# Modeling the Iron Making Route in gPROMS

## Advanced Process Modelling Forum 2015

## Modeling the Iron Making Route in gPROMS

**Process Simulation @ Primetals**
**Iron Making Department**

**London, 22.04.2015**

**Bernd Weiss**

### Content

# Who we are – in short

Technology, engineering, automation and electrical engineering for metallurgical plants in the areas of:

- New plants
- Modernization
- Service

## History

- 1956 – 1987: part of voestalpine (Austrian integrated iron and steel works), internal and external engineering projects, increase in project size and complexity
- 1988: foundation of "Voestalpine Industrieanlagenbau Ltd."
- 1995 – 2005: excarvation from voestalpine to VA TECH holding
- 2005 – 2014: Siemens acquiring VAI, formation of Siemens VAI and integration to Siemens group
- 2015: Joint venture of Mitsubishi-Hitachi Metals Machinery Inc. and Siemens, formation of Primetals Technologies

# Who we are - portfolio

### IRONMAKING

- Beneficiation
- Agglomeration
- Blast furnace
- Smelting reduction, direct reduction

### STEELMAKING & LONG ROLLING

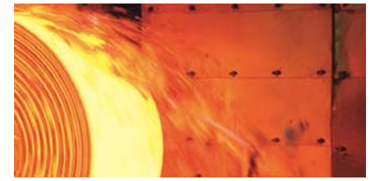
- Converter plants
- Electric steelmaking
- Stainless steelmaking
- Secondary metallurgy
- Long rolling
- Minimills

### CASTING & ENDLESS STRIP PRODUCTION

- Continuous casting
- Arvedi ESP lines (endless strip production)

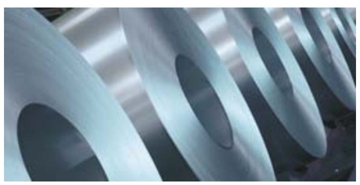
### STRIP CASTING

- Thin-strip casting



### HOT ROLLING

- Hot rolling mills
- Aluminum rolling mills
- Other nonferrous mills



### COLD ROLLING

- Cold rolling mills
- Aluminum rolling mills
- Other nonferrous mills

### PROCESSING & TUBE MILLS

- Strip processing lines
- Tube and pipe mills

### ECO SOLUTIONS

- Gas cleaning
- Energy efficiency
- By-product recycling
- Water treatment
- Process & technology consulting

### ELECTRICS & AUTOMATION

- Ironmaking
- Steelmaking
- Continuous casting
- Rolling and processing
- Modernization (packages and products)

### METALLURGICAL SERVICES

- Spares and components
- Electrical and mechanical maintenance and repair services

# What we do

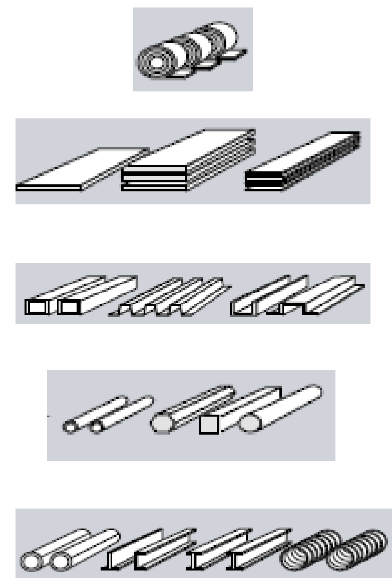
# What we have to achieve


Coal / Coke


Lump ore


Fine ore


Pellets



## The motivation

- In the past - process calculations mostly MS Excel and partly ChemCAD
- MS Excel for mass- and energy balance calculations
  - Easy to use by everybody
  - But significant limitations:
    - Confusing set up of routines – organically grown
    - No thermodynamics directly implemented, no equilibrium routines
    - No flow-sheeting tool
    - Standardization hardly possible
- ChemCad for additional tasks
  - Flow sheeting tool, easy to use
  - Not capable in handling metallurgical systems at all (plants, chemistry)
- Problems
  - Significant work effort in MS Excel for adaption of balances to customer needs (deviation from standard plant concepts)
  - Consortial projects - no lumped mass/energy balance possible due to usage of different tools, deviations at interfaces
  - Only uni-directional calculations possible in complex MS Excel workbook set ups
  - Linkage of various plants to one flow sheet not possible
  - ...
- Investigation/evaluation on state of the art of flow sheeting tools

# How we approached gPROMS

## The motivation – evaluation results

- Main problems:
  - Main metallurgical unit operations not available (melter gasifier, shaft, fluidized bed, …)
  - Customizing options not satisfying: user defined unit operations, user defined chemical components/materials
  - Standard data interfaces (to MS Excel, MS Access, HSC, …) not capable/existing
  - Performance of calculation of design specifications not satisfying

- Chemical problems:
  - Physical and chemical properties of species relevant for metallurgy not available
  - No handling of solids available, heterogeneous equilibrium calculations not feasible

- Specific problems:
  - Relevant species not even implemented, calculation of inverse problems not possible
  - Convergence problems, temperature ranges of physical properties, …

- **Result**
  - **No state of the art tool is capable of performing metallurgical flow sheet calculations, therefore:**
  - Tool must be customizable (for models, species, …) and/or linkable to thermodynamic software
  - **Evaluation result: gPROMS in combination with ChemApp and FactSage**
  - **Go to market chance: after development of tool – option for commercialization**

# How we approached gPROMS

## The challenge

- Standardization of
  - Thermodynamic data and calculation routines
  - Unit operations

- Easier process modelling due to flow sheeting environment
  - Higher flexibility
  - Linkage of any unit operation/plant model with each other
  - Faster adaptions

- Elaboration of metallurgic unit operation library for standard and alternative iron/steel making route

- Extension of chemical and calculation possibilities compared to MS Excel

- Steady state calculations

# How we approached gPROMS

## The approach

- Software approach
  - gPROMS and FactSage licenses acquired
  - ChemApp licenses acquired, interface in between gPROMS and ChemApp elaborated by PSE

- Vision: **set up of full model library for Primetals portfolio in 3 phases**
  - Phase 1:
    - Iron making department internal feasibility
    - Implementation of Finex, Corex, Corex gas based Midrex, Midrex, pellet and sinter plants
  - Phase 2:
    - Distribution to other Primetals departments, implementation of blast furnace, BOF, etc.
  - Phase 3:
    - Commercialization: studies for customers, possibly also sale of software tool together with metallurgical library

- Implementation approach:
  - Low fidelity models
    - Documentation of former MS Excel models and implementation in gPROMS, validation of gPROMS models against MS Excel
    - Usage for pre-projects, projects, standard operational analyses
  - High fidelity models
    - For selected aggregates with task of specific scientific investigations, multi zone models, etc.

