fine ore

Concentrate

Preparation



Pellet Plant



Sinter Plant

Coal > Coke

Lump ore

Fine ore

Pellets

Sinter

Ironmaking Processes

Blast Furnaces

FINEX®

COREX®

DR Plants/ MIDREX®

Products

Hot Metal

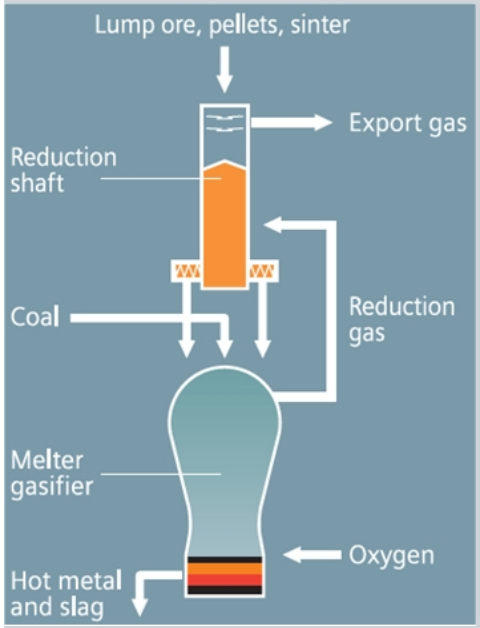
Hot Briquetted Iron

Direct Reduced Iron

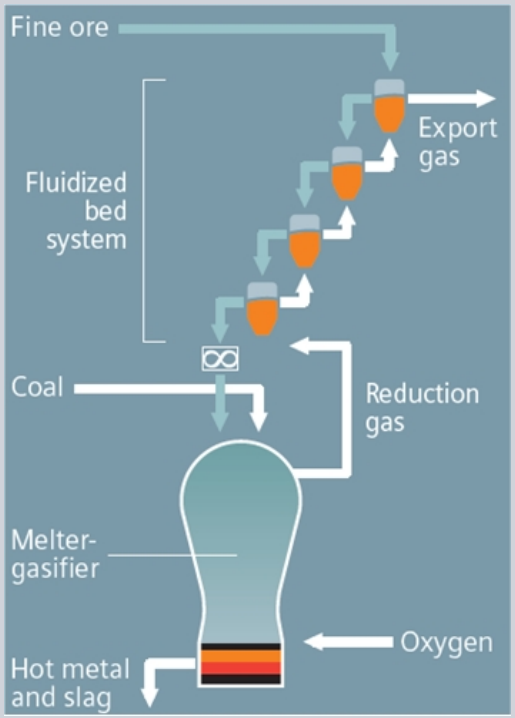
Steelmaking / Market

Ironmaking processes

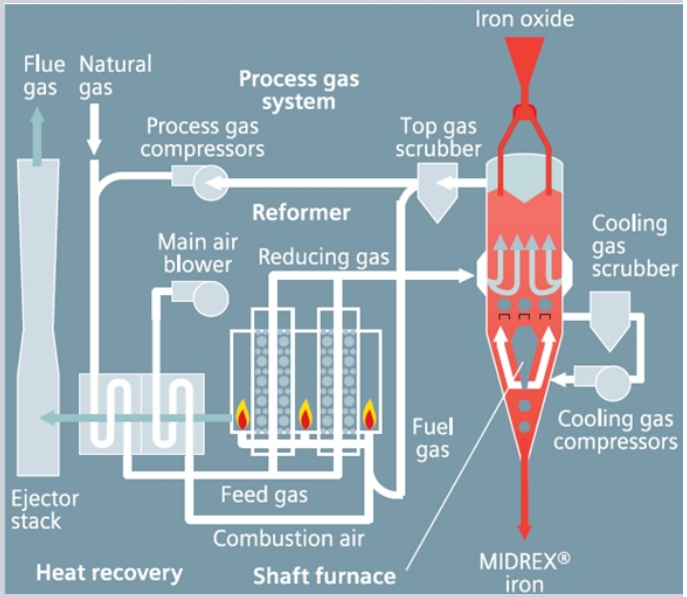
- Processes besides conventional blast furnace iron making route:



