

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

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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



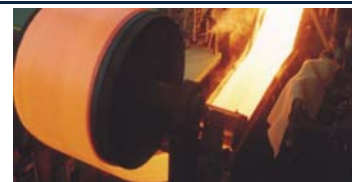
STEELMAKING & LONG ROLLING

- 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



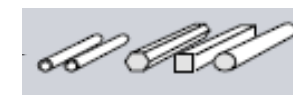
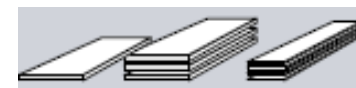
Lump ore



Fine ore



Pellets



How we approached gPROMS

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 (melting 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 adaptations
- 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.

How we approached gPROMS

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

How we approached gPROMS

The approach

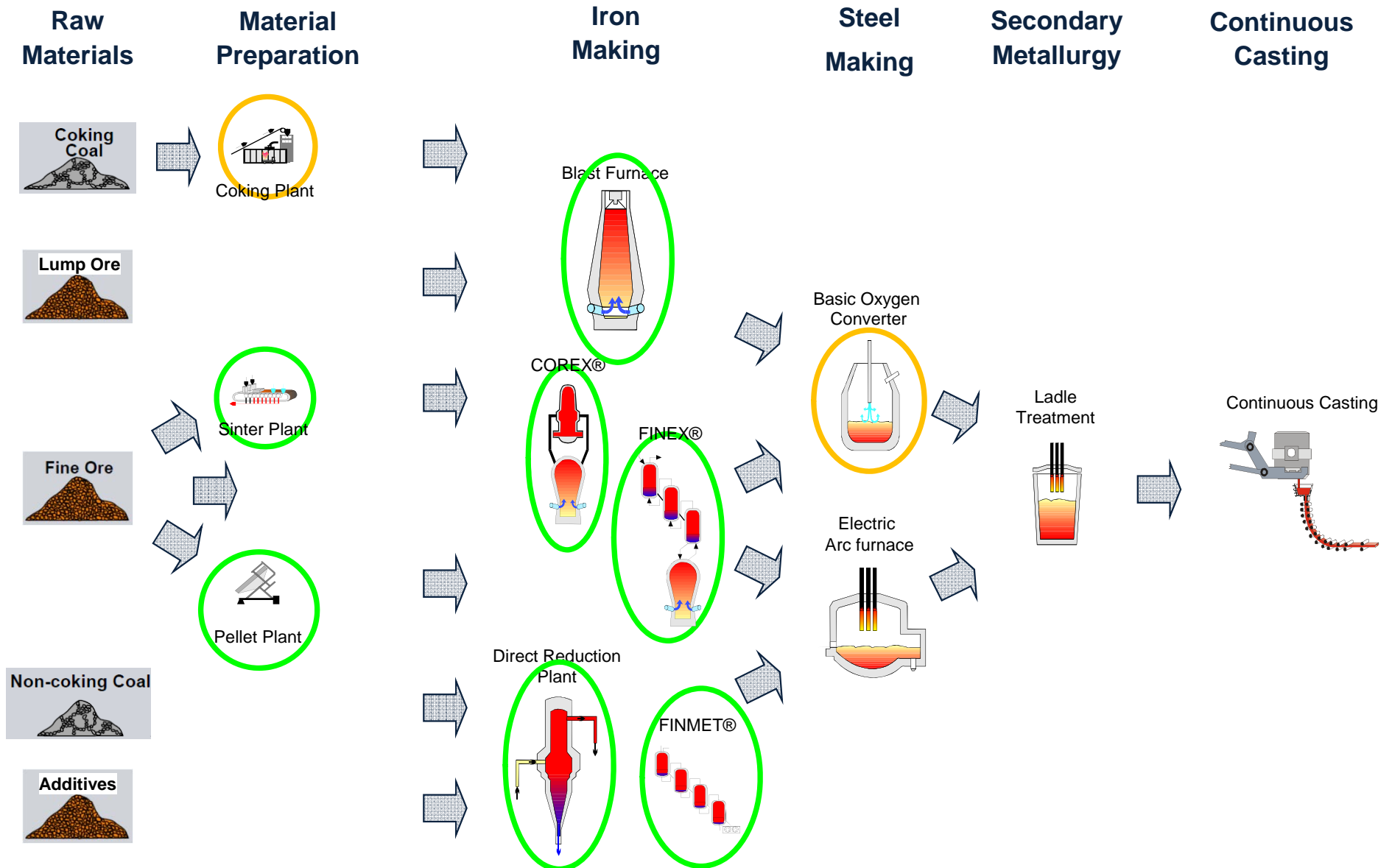
- Thermodynamics
 - Multiflash
 - IAPWS95 steam tables
 - FO Lookup table for metallurgic species enthalpies
 - ChemApp linkage
 - Rist routine and Baur Glaessner approach for basic metallurgical calculations
- Unit operations
 - Sources: introduction of raw materials into flow sheets (solids, gas, water, 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, CO₂ sequestration, mixer, compressor, pumps, CH₄ 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

Purge_Bustle (source_gas)

Temperature units: degrees Celsius
 Pressure units: barg
 Composition specification: mol %
 Flowrate specification: Nm3/tHM

Specify

☒ Temperature: 25 °C
☒ Pressure: 4 bar(g)
☒ Composition: ☐ Uniform for entire array ☒ Per element

gas	mol %
H2	0
H2O_gas	0
H2S	0
O2	0
CO	0
CO2	0
CH4	0
C6H6	0
N2	100
Ar	0
SO2	0

☒ Vol. flow rate: ☐ Uniform for entire array ☐ Per element
 5.6 m³/t (tHM)

Coal1_MG (source_coal_comb)

Input type: direct
 Temperature units: degrees Celsius
 Flowrate specification: dry flow
 Flowunit specification: kg/t (tHM)