## The implementation approach

- Implementation split
  - Internally
  - Vienna university of technology (in terms of a PhD thesis)
  - PSE
    - Premium software support
    - Engineering days

- Partner voestalpine
  - Suffering of having no possibility for overall integrated steel plant consumption figures balancing, investigations on internal cycles of material, etc.
  - Contributes financially
  - Contributes technologically
    - Operation data
    - Knowledge exchange

- Primetals UK
  - Blast furnace/hot blast stoves group involved in model development for standard iron making route
  - Contributes technologically

## The approach

- Thermodynamics
  - Multiflash
  - IAPWS95 steam tables
  - FO Lookup table for metallurgic species enthalpies
  - ChemApp linkage
  - Rist routine and Baur Glaessner approach for basic metallurgical calculations

- Unit operations
  - Sources: introduction of raw materials into flow sheets (solids, gas, water, coal/coke, fluid fuels, database linkage)
  - Splitters: dust, fraction/volume based, gas/fluid, gas/solid, …
  - General: heat exchangers (condensator, gas/gas, gas/water), scrubbers, burners, steam drum, direct/indirect heaters, $CO_2$ sequestration, mixer, compressor, pumps, $CH_4$ reformer, …
  - Metallurgic: fluidized bed reactors, melter gasifier, reduction shaft, blast furnace, pelletizing plant, sinter machine, LD converter
  - Solids: bag house filter, electrostatic precipitator, cyclone solid/gas, coal briquetting, DRI compacting

- Additionally
  - Import of data from MS Excel raw material data base, export of calculation results to MS Excel
  - Initialization procedures

# How we approached gPROMS

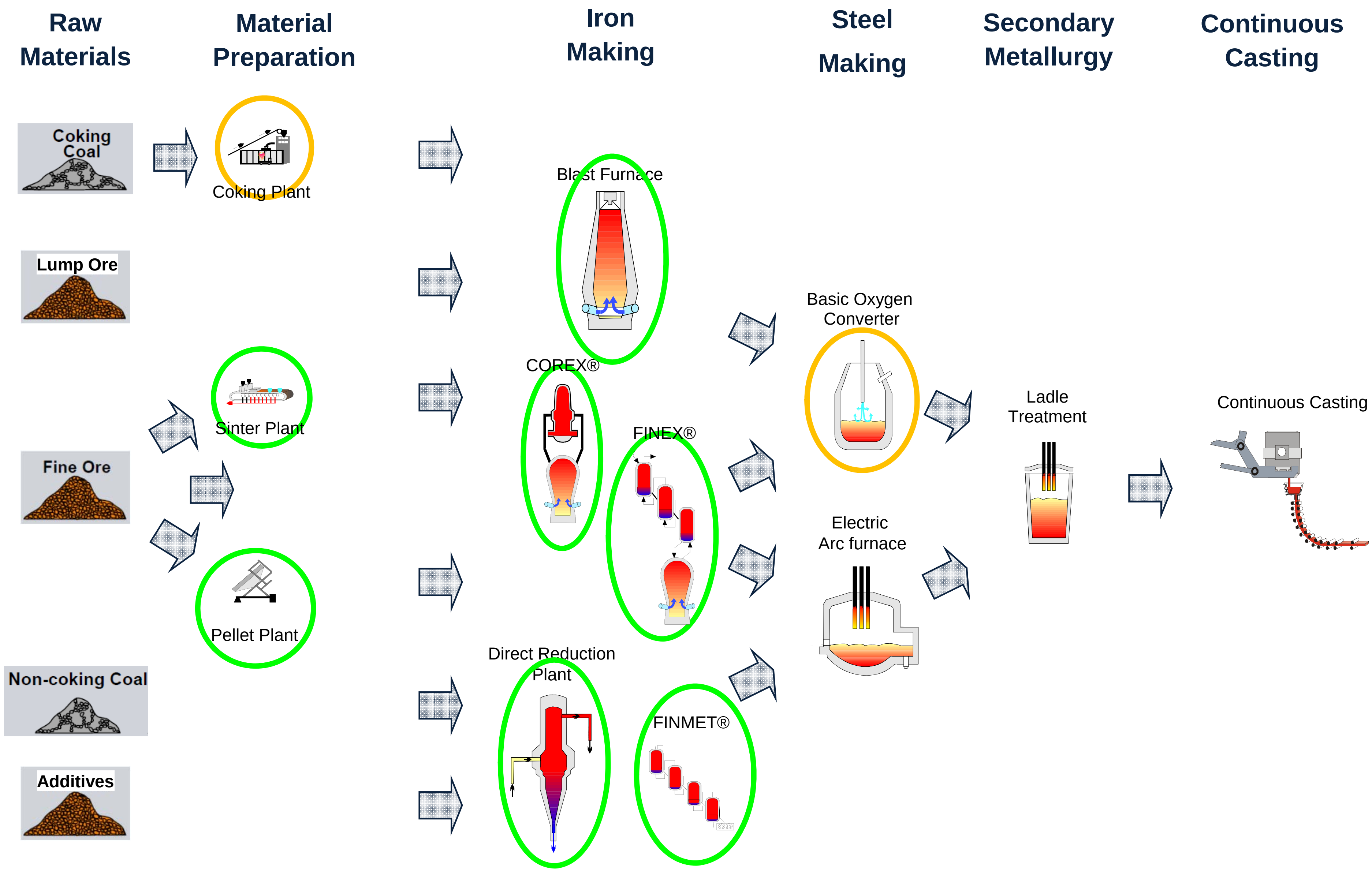
## The approach

- Library structures
  - Mainly mass balances based on conversion and distribution coefficient calculations
  - Specific reactions with equilibrium approach
  - Enthalpy balances via FO lookup table
  - Hierachial set ups with sub models

- Connection ports
  - Currently mass, temperature, pressure and compositions transported
  - Extension to particle size distributions, densities, enthalpies possible
  - All in SI units

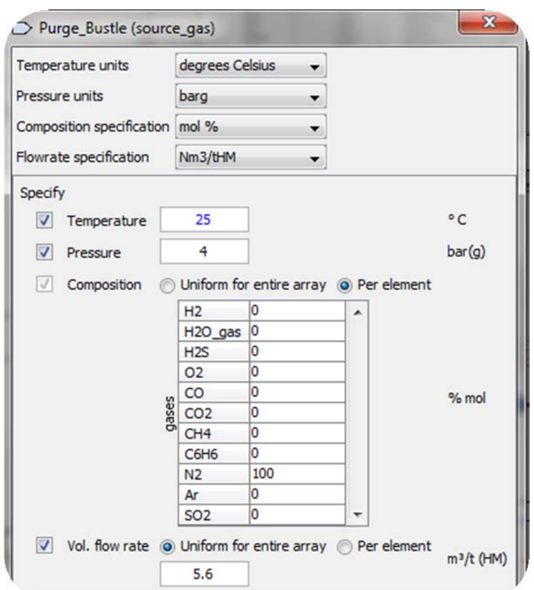
- Additional sub models for
  - Gas viscosities
  - Material properties
  - Declaration of ordered sets for species groups (solids, gases, fluid fuels, hot metal, slag, …)
  - Combustion calculations with adiabatic gibbs equilibrium (Multiflash)