Corex®



Finex®



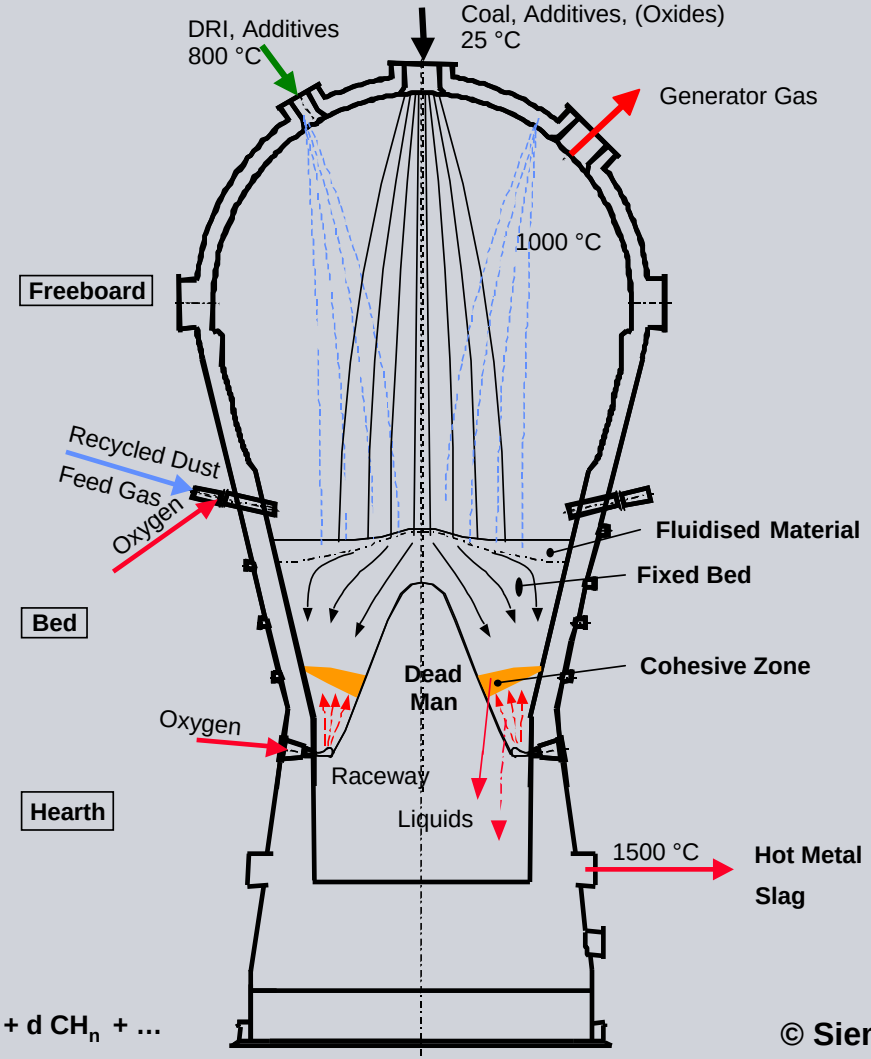
Midrex®

Chemical challenge - melter gasifier

SIEMENS VAI

• Metallurgy

$FeS + CaO \rightarrow FeO + CaS$
$2\,FeO + Si \rightarrow 2\,Fe + SiO_2$
$FeO + Mn \rightarrow Fe + MnO$
$3\,Fe + C \rightarrow Fe_3C$



• Calcination

$CaCO_3.MgCO_3 \rightarrow CaO.MgO + 2\,CO_2$
$CaCO_3 \rightarrow CaO + CO_2$

• Reduction

$FeO + CO \rightarrow Fe + CO_2$
$FeO + C \rightarrow Fe + CO$
$MnO + C \rightarrow Mn + CO$
$SiO_2 + 2\,C \rightarrow Si + 2\,CO$

• Gasification

$C + O_2 \rightarrow CO_2$
$CO_2 + C \rightarrow 2\,CO$
$C + 1/2\,O_2 \rightarrow CO$

• Sulphur

$CaO + H_2S \rightarrow CaS + H_2O$
$MgO + H_2S \rightarrow MgS + H_2O$

• Gas Reactions

$C + H_2O \rightarrow CO + H_2$
$CO + H_2O \rightarrow H_2 + CO_2$
$C + CO_2 \rightarrow 2\,CO$
$CH_4 \rightarrow 2\,H_2 + C$