Specify

☒ Brand name: "Coal A"
☒ country: "Country"
☒ Carbon type: coal
☒ mass_percent_proximate: ☐ Uniform for entire array ☒ Per element

components proximate input	%
volatile	25.43
ash	9.01

☒ mass_percent_ultimate: ☐ Uniform for entire array ☒ Per element

components ultimate input	%
C	77.88
H	4.23
N	1.33
S_vol	0.42

☒ mass_percent_ash: ☐ Uniform for entire array ☒ Per element

components ash	%
Fe2O3	8.85
CaO	3.25
MgO	2.38
SiO2	52.72
Al2O3	27.34
MnO	0.12
TiO2	0.91
Na2O	0.41
K2O	0.93
P2O5	1.53
SO3	0.69
rest	0.861

☒ Temperature: 25 °C
☒ Moisture: 5 % kg/kg
☒ Dry mass rate: ☐ Uniform for entire array ☐ Per element
 230.6 kg/t (tHM)

Ore1_RS (source_ore_comb)

Input type: direct
 Temperature units: degrees Celsius
 Flowrate specification: dry flow
 Flowunit specification: kg/t (tHM)

Specify

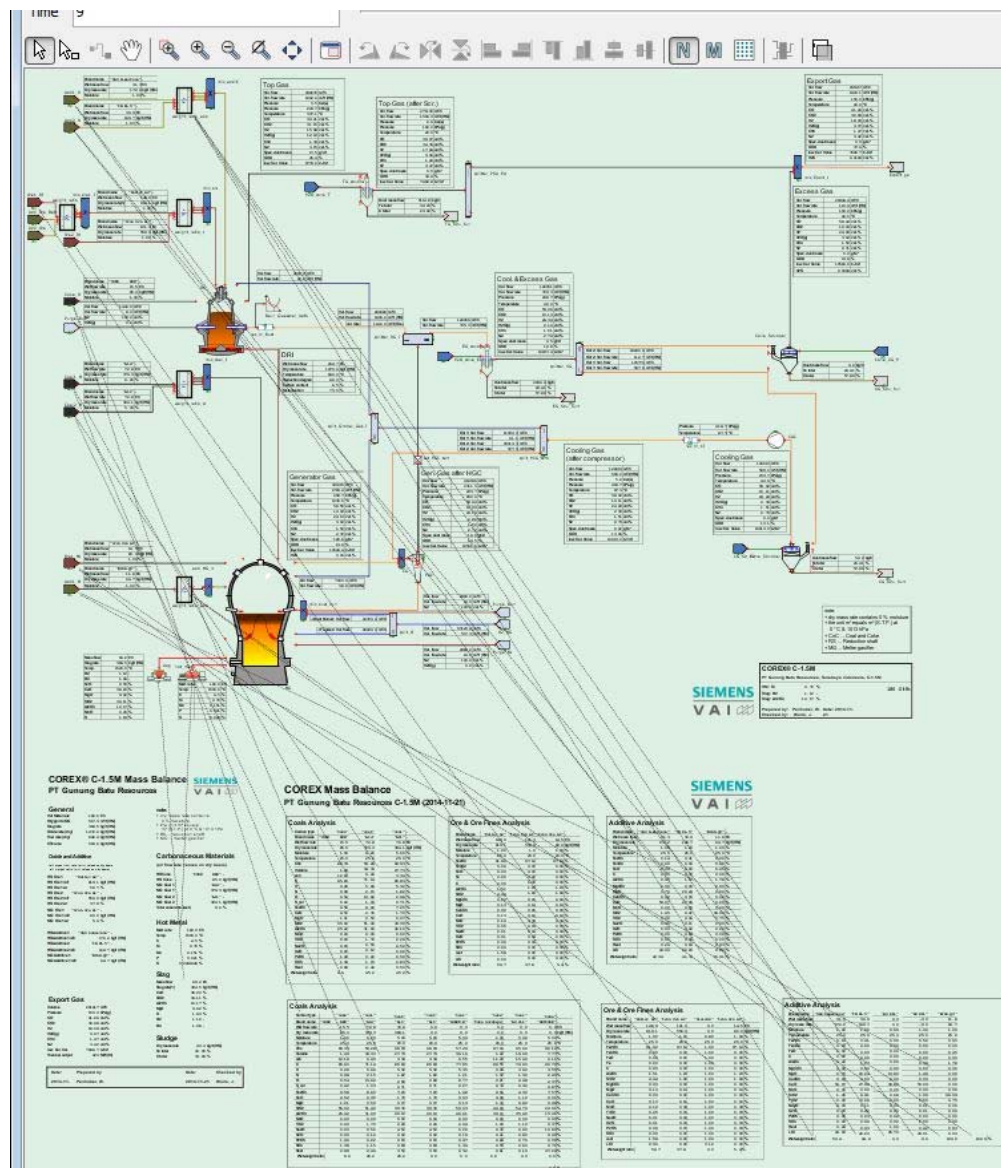
☒ Ore Short Name: "Brand"
☒ Country: "Country"
☒ Mass percent: ☐ Uniform for entire array ☒ Per element

solid in	% kg/kg
Fe2O3	93.32
Fe3O4	0
FeO	0.05
Fe	0
C	0
Al2O3	1.50
SiO2	2.42
MgCO3	0
MgO	0.21
CaCO3	0
CaO	0.77
MnO	0.46
TiO2	0.06
Na2O	0.02
K2O	0.03
P2O5	0.03
SO3	0.01
Rest	1.02