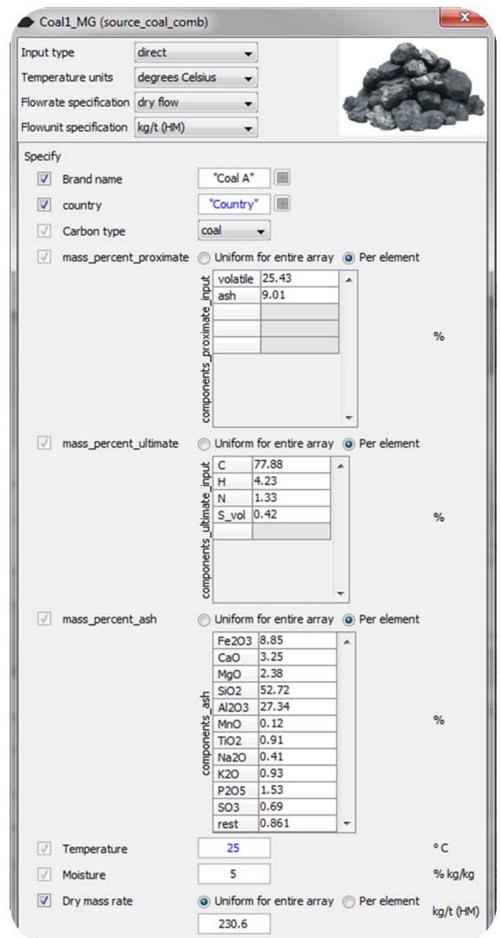
# What is the status

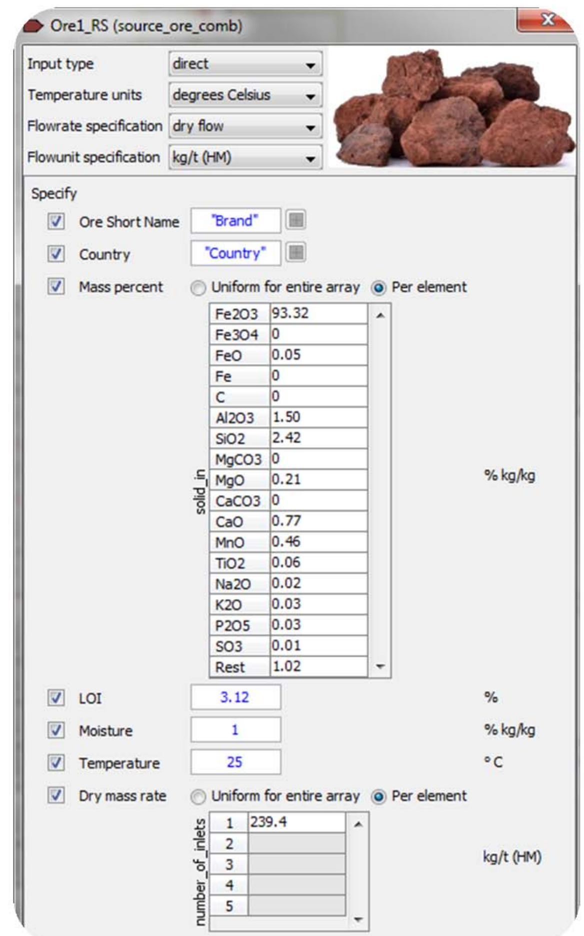


# How does it look like

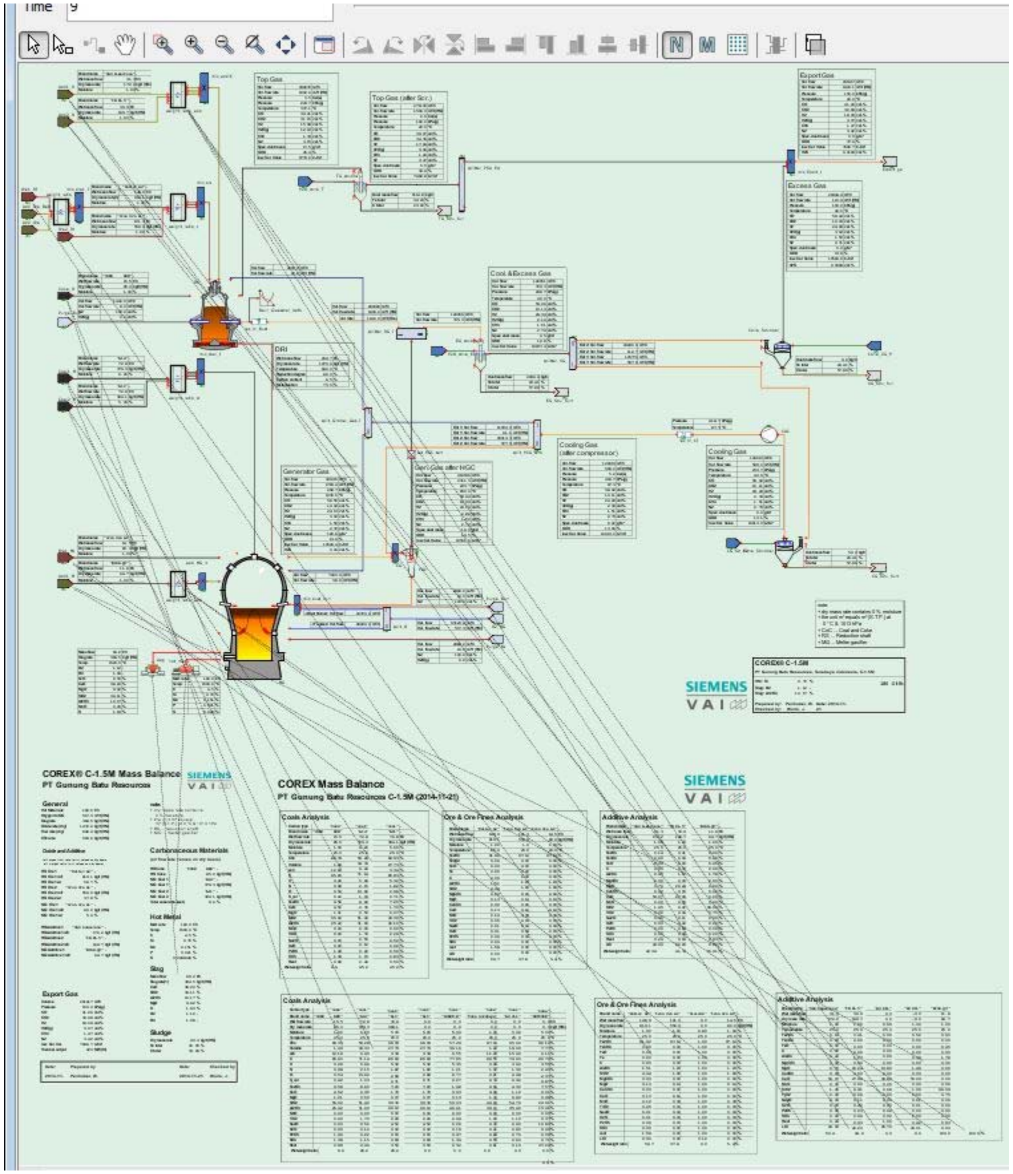
- Ore/additives/coal/coke/gas sources
- Direct entries/database (Excel) for stream analysis
- Flow values (absolute/on melting rate basis)
- Temperature + pressure