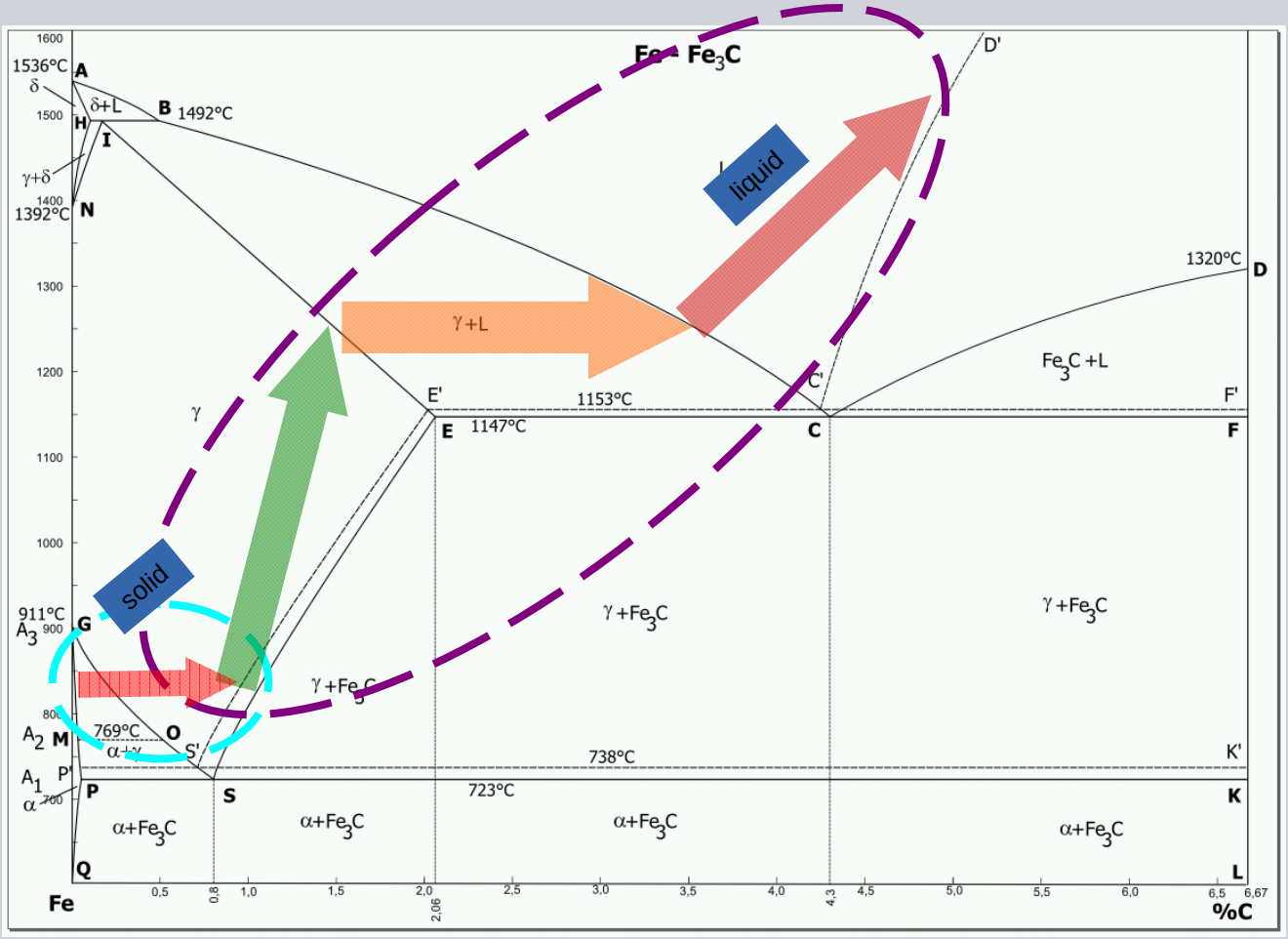
• Coal Pyrolysis

$Coal \rightarrow a\,CO + b\,H_2 + c\,N_2 + d\,CH_n + \ldots$

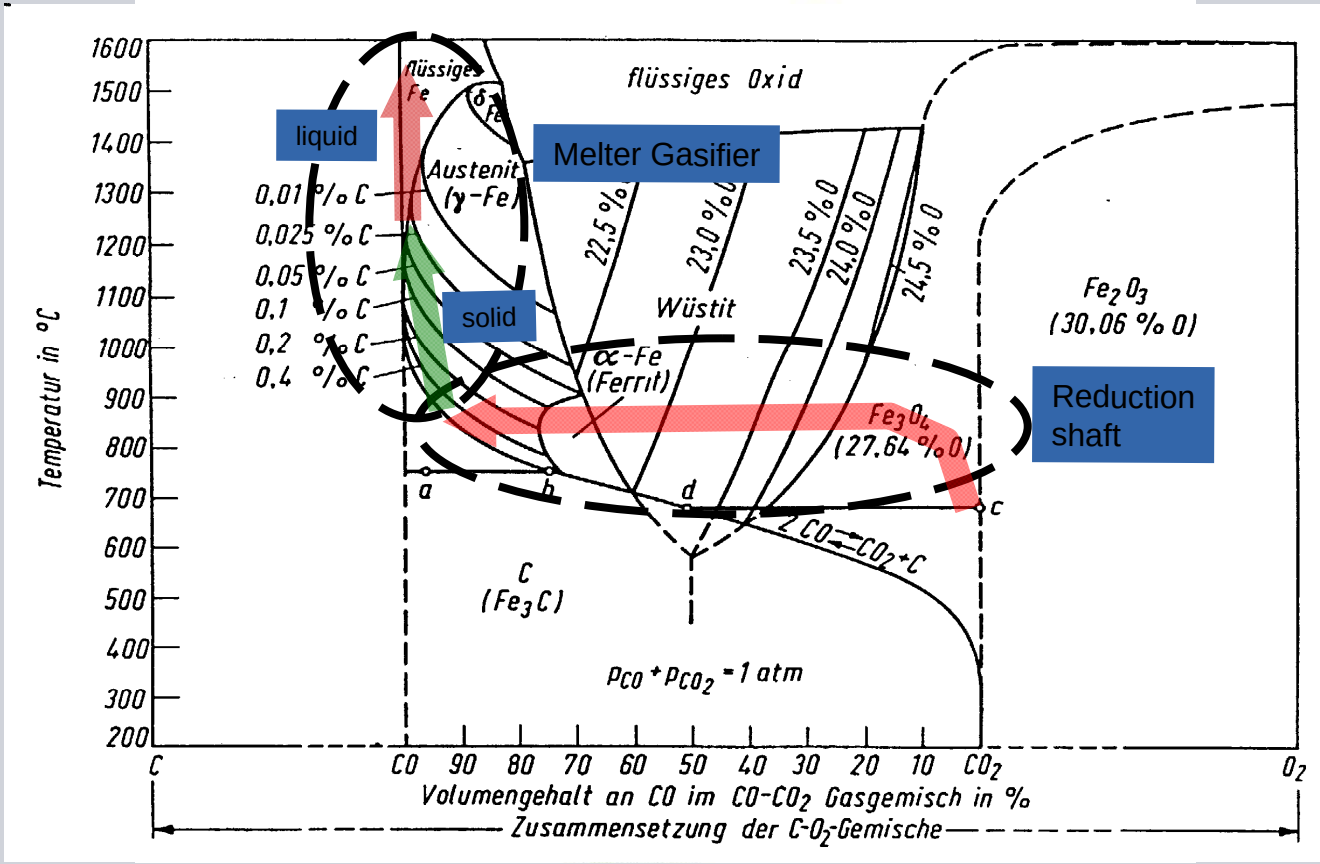
Chemical challenge

Melter Gasifier

Reduction Shaft



Chemical challenge



Approach to gPROMS

Motivation

- Increased complexity of process development
- Increased flexibility for process setup on customer demands
- Additionally:
  - No standardized thermodynamics, flow sheeting

Approach to gPROMS

- Evaluations on state of the art in process simulation
  - Internal, external, guided with PSE
- Outcome: no standard process simulation tool suitable
  - Lack of thermodynamics
  - Unit operations
- Descision for gPROMS due to its flexiblity, customizability and functionality

Development approach

Two parallel implementations

- Low fidelity approach
  - Based on existing internal routines
  - Substitution of MS Excel implementations
  - Utilisation for “every day” project work
  - Global aim - implementation of overall iron and steelmaking routes
    - Conventional (sinterplant, pelletising plant, coking plant, blast furnace, converter)
    - Alternative (sinterplant, pelletising plant, Corex, Finex, converter)