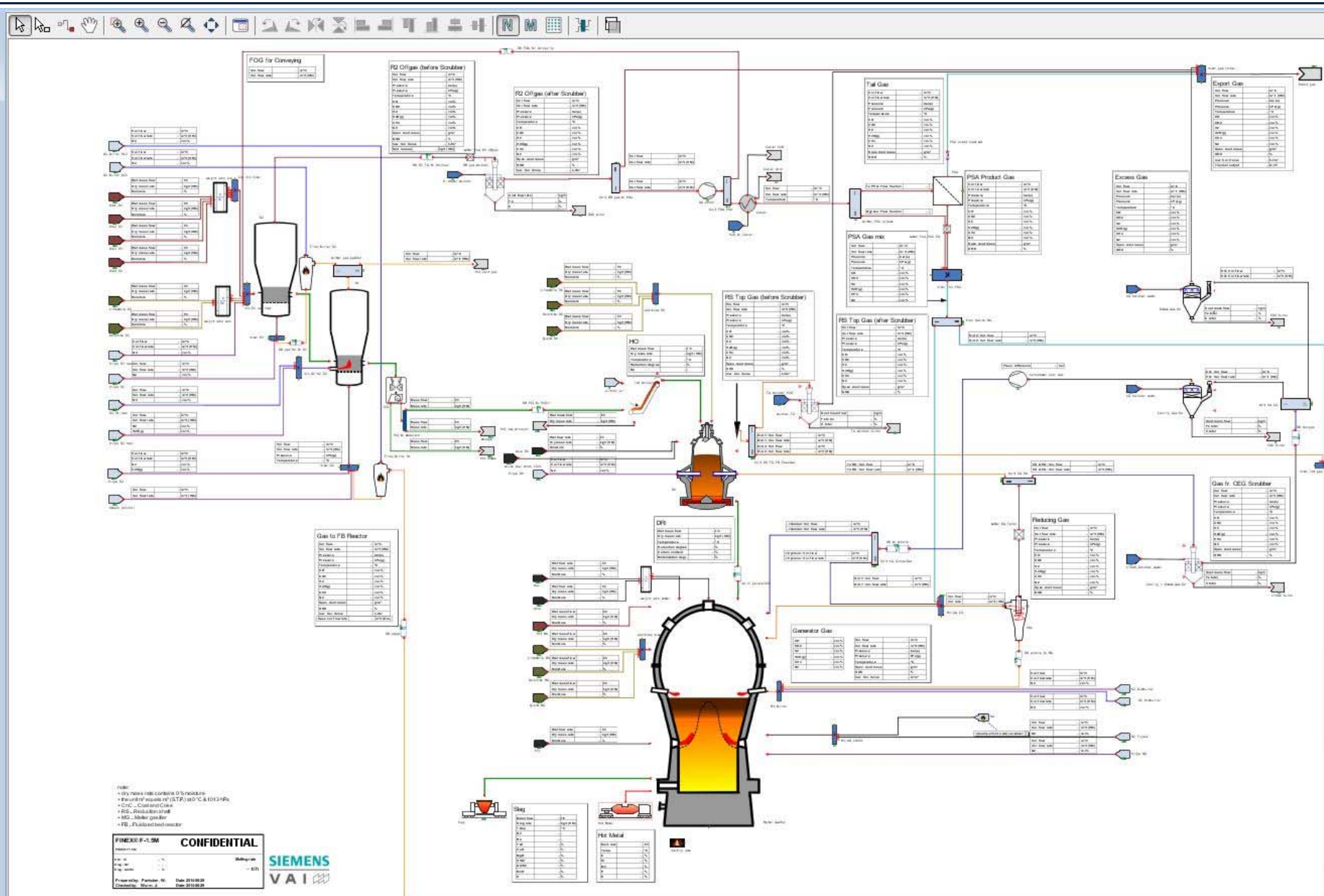
☒ LOI: 3.12 %
☒ Moisture: 1 % kg/kg
☒ Temperature: 25 °C
☒ Dry mass rate: ☐ Uniform for entire array ☒ Per element