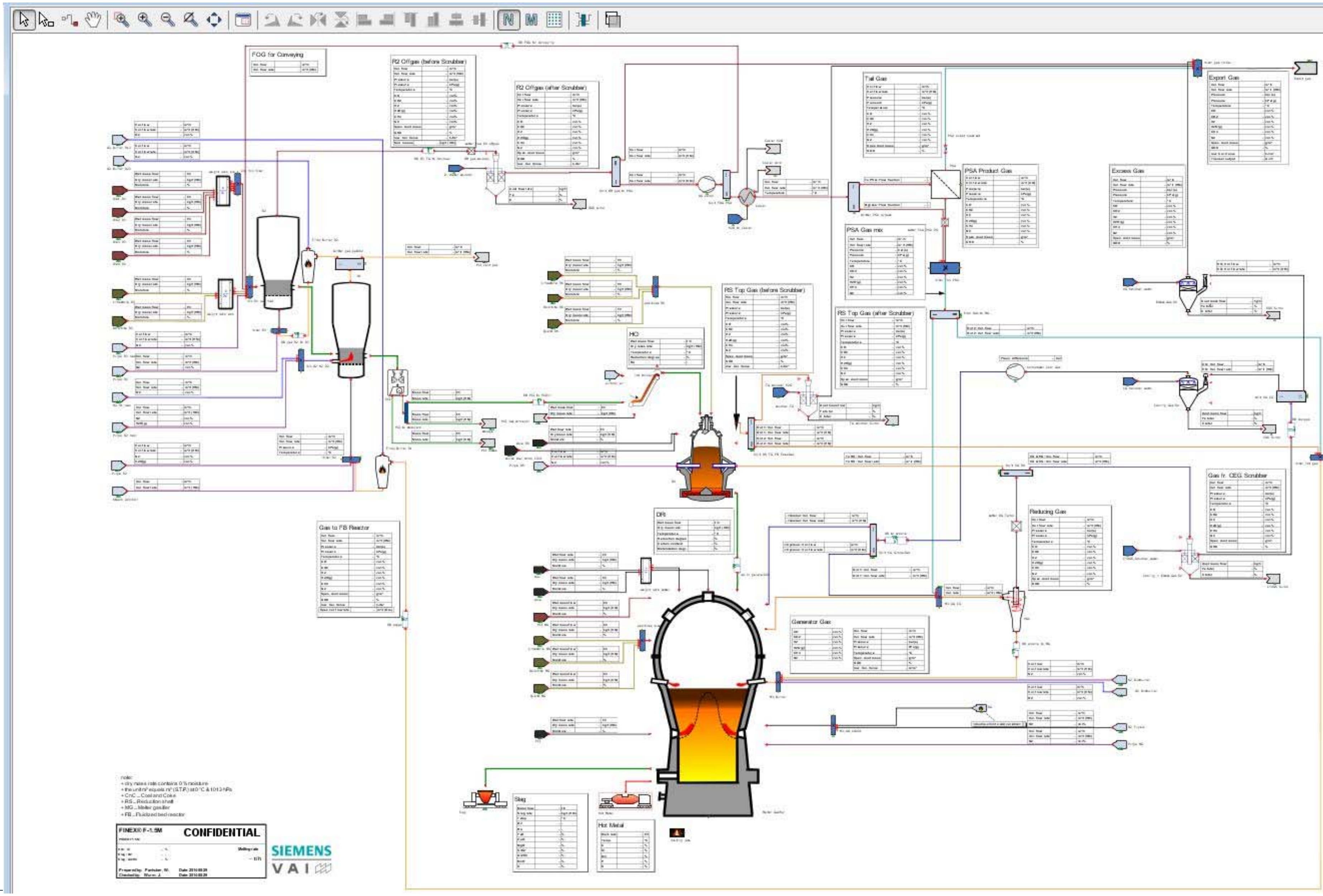



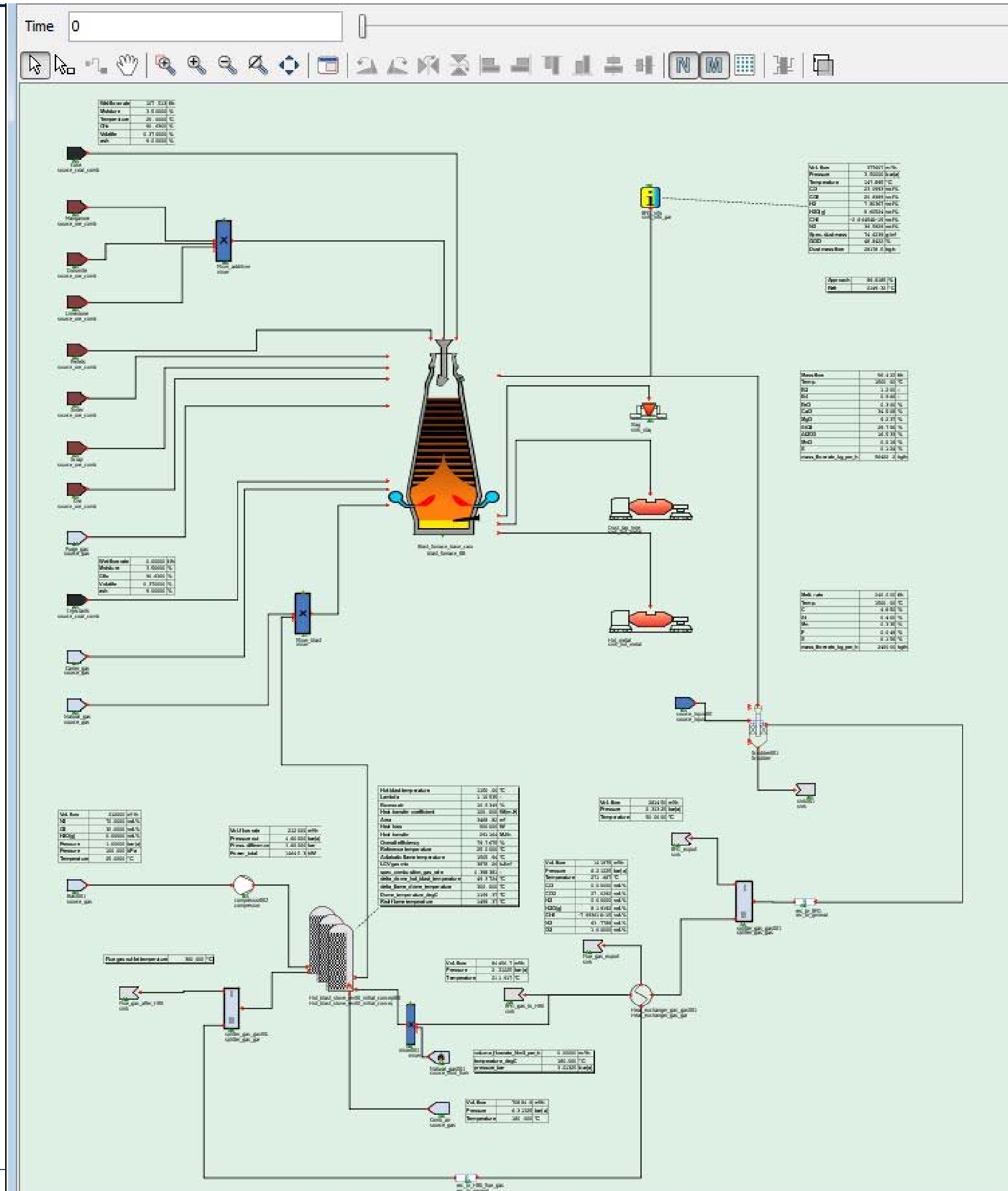
# How does it look like



# How does it look like

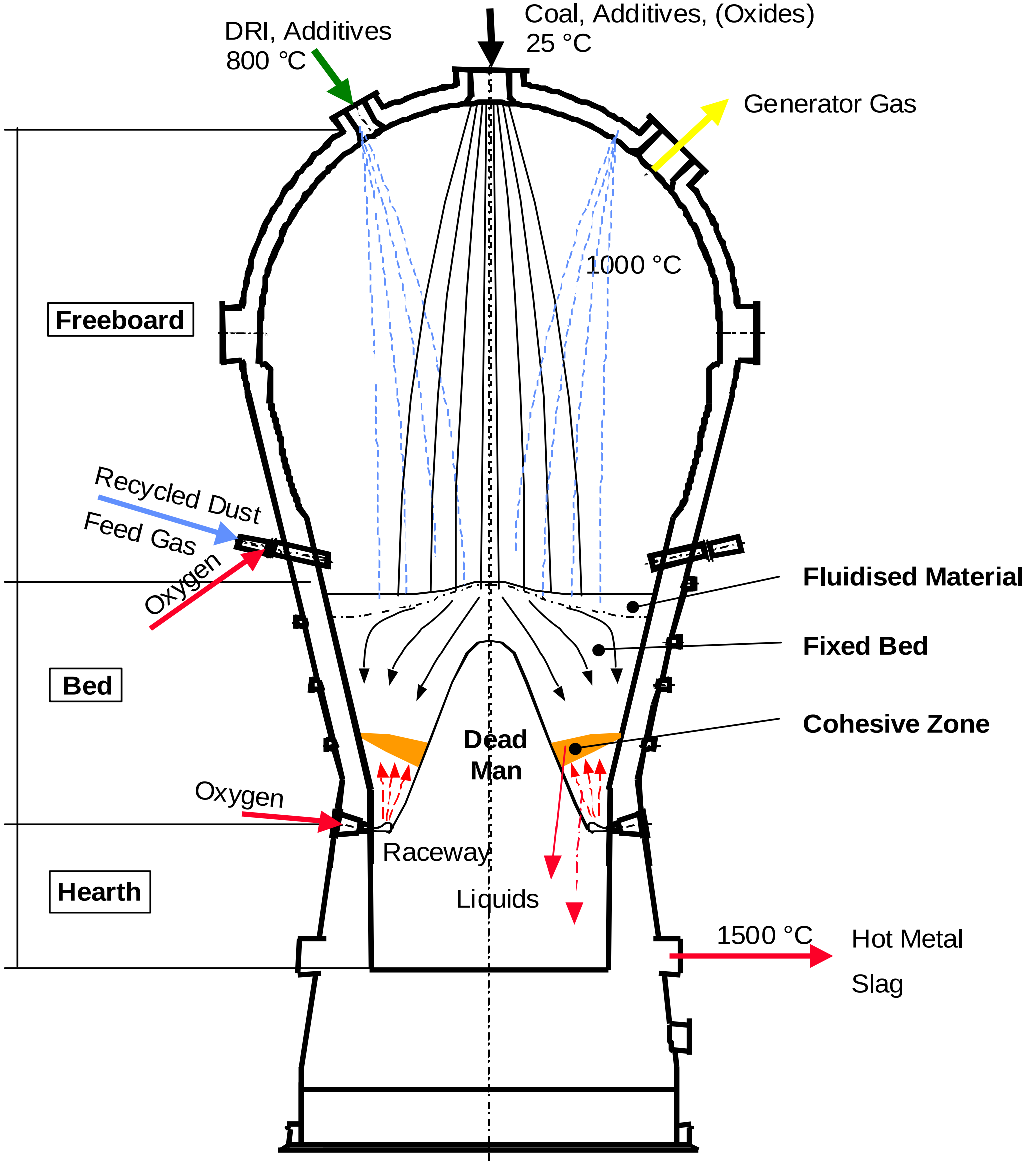


# How does it look like

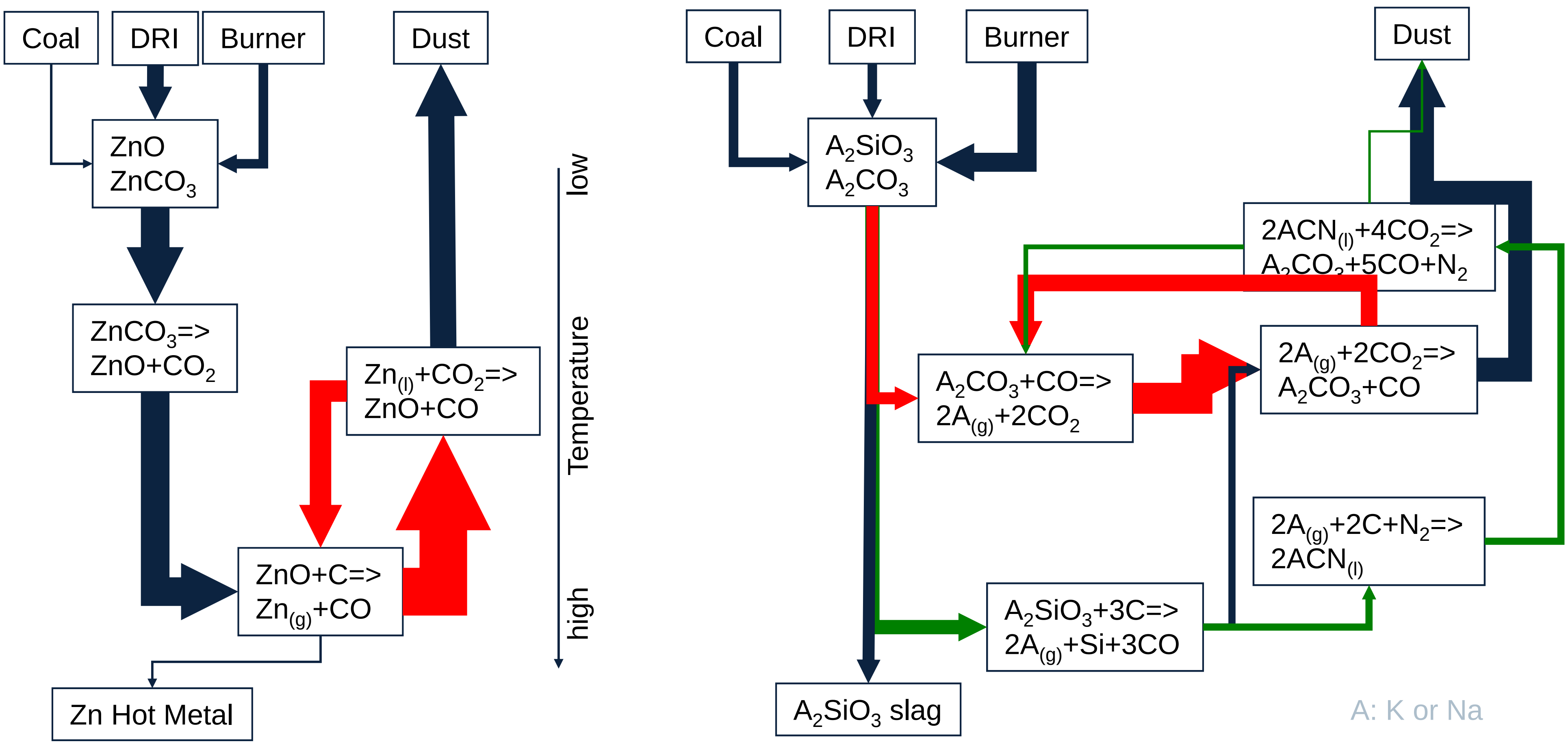


## Open items library

- Species extension for more detailed consideration of internal material cycles
  - Increasing from 60 to 130 species – inclusion of problematic trace materials
  - Going along with extension of thermodynamic data
  - Adding of functionalities/chemistry to core unit operations
  - First trials show already significant increase of calculation time



# What is still to do



# What is still to do

## Open items library

- Extending the amount of models
  - Utilities (water treatment plants, power plants, air separation unit)
  - Additional steel making units

