# Max H2 DR

Maximise H2 Enrichment in Direct Reduction Shaft Furnaces

# Benchmarking of developed steelmaking chain models

## Benchmarking of the tools of the multipurpose toolkit based on simulations of a standard integrated steelworks

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Sensitivity: general

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# 1. Introduction

The report investigates the material and energy balance of a European integrated standardized steel mill (EU SSM) with 4 $Mt_{HRC}$pa capacity and interconnection development of the developed modelling tools.

EU SSM operates with a Blast furnace – Basic oxygen furnace (BF – BOF) route, that is established as a "business as usual"; i.e. Reference scenario in the context of the MaxH2DR project Task 3.1: Adaptation and extension of available models and interconnection development.

EU SSM IRMA flow-sheet is built using as basis the system boundaries as agreed in the MaxH2DR general assembly work package 3 meetings in Brussels on 17-18th October 2022 and in Pisa on 27-28th March 2023, as follows:

- Final product:            Hot rolled coil

- Steel mill productivity:       4 $Mt_{HRC}$pa

- Number of Blast furnaces:     2

- Hot metal output ratio BF's:    60 : 40 in mass

- Availability Blast furnaces:     8760 hpa (100 %)

- Number of Cokes plants:       2

- Number of Sinter; Pellet; Coal grinding plants:    1; 1; 1

- Own/ Merchant pellets ratio:    1 : 2 in mass

EU SSM is comprised of raw materials section, iron and steel making units and gas – energy section. Material - energy balance of the raw materials, iron and steel making plants is elucidated using Tata Steel in-house IRMA flow-sheeting tool. Raw materials, iron and steel making plant (i.e. sub - process) models in the TS RD library were re – evaluated according to settings and boundary conditions established for the EU SSM (See Section **3.1**). These sub – processes are inter - connected with material – energy blocks on the main IRMA lay-out, to generate the "site wide steel mill model".

Process models of the gas - energy section were developed by SSSA using commercial Aspen One engineering suite and in particular the Aspen Plus tool. The models include all the units generally included in EU SSM concerning process off gases treatment, processing and recovery as well as for the production of steam, electricity and technical gases. The type, size, setting and efficiencies of the processes/plants have been selected for fitting with previously defined and reported system boundaries and for being representative of the current configurations of the majority of the EU SSM.

**Table 1** shows the sub-processes included in the EU SSM and the employed modelling tools.

Site wide model exchanges relevant data with the gas – energy section of the SSSA tool mainly comprised of;

- **Demand - Site Wide:** Mixed fuel gases (thermal energy for the works), electricity, steam and utility gases (e.g. $O_2$, $N_2$)
- **Supply – Site Wide:** Process off gases from the Cokes plants, Blast furnaces and Basic oxygen steel plant (i.e. Cokes oven gas, Blast furnace gas and Basic oxygen steel plant gas)
- **Supply – Gas Energy section:** Mixed fuel gases (thermal energy for the works), electricity, steam and utility gases (e.g. $O_2$, $N_2$) to satisfy site wide demands

In the course of development of this deliverable report, the interconnection IT infrastructure of the database (DB) development for the automatic interactions was still ongoing (See Section **3.3.3.2**) for details in the status of the DB development).

Table 1. Sub-processes in the Standard EU Steel Mill and modelling tools

| Section | Sub - process | Modelling tool |
|---|---|---|
| Raw Materials | Sinter plant | IRMA |
| | Pellet plant | IRMA |
| | Cokes plant 1 & 2 | IRMA |
| | Coal grinding line | IRMA |
| Iron and steel making | Blast furnaces 1 & 2 | TS HMB integrated in IRMA |
| | Basic oxygen steel plant | TS TCM integrated in IRMA |
| | Casters | Black box[1] in IRMA |
| | Hot strip mill | Black box in IRMA |
| Gas – energy | BFG Treatment area | Aspen Plus |
| | BOFG Treatment area | Aspen Plus |
| | COG Treatment area | Aspen Plus |
| | Mixing and Enrichment Station | Aspen Plus |
| | Auxiliary Boilers | Aspen Plus |
| | Power plant | Aspen Plus |
| | Air Separation Unit | Aspen Plus |