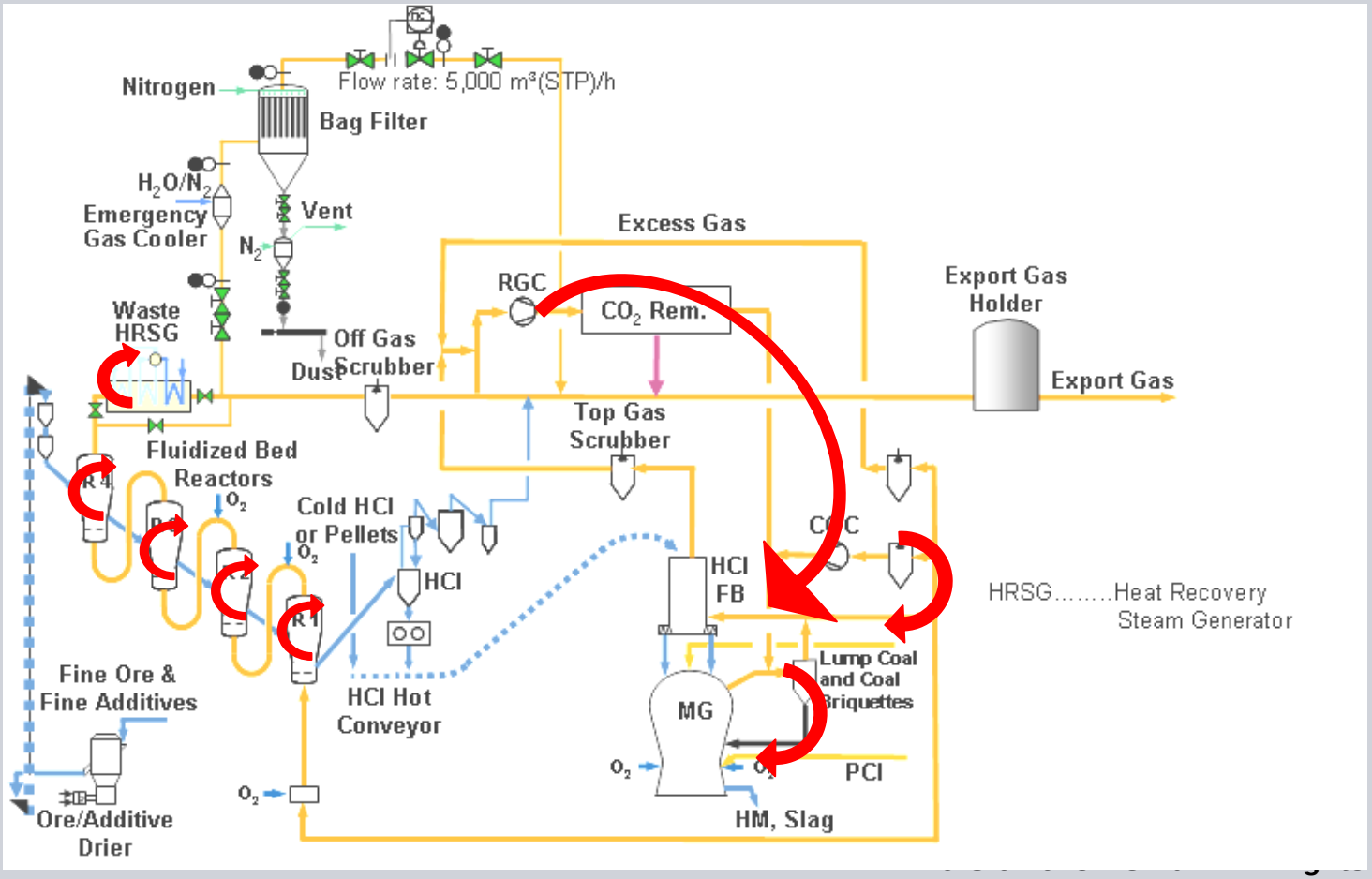
- High fidelity approach
  - Only for selected unit operations
  - Extended thermodynamic routines by using an interface to ChemApp
  - Utilisation for scientific investigations

Low Fidelity Approach

- Full capable metallurgic unit operation library building large flow sheets
- Based on conversion and distribution coefficient calculations as complex chemistry was not available
- Utilization of:
  - FO look up table for enthalpy calculations (based on HSC Chemistry 6.0)
  - IAPWS95 for steam parameters
  - Multiflash gibbs equilibrium for combustion calculations
  - MS Excel interface for results export
  - Linkage to MS Access ore/coal data base for raw material data import
- Challenges:
  - Process abstraction => MS Excel tool move to flow sheeting tool
  - Initialisation procedures (recycles, non linear equation systems)