- Update to gPROMS 4.1

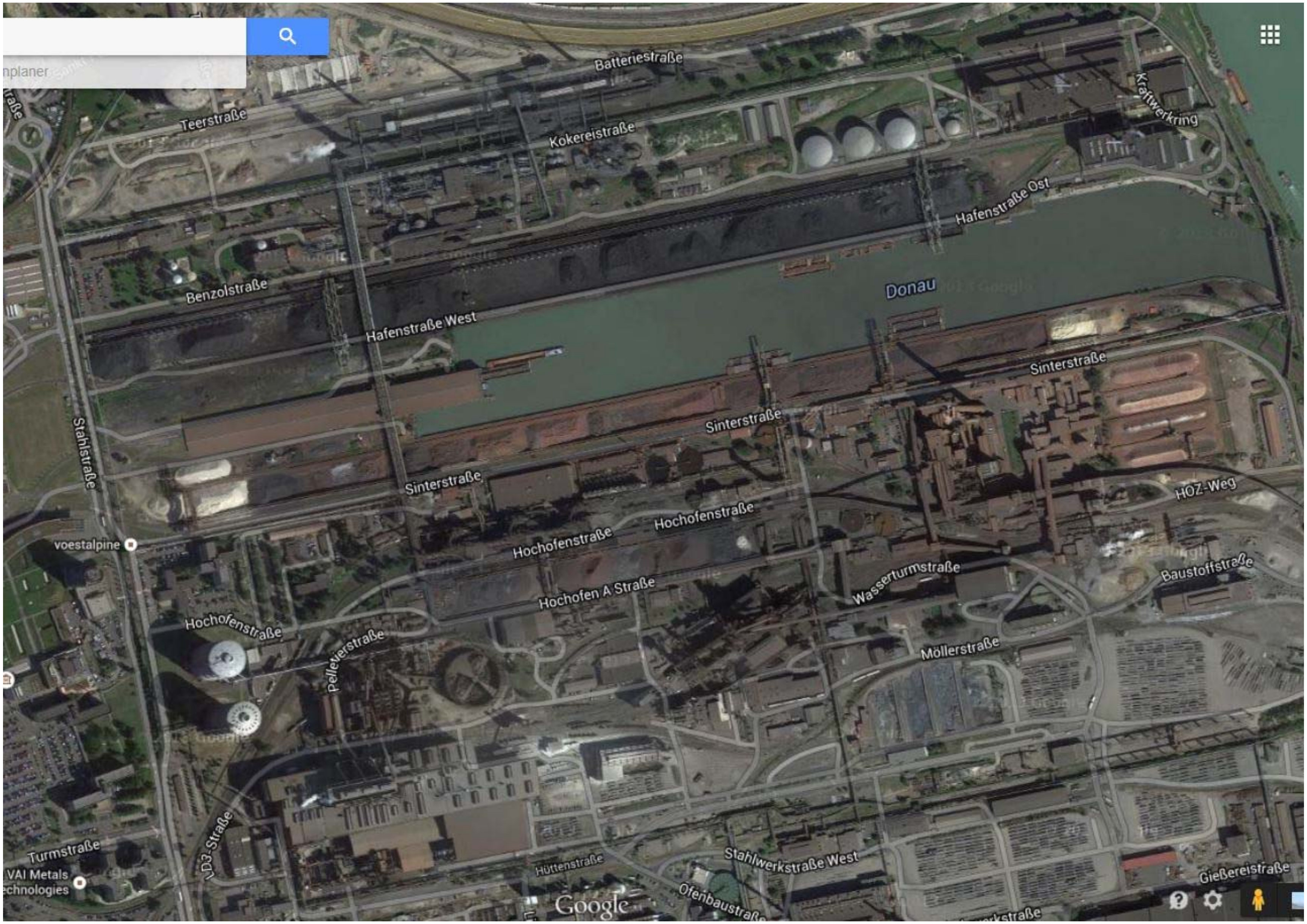
- Simplified sales application

## Open items flow sheets

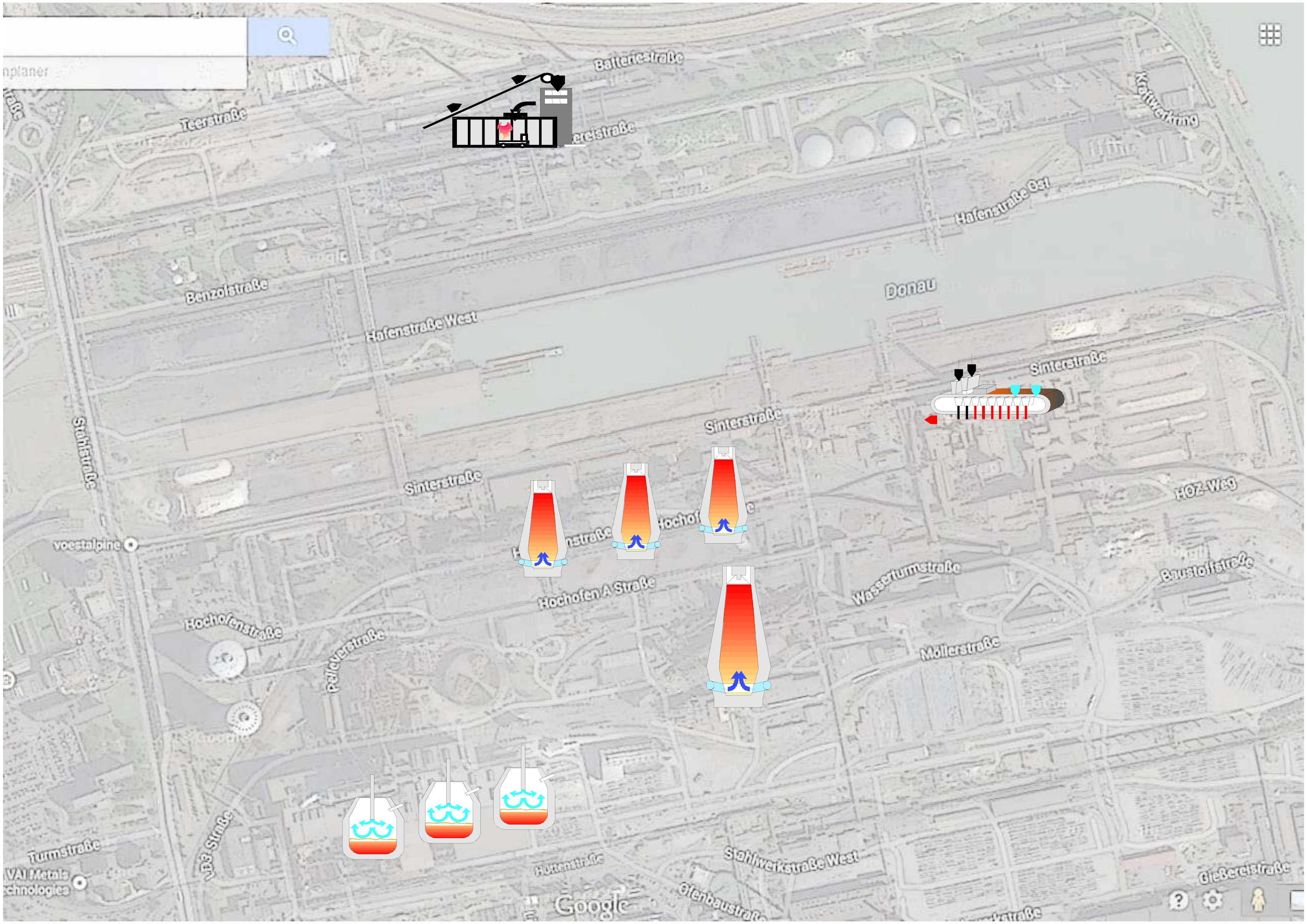
- Set up of integrated steel plant flow sheet
  - Usage of ready part-plant models to a lumped integrated steel plant flow sheet
  - Integration of material recycles:
    - Sludge: dewatering, drying and recycle to sinter and pellet plant (high iron and carbon content)
    - Dust: from dry dedusting units back to sinter and pellet plant (high iron content)

- Robust comparison of standard iron making route with the alternative iron making route
  - Comparison of blast furnace route with Corex/Finex processes