The following is considered to be out of scope: economic evaluation, including costing of equipment or cash flow analysis; definition of control loop logics; detailed P&IDs. However, simple "control" units have been included in the gas-energy models for allowing the right interpretation of demands from site wide model and the suitable distribution of heat (by mixing gases), steam, electricity and technical gases. In addition, as already anticipated, a complex IT structure have been developed for allowing both collecting info and data related to all the investigations provided in the project with the developed models as well as for allowing the interactions between the different tools.

ABO AML model will provide configurations and operation regimes to IRMA to simulate different system configurations and operational schemes in different stages of a transition towards H2 enriched – direct reduced iron (DRI) and steel making. In this report, current status in the benchmarking of ABO AML model is included. This includes descriptions of the system units and process flows included in the model as well as example model outputs representing operational schemes with a BF-BOF configuration and a configuration featuring hydrogen-based reduction. Model development is set to progress towards further alignment with the reference scenario, aiming at an extensive analysis of possible transition pathways.

## 1.1 Units

Generally, the SI-units will be used throughout the documentation, although pressure will be specified in bara and barg and temperature in °C.

Normal conditions are defined as:

- Pressure: 1,01325 bara
- Temperature: 0.0°C

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[1] Simplified models in which material and energy balances are established using fixed product yield and energy demand nominal to production rate (See Section **3.1.2.3 Casters and Hot strip mill**).

# 2. Basis of design and raw materials data

Ambient conditions specify material streams input temperature and pressure in the ambient conditions of the EU SSM IRMA model:

Ambient Pressure                    1 bara
Ambient Temperature                 15 °C
Low pressure steam                  4 bara
Medium pressure steam               15 bara
High pressure steam                 44 bara

In the next sub-sections, specifications of the gaseous, solid and liquid streams that are input to the EU SSM IRMA and ASPEN boundaries (See **Table 1**) are explained.

## 2.1 Gaseous streams

**Table 2** shows the chemical composition, temperature and pressure of NG, Air and Oxygen (low and high purity). Natural gas and Oxygen stream delivery pressures are as supplied from the gas – energy section. Concerning Oxygen, the current version of ASU model provides oxygen with a purity of 95.51% (see Section **3.2.7**); further improvements will allow providing the two oxygen qualities.

Table 2. Chemical composition, temperature and pressure of Natural gas, Air and Oxygen

|  | Natural Gas | Air | Oxygen (low purity)* | Oxygen (high purity) |
|---|---|---|---|---|
| $C_2H_6$, %$_{mols}$ | 4.50 | 0 | 0 | 0 |
| $CH_4$ | 90.50 | 0 | 0 | 0 |
| CO | 0.00 | 0 | 0 | 0 |
| $CO_2$ | 1.50 | 0.03 | 0 | 0 |
| $H_2$ | 0.00 | 0 | 0 | 0 |
| $H_2O$ | 0.00 | 1.19 | 0 | 0 |
| $N_2$ | 2.00 | 78.16 | 4.49 | 0.05 |
| $O_2$ | 0 | 20.62 | 95.51 | 99.95 |
| Rest | 0 | 0 | 0 | 0 |
| Temperature, °C | 15.00 | 15.00 | 35.00 | 35.00 |
| Pressure, bara | 15.00 | 1.00 | 8.00 | 8.00 |
| LHV, MJ/Nm³ | 35.88 | NA | NA | NA |

* as delivered by current version ASU

## 2.2 Solid streams

### 2.2.1 Ferrous streams and fluxes

The fine ore blend input chemistries to the PP and SP IRMA models were generated based on the target oxide pellet and sinter chemistries (modelling methodology is explained in Sections **3.1.1.1 Sinter Plant** and **3.1.1.2 Pellet Plant**). Lump ore (to BF) chemistry is as retrieved from relavant literature [1].

Table 3 shows chemical compositions of the pellet ore mix, sinter ore mix and lump ore.