Low Fidelity Approach

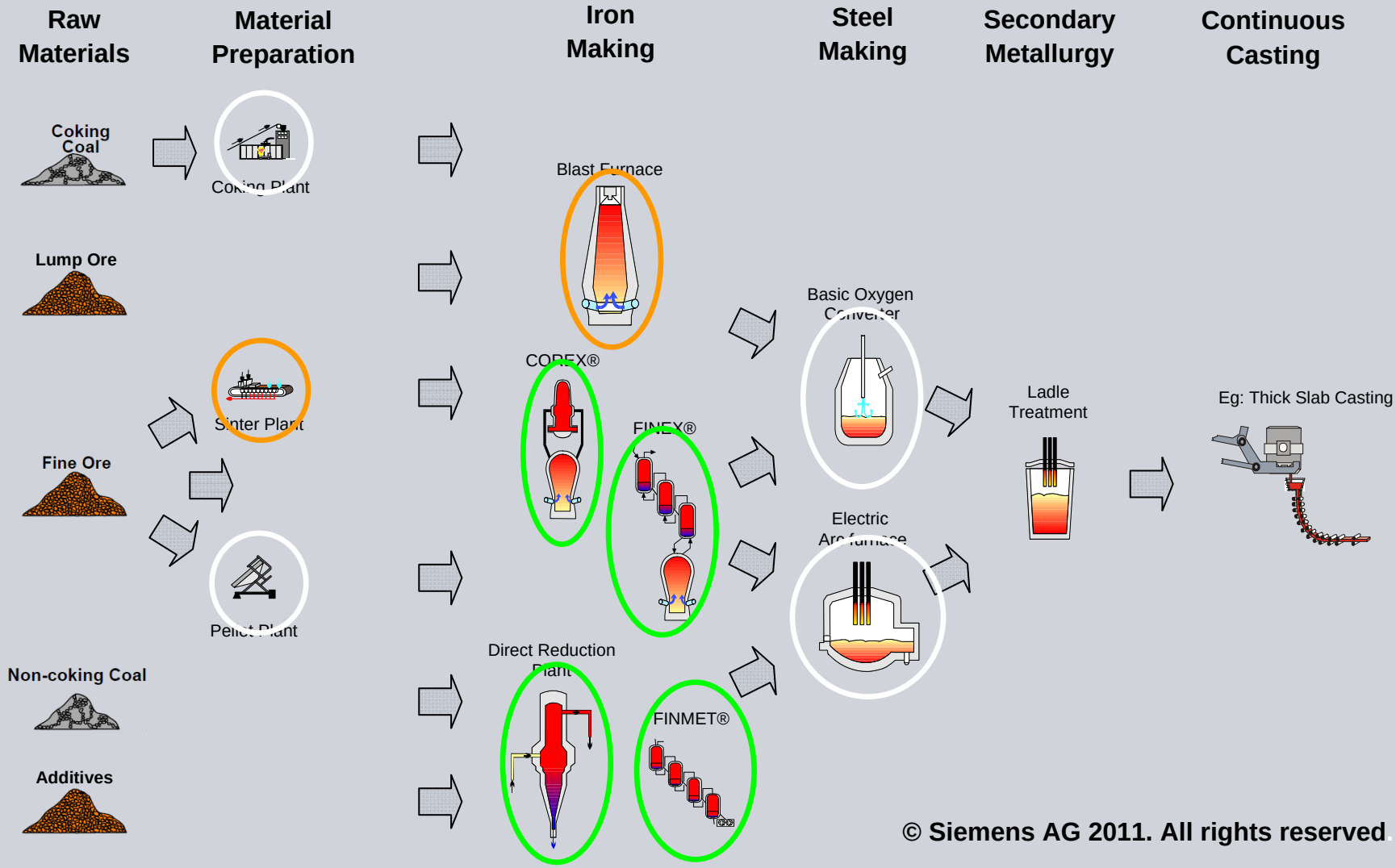
Initialisation - Recycles



Low Fidelity Approach - Status

- Blast furnace ironmaking route
  - Sinter machine pending
  - Blast furnace started
  - Hot blast stoves + slag granulation envisaged
- Alternative ironmaking route
  - Corex® finished
  - Finex® finished
  - Midrex® + Corex gas based Midrex® process pending
- Outlook
  - Steelmaking:
    - BOF
    - EAF
  - Additionally:
    - Air separation unit
    - Power plants