number of inlets	kg/t (tHM)
1	239.4
2	
3	
4	
5	

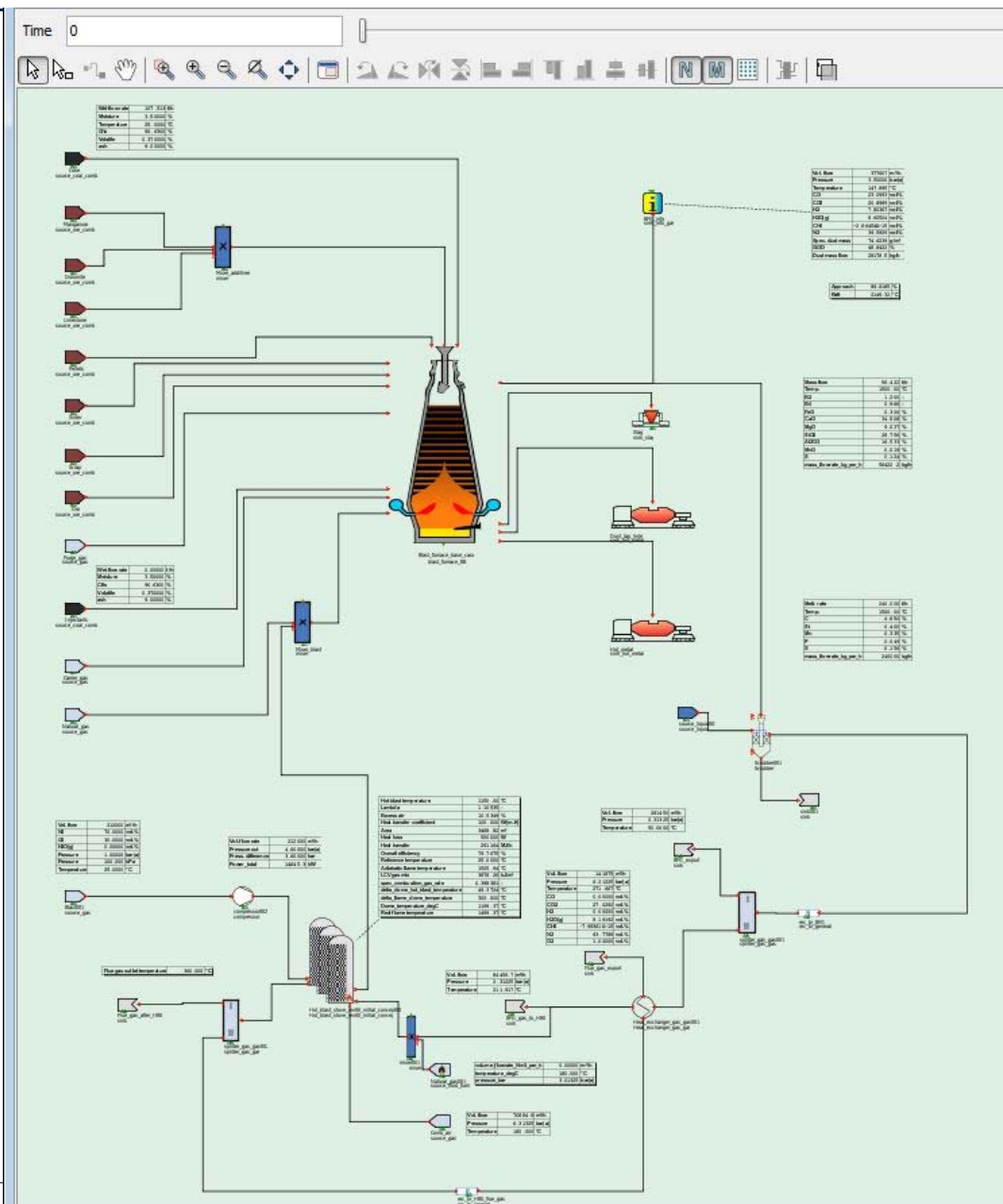
How does it look like



How does it look like