# What is still to do



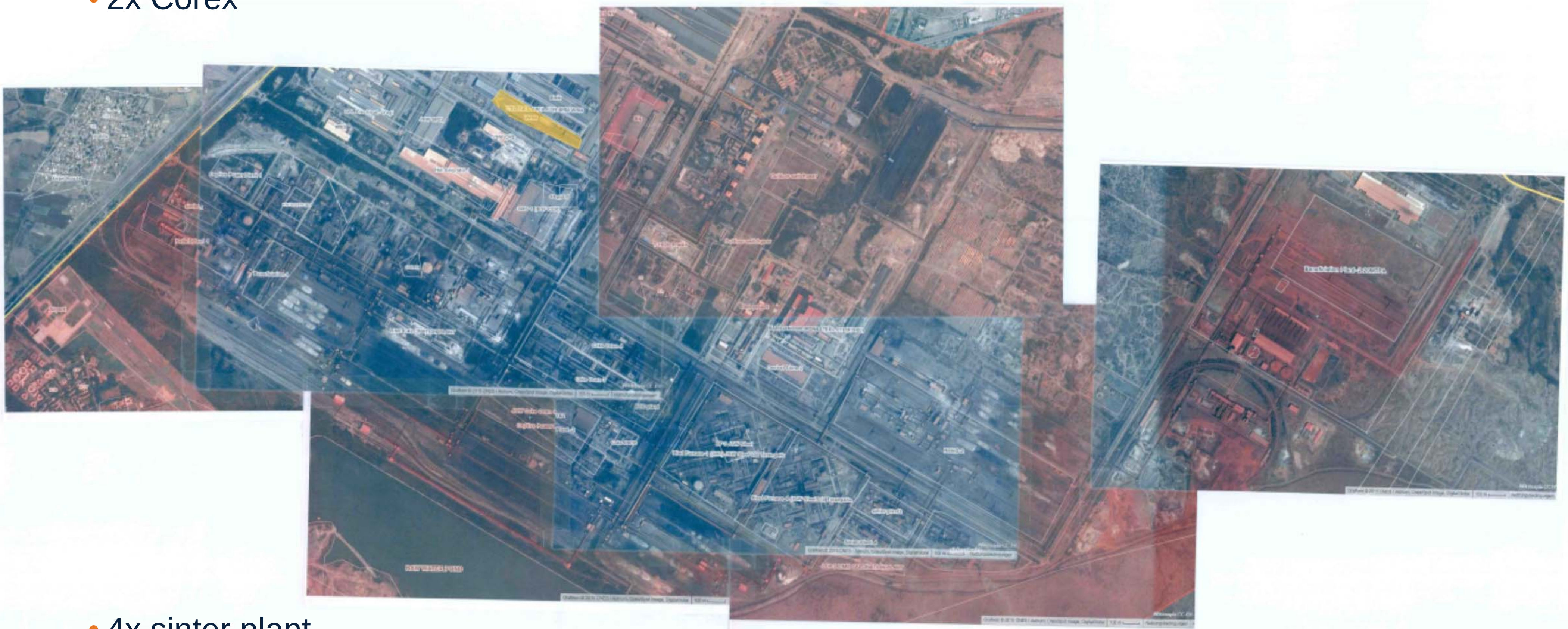
# What is still to do



## What is still to do

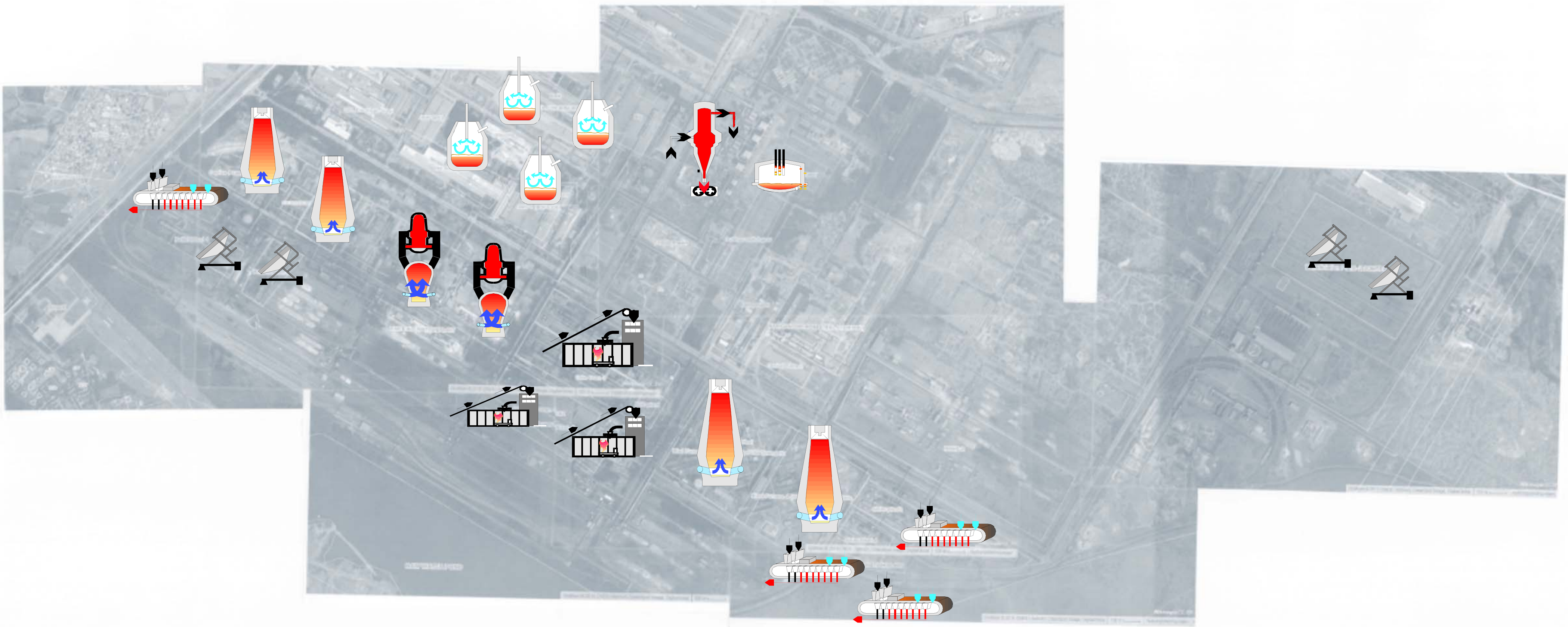
### Example: 12 MTPA full integrated steel plant

- 4x blast furnace
- 2x Corex

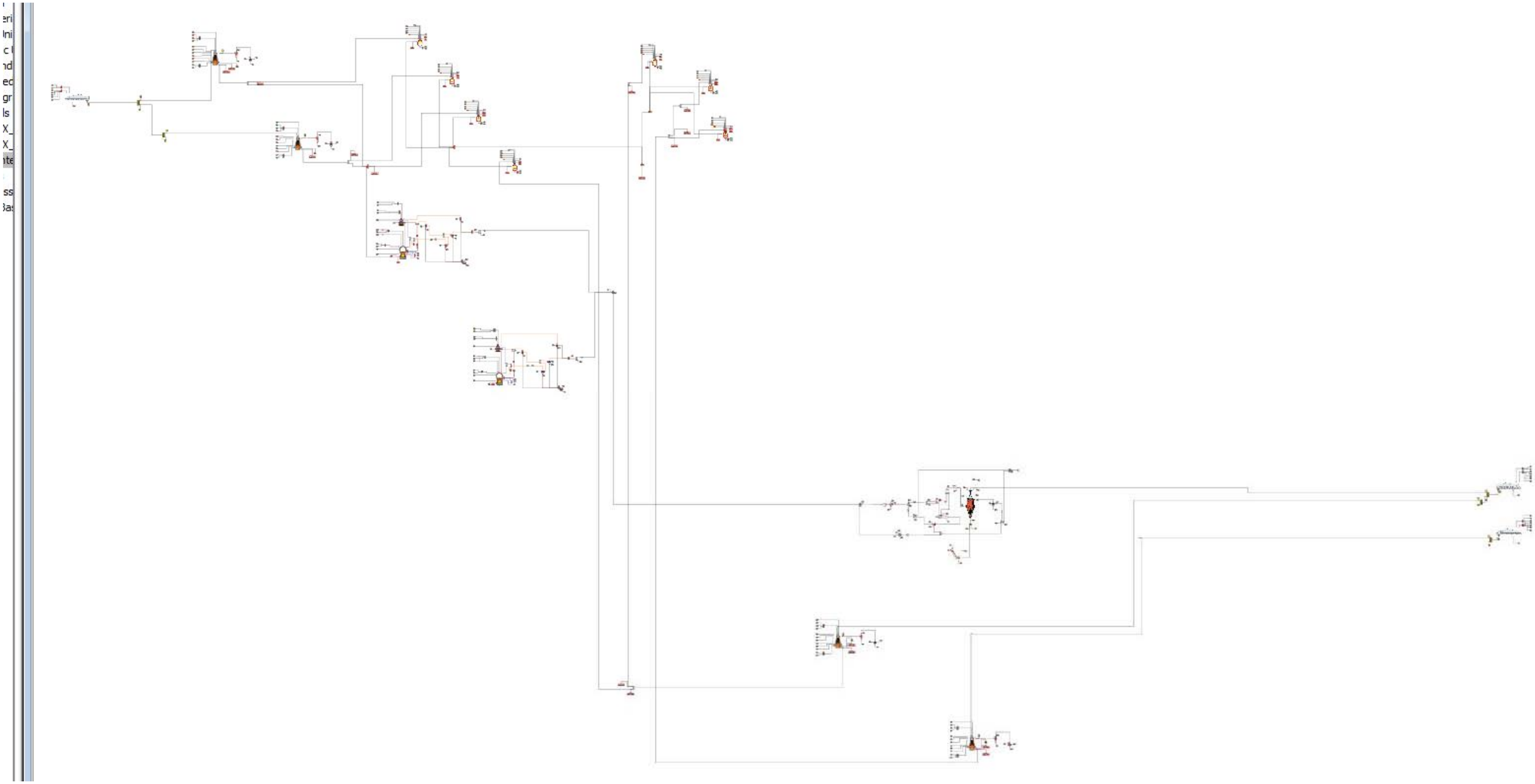


- 4x sinter plant
- 7x LD converters
- 4x pelletizing plant
- 4x coke plant
- 1x DR plant
- 1x Electric arc furnace
- 1x power plant

# What is still to do



# What is still to do



# What are the benefits

- Faster adaption to customer needs
  - Significantly increased flexibility/velocity in calculations during process adaptions
  - Less internal working ours for handling of enquiries
  - Shorter response times to enquiries

- Easier process development
  - gPROMS extends possibilities compared to former tools

- Reduction of NCCs
  - Consortia projects – up to 3 or more external technology partners
  - Generation of lumped balances in former times not possible
  - Now most technologies are covered in gPROMS

- Development of a model library which is currently not commercially available for metallurgy

## Contact

**Bernd Weiss**
MT IR TI DR

**Primetals Technologies**

Turmstrasse 44
4031 Linz
Austria

**M** +43 (664) 8844 8330

**E** bernd.weiss@primetals.com

**primetals.com**

PRIMETALS TECHNOLOGIES

# THANK YOU