Low Fidelity Approach - Status

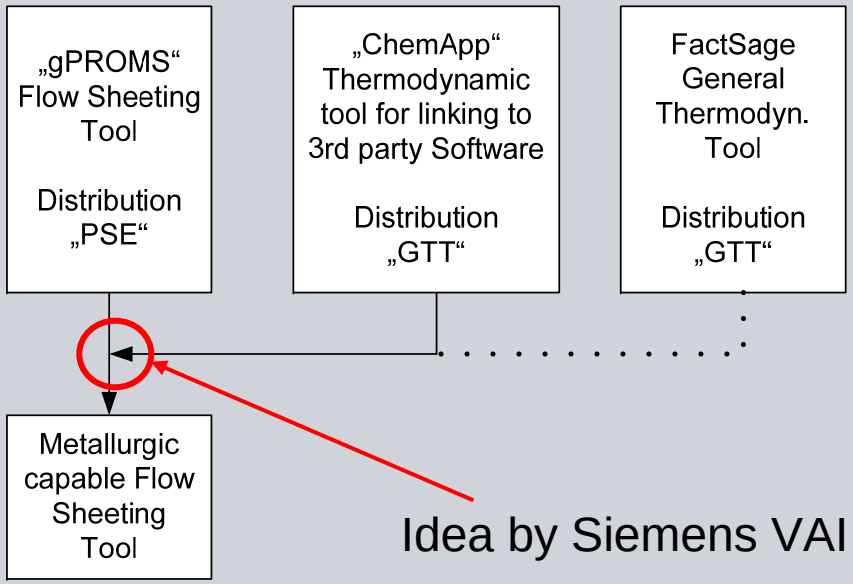


High Fidelity Approach

- Idea: full thermodynamic implementation of selected unit operations for scientific investigations

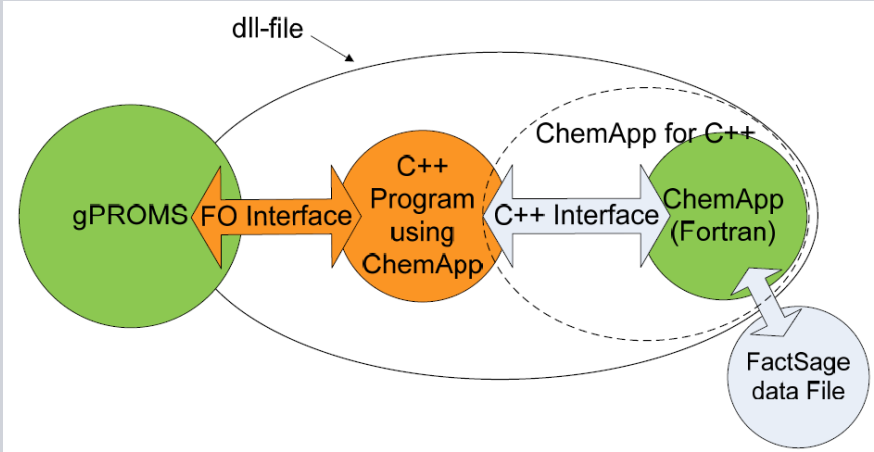
- Basis: FactSage + ChemApp
  - **FactSage**: provides thermo chemical data and tools for thermodynamic calculations incl. GUI with fully capable metallurgic libraries
  - **ChemApp**: Calculation engine linkable to 3rd party software containing a rich set of subroutines for complex, multiphase chemical equilibria. It has to be fed with species data provided by FactSage

- Precondition: Interface gPROMS - ChemApp
  - Linkage as a dynamic link library
  - Input file on chemical system from FactSage
  - Preselection of phase information/settings in FactSage