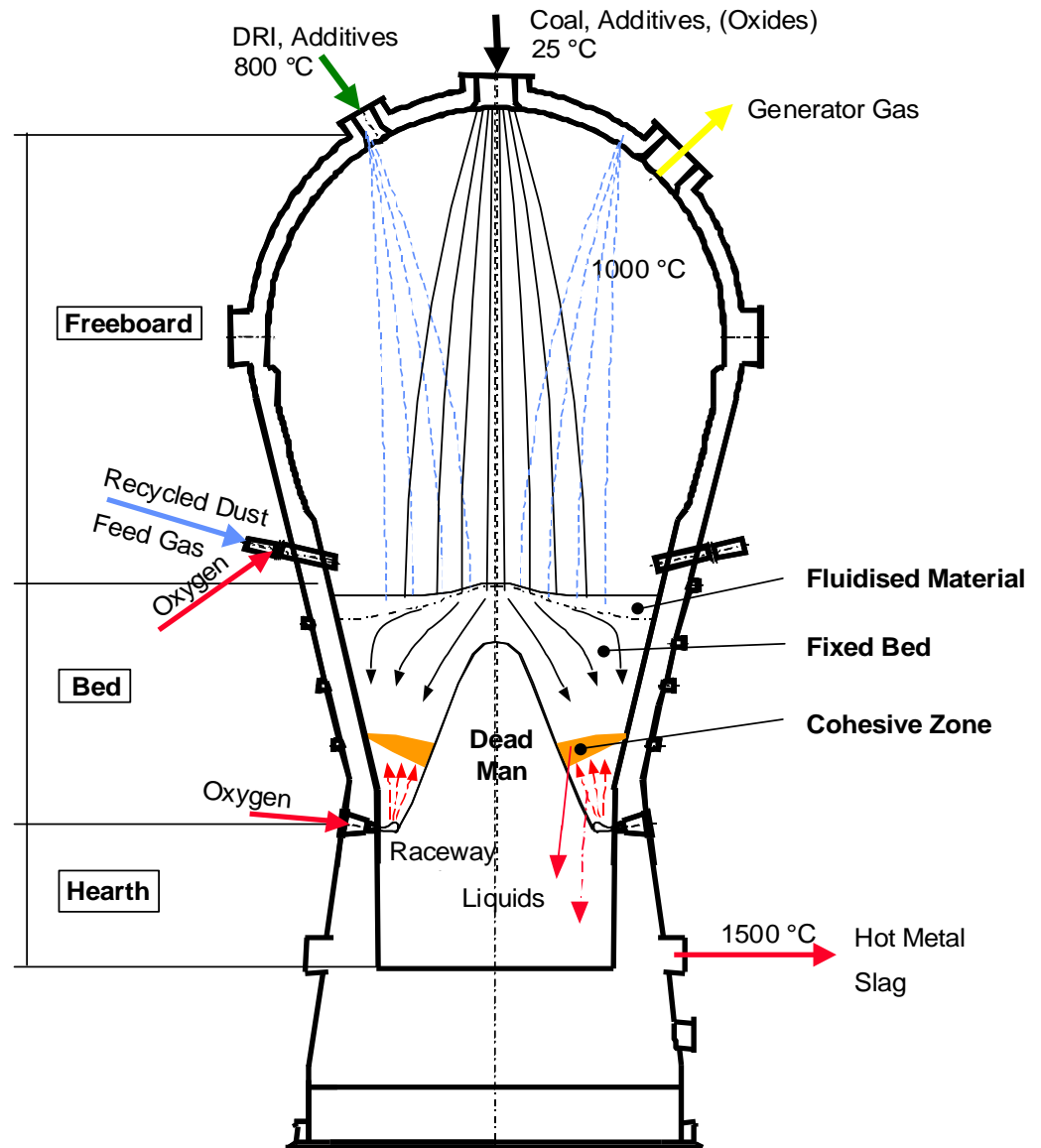
How does it look like



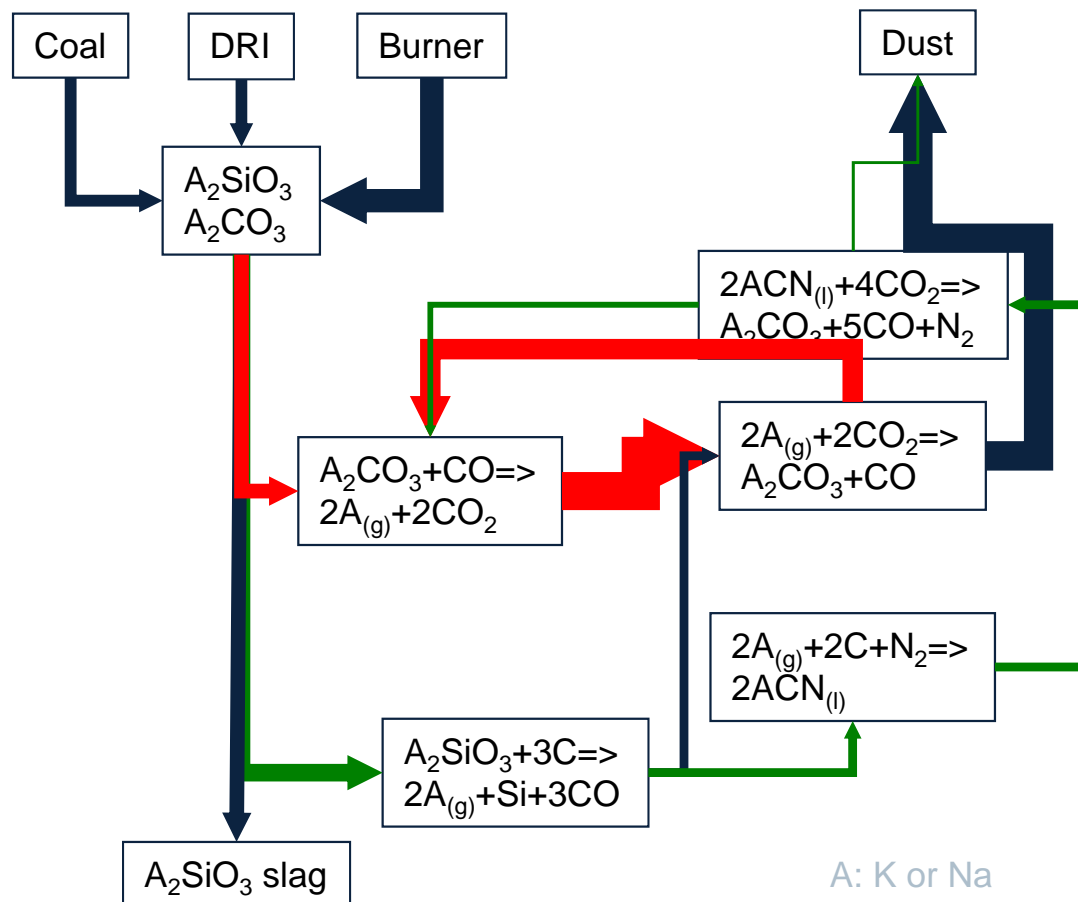
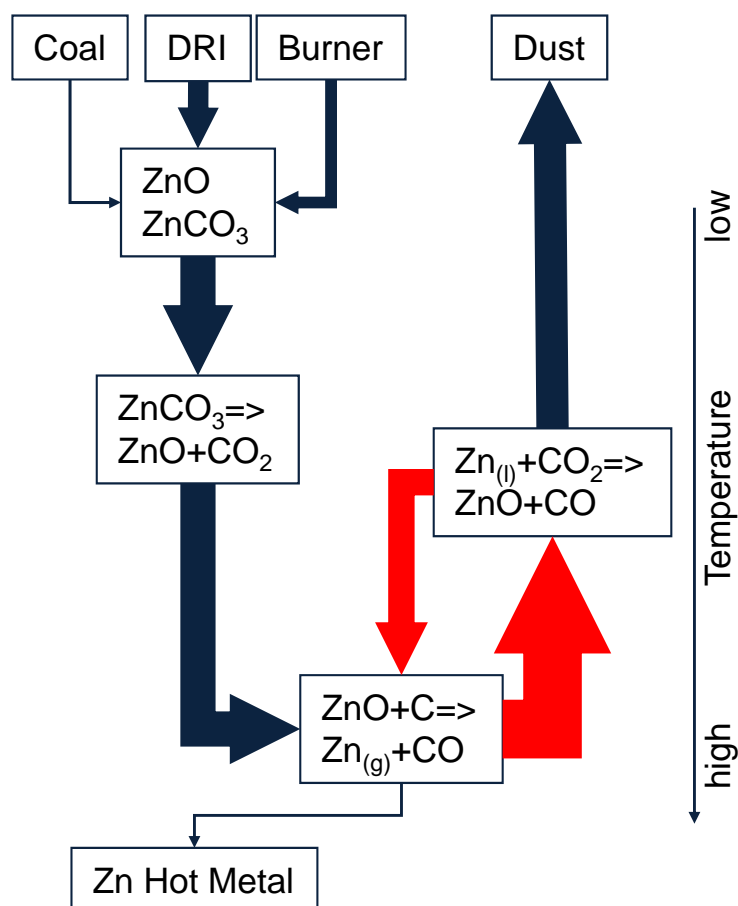
What is still to do