Table 3. Chemical composition of the pellet ore mix, sinter ore mix and lump ore

|  | Pellet Ore Mix | Sinter Ore Mix | Lump Ore |
|---|---|---|---|
| $Al_2O_3$, %mass | 0.15 | 1.04 | 1.35 |
| C | 0.12 | 0.09 | 0.00 |
| CaO | 0.36 | 0.29 | 0.07 |
| T.Fe (%) | 66.86 | 62.04 | 61.90 |
| $Fe_2O_3$ | 56.79 | 76.26 | 88.5 |
| $Fe_3O_4$ | 37.48 | 12.02 | 0.00 |
| $H_2O$ (liq.) | 0.00 | 2.37 | 0.00 |
| MgO | 0.25 | 1.30 | 0.08 |
| MnO | 0.20 | 0.21 | 0.09 |
| $SiO_2$ | 4.44 | 4.85 | 3.67 |
| Rest | 0.20 | 1.55 | 6.17 |

Chemical compositions of bentonite, limestone, olivine and burnt lime that are input material streams to EU SSM IRMA model were defined based on the relevant literature data [2]- [6] and expert opinion in the TS RD to generate aggrevated chemistries for these streams (See **Table 4**).

Table 4. Chemical composition of the fluxing agents

|  | Bentonite | Limestone | Olivine | Burnt Lime |
|---|---|---|---|---|
| $Al_2O_3$ | 19.86 | 1.1 | 0 | 0.26 |
| CaO | 6.85 | 0 | 0.32 | 69.40 |
| $CaCO_3$ | 0 | 88.7 | 0 | 22.97 |
| FeO | 0.46 | 0 | 7.24 | 0 |
| $Fe_2O_3$ | 4.97 | 0 | 0 | 0.76 |
| MgO | 3.31 | 1.73 | 48.25 | 1.65 |
| Mn | 0.04 | 0 | 0 | 0 |
| S | 0.83 | 0 | 0 | 0 |
| $SiO_2$ | 62.67 | 5.06 | 41.72 | 4.51 |
| Rest | 1.01 | 3.41 | 2.47 | 0.45 |

## 2.2.2 Carbonaceous streams

Coking coal, PCI coal and anthracite are import solid carbonaceous streams to the EU SSM for energy supply and reducing agent purposes in the iron and steel works. Chemical composition of the solid carbonaceous streams were defined based on the relevant literature data [6]- [8]and evaluated in the TS RD to generate aggrevated chemistries for these streams (See **Table 5**).

Table 5. Chemical composition of the carbonaceous streams

|  | PCI Coal blend | Coking Coal blend | Anthracite |
|---|---|---|---|
| $Al_2O_3$ | 2.58 | 2.92 | 3.65 |
| C | 81.35 | 83.49 | 76.42 |
| CaO | 0.21 | 0.24 | 0.61 |
| $Fe_2O_3$ | 0.83 | 0.94 | 0 |
| $H_2$ | 4.22 | 4.13 | 2.70 |

| | | | |
|---|---|---|---|
| MgO | 0.10 | 0.11 | 0.15 |
| $N_2$ | 1.91 | 1.23 | 0.19 |
| $O_2$ | 3.85 | 1.05 | 5.96 |
| $SiO_2$ | 4.33 | 4.89 | 8.57 |
| S | 0.35 | 0.69 | 0.19 |
| MnO | 0.01 | 0.01 | 0.005 |
| Rest | 0.26 | 0.30 | 1.56 |

## 2.3 Liquid streams

In gas-energy Aspen-based models also water is used that, for simplicity and since water treatment is out of the scope of the investigations, has been assumed as pure water at 30°C (common temperature of water after cleaning and cooling sections). In COG treatment also a flushing liquor has been used with a concentration of 5.5 g/L of ammonia.