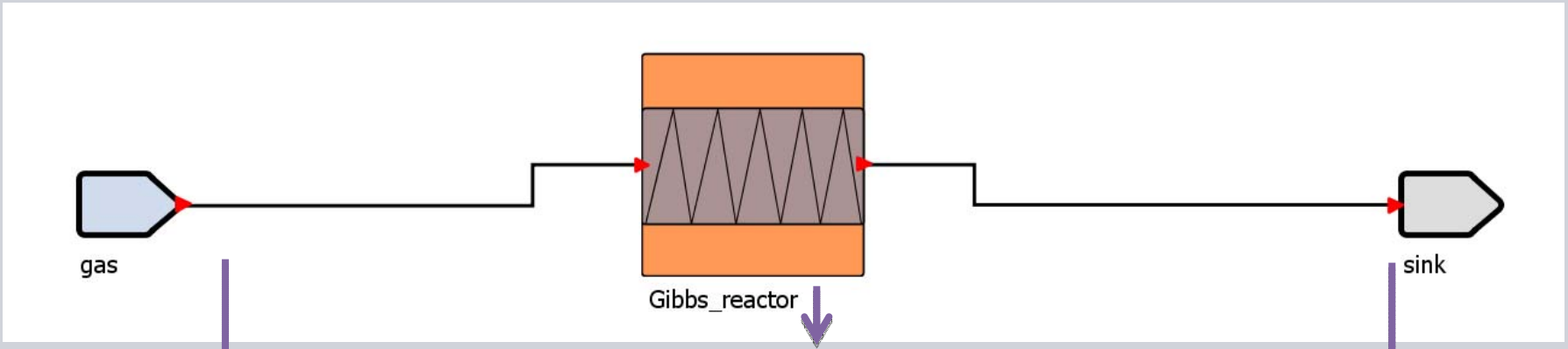


High Fidelity Approach

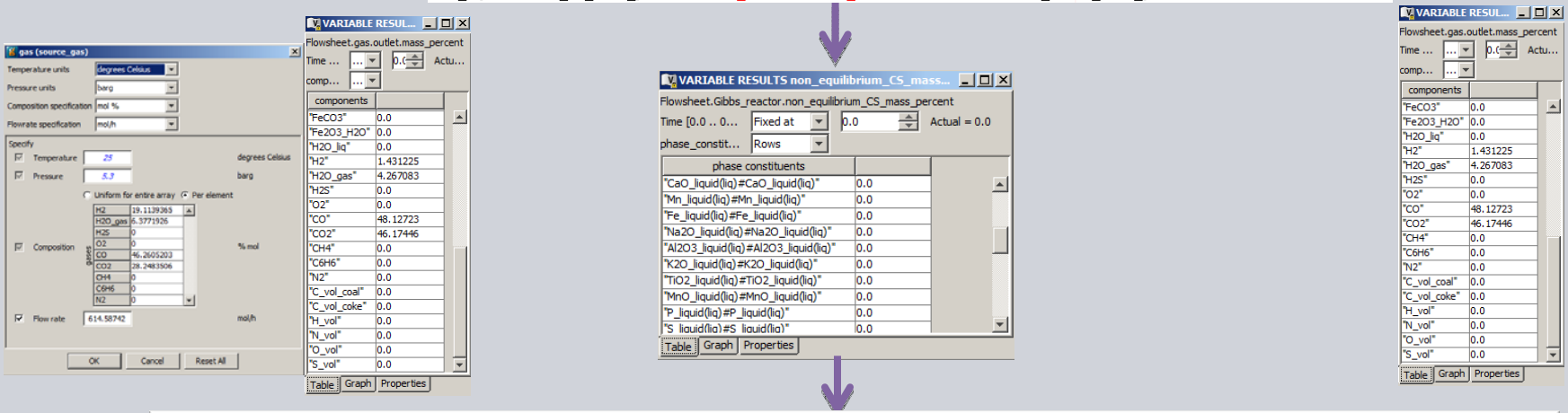
- Procedure
  - **FactSage**: .dat/.cst file is created based on all elements/species of the problem statement and expected solutions
  - **ChemApp**: installed
  - **Interface ChemApp - gPROMS**: .dll file stored in fo-folder in installation directory
  - **gPROMS**: .dat/.cst file stored under miscellaneous files



High Fidelity Approach




```
non_equilibrium_CS_mass_percent("Fe2O3_hematite(s)#Fe2O3_hematite(s)")= normalised_inlet_mass_percent("Fe2O3");
non_equilibrium_CS_mass_percent("Fe3O4_magnetite(s)#Fe3O4_magnetite(s)")= normalised_inlet_mass_percent("Fe3O4");
non_equilibrium_CS_mass_percent("K2O_solid(s)#K2O_solid(s)")= normalised_inlet_mass_percent("K2O");
```




```
# Equilibria calculation
equilibrium_CS_mass_percent = phys_prop_CS.EquilibriumAmount(temperature , pressure , non_equilibrium_CS_mass_percent() ) ;
```



```
outlet.mass_percent("FeO")      = equilibrium_CS_mass_percent("FeO_wustite(s)#FeO_wustite(s)");
outlet.mass_percent("Fe2O3_H2O")= equilibrium_CS_mass_percent("Fe2O3(H2O)_solid(s)#Fe2O3(H2O)_solid(s)");
outlet.mass_percent("FeCO3")    = equilibrium_CS_mass_percent("FeCO3_siderite(s)#FeCO3_siderite(s)");
```

High Fidelity Approach

- Problems
  - Phase and solution systems selection in FactSage prior to .cst/.dat file
  - Model abstraction: equilibria not reached in real processes
    - “distance to equilibrium” approach
    - Temperature approach
    - Further evaluations on possible solution systems selection to be used from FactSage

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