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

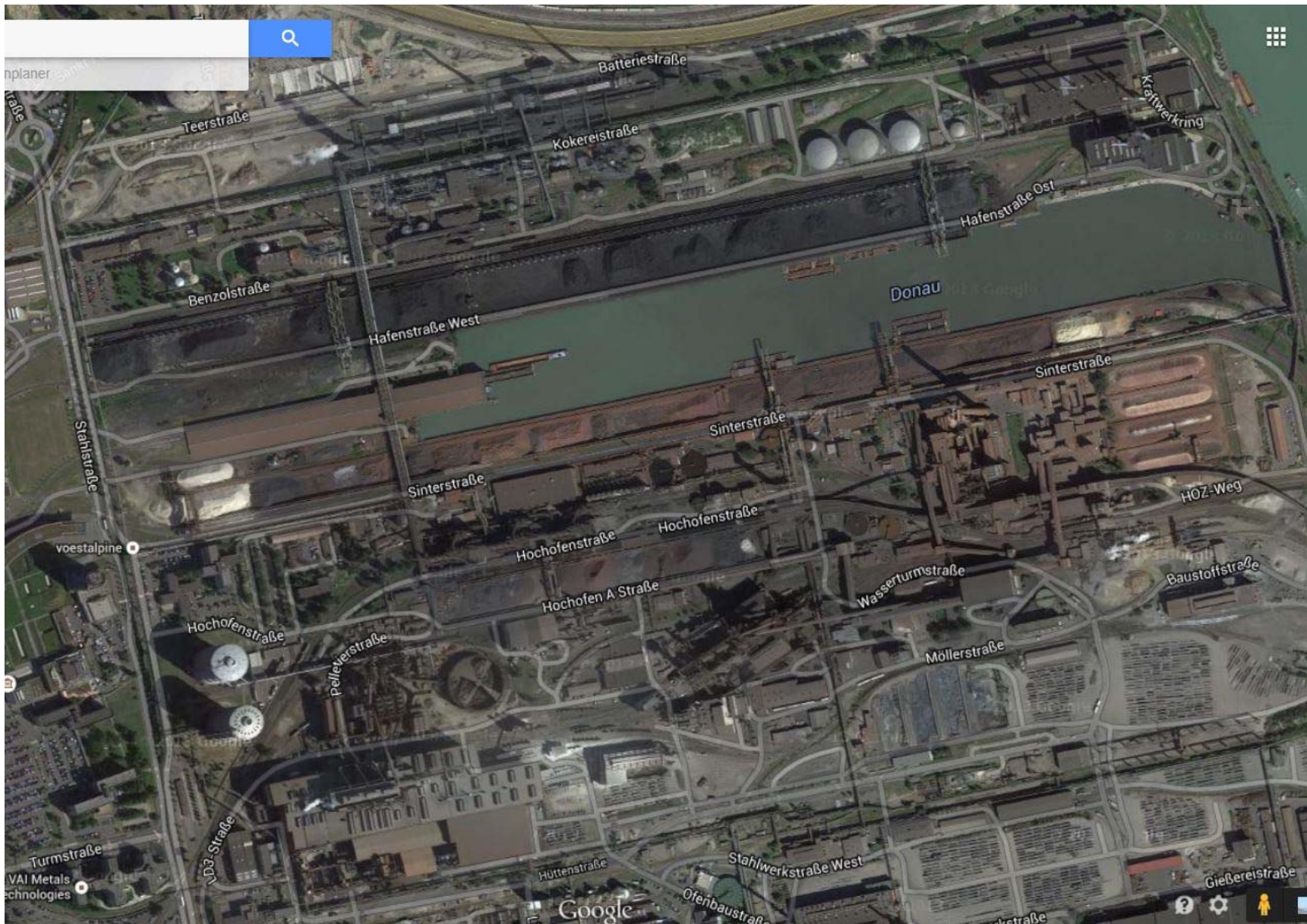
Open items library

- 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

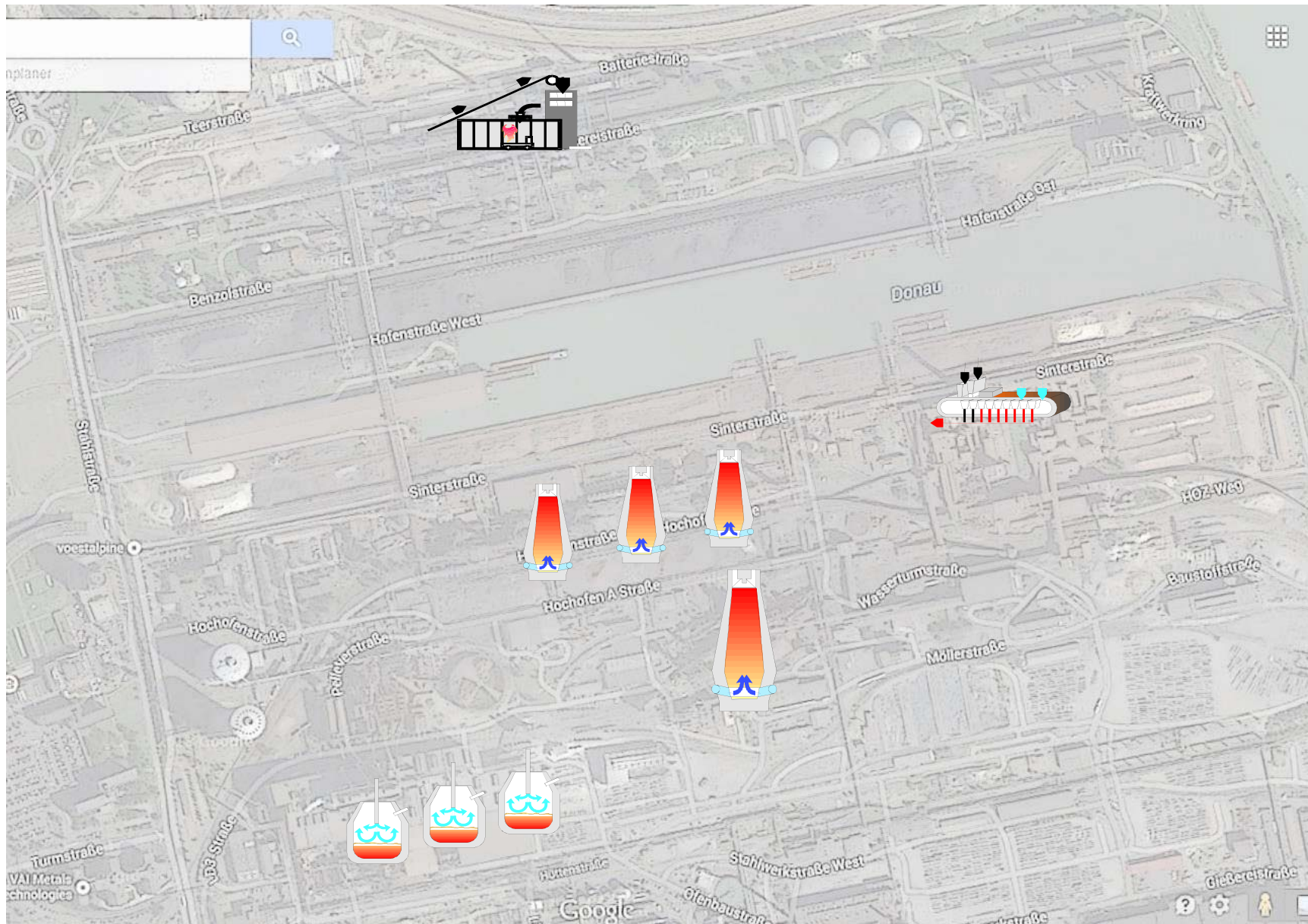
Open items flow sheets

- 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



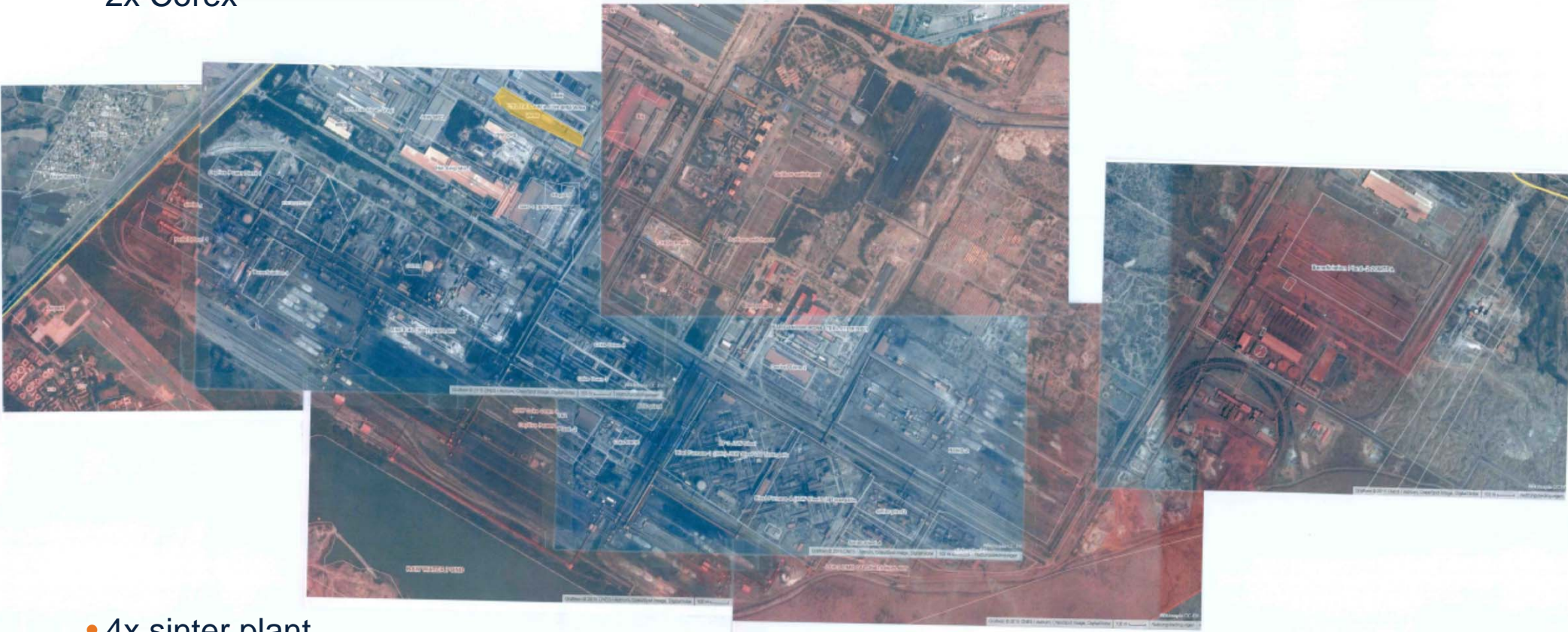
What is still to do



What is still to do

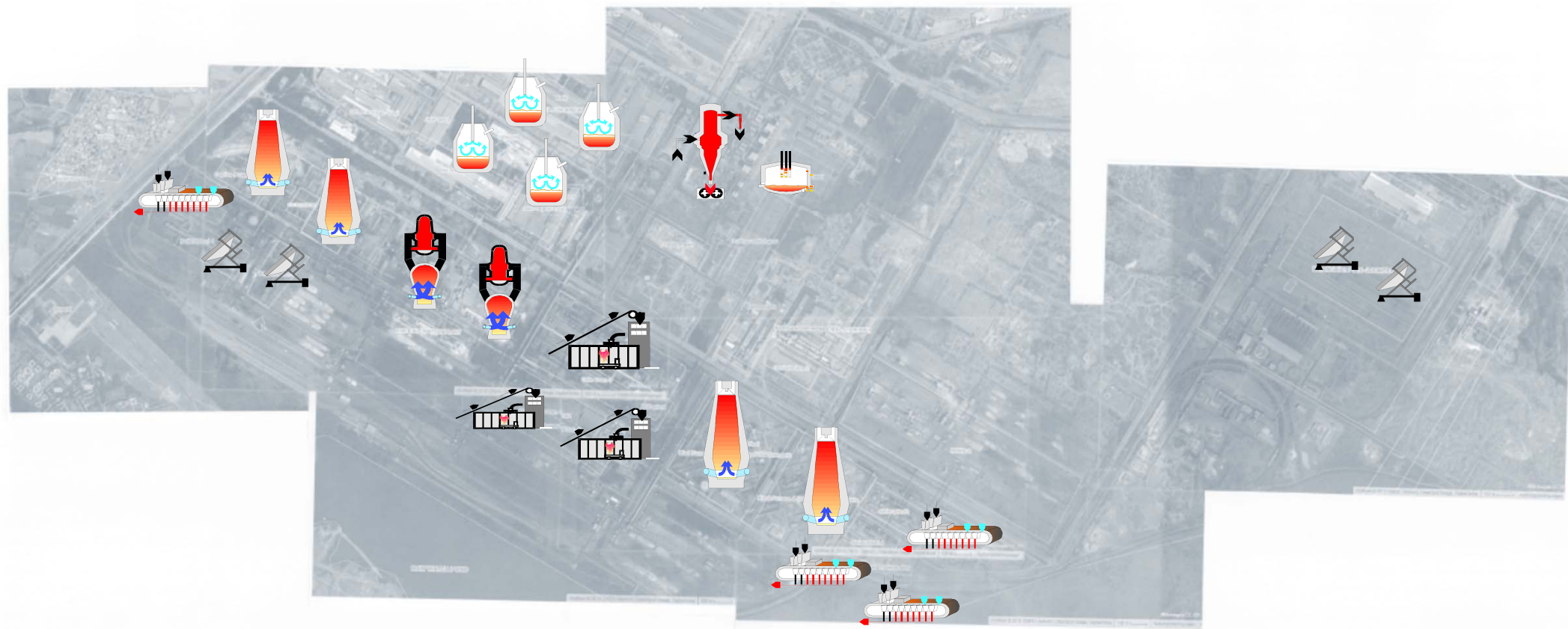
Example: 12 MTPA full integrated steel plant

- 4x blast furnace
- 2x Corex

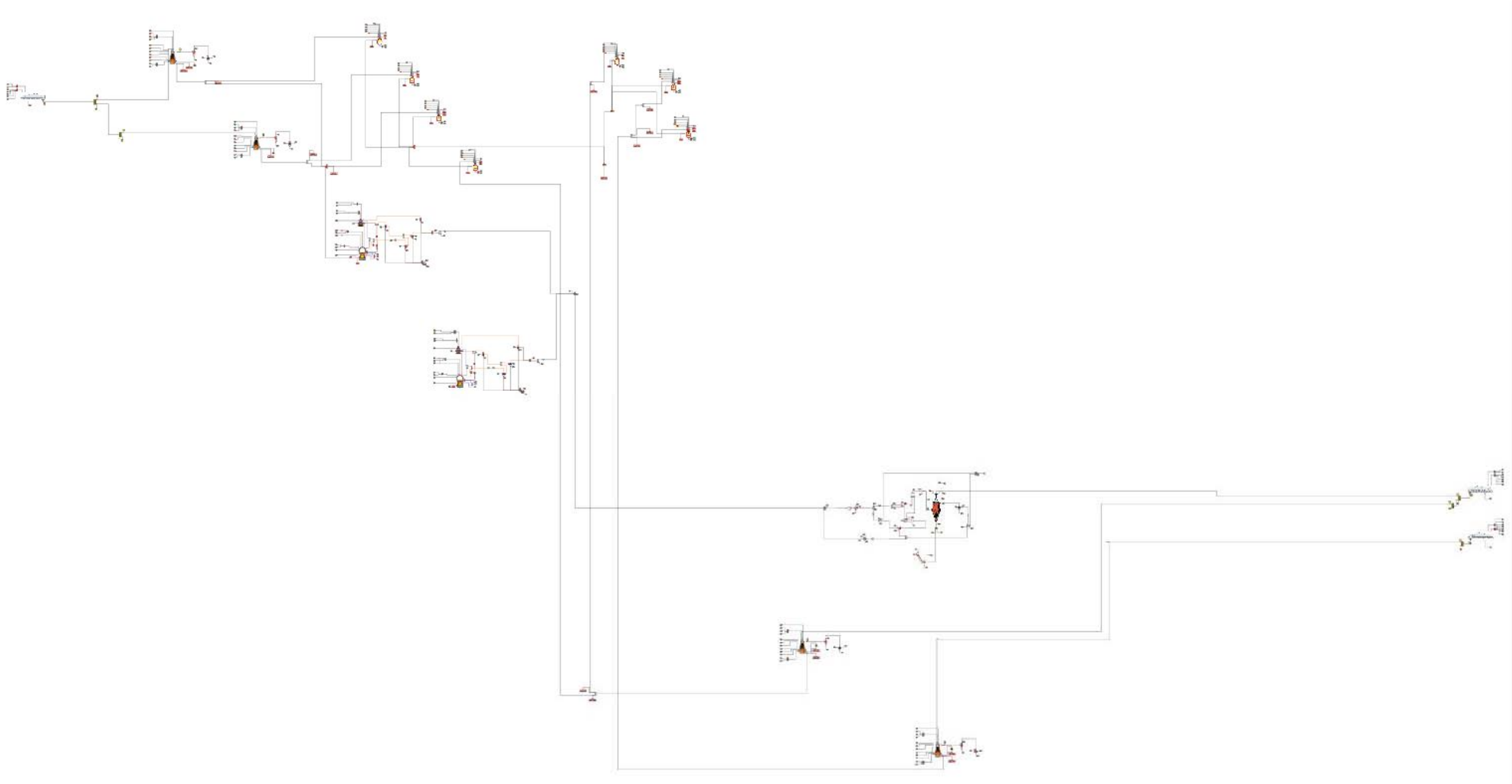


- 4x sinter plant
- 7x LD converters
- 4x coke plant
- 1x Electric arc furnace
- 4x pelletizing plant
- 1x DR plant
- 1x power plant

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 adaptations
 - 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**

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