# 3. Methodology

## 3.1 Standardized Integrated Steelworks IRMA model

The IRMA process models consist of interconnected unit operations that include heating - cooling, mixing – separation, chemical reactions, compression - turbine and chemical equilibrium (of multicomponent, multiphase systems). In the model convergence, Quasi-Newton Bounded mathematics is selected as a solver type. Flow-sheet solver accuracy of 0.1 tons, 1 °C, 0.1 GJ and 1 % are selected as accuracies in the fields of total mass, temperature, enthalpy and mass fraction. In this version, ChemApp v4.1.2.0 and Factsage data: Equilib v5.2.0 are used for thermodynamic data (e.g. enthalpy) estimation .

In this section the EU SSM IRMA Model settings – set points in the sub-processes and plant target solvers are described. Settings in the IRMA model (unless specified as calculation output) are constant values, retrieved using relevant expert opinions in the fields, literature data (specified in the report where relevant) and ULCOS SP9 – WP4 Reference data [9].

IRMA reports mass -energy balance in scalar kg/ tons and MJ/ GJ scales, respectively. In this work, tons and GJ scales are used with hourly time intervals to express in the mass and energy flow rates in tons/hr and GJ/hr.

### 3.1.1 Raw materials section modelling in IRMA

In this section, methodology modelling of the sinter, pellet, coal grinding-drying and cokes plants 1 and 2 that are included to the raw materials section of the EU SSM IRMA model are explained.

### 3.1.1.1 Sinter Plant

The sinter plant process considered in this model consists of conventional ('air breathing') sintering without waste gas recirculation. For the sinter plant mass-energy balance model, the basic unit operations of the sintering process were considered as follows:

- Mixing of iron ores, fluxes, reverts and carbon source, and granulation with addition of water.
- Ignition at a pre-defined oxygen excess, interfacing with the work of consortium partners on the WAG network and WAG composition.
- Calcination/decomposition of fluxes and breeze/anthracite combustion.
- Sinter ferrous component nett reduction/reoxidation reactions using an FeO-content setpoint to determine nett energy requirement.
- A flue gas 'post-combustion' unit operation, where the stochiometrically required $O_2$ and CO of the net reduction/reoxidation are combusted to reflect the contribution thereof to the mass-energy balance.
- An energy convergence operation where the process carbon requirement is adjusted to obtain a pre-defined sinter bed total heat content.
- Sinter cooling and screening to obtain a final product sinter at ambient temperature for use in the BF model module.

**Table** 6 shows the input – output streams of the SP. Pellet fines, mill scale, coke breeze and BFG dust are recycled in the SP produced as side product / waste streams in the PP, HSM, CP, BF, respectively.

Table 6. Material input – output streams of the SP

| Input streams | | Output streams |
|---|---|---|
| Fine iron ore | BFG dust | Sinter |
| Pellet fines | Burnt lime | Flue gas |
| Mill scales | Olivine | Water vapour |
| Anthracite | Mixed fuel gas | |
| Coke breeze | Air | |
| Limestone | MP steam | |

The governing chemical reactins in the SP are listed in **Equation 1** - **Equation 13**. They are grouped into flux calcination (**Equation 1** and **Equation 2**), ferrous reduction/oxidation (Equation 3 - Equation 8), and solid carbon and mixed fuel gas combustion (**Equation 9** - **Equation 13**).

$$CaCO_3 = CaO + CO_2 \qquad \text{Equation 1}$$

$$FeMgSiO_4 = FeO + MgO + SiO_2 \qquad \text{Equation 2}$$

$$3.Fe_2O_3 + CO = 2.Fe_3O_4 + CO_2 \qquad \text{Equation 3}$$

$$Fe_3O_4 + CO = 3.FeO + CO_2 \qquad \text{Equation 4}$$

$$FeO + CO = Fe + CO_2 \qquad \text{Equation 5}$$

$$Fe + O_2 = 2FeO \qquad \text{Equation 6}$$

$$6.FeO + O_2 = 2.Fe_3O_4 \qquad \text{Equation 7}$$

$$4.Fe_3O_4 + O_2 = 6.Fe_2O_3 \qquad \text{Equation 8}$$

$$2.C_{breeze+C-bearing\ reverts} + O_2 = 2.CO \qquad \text{Equation 9}$$

$$2.CO + O_2 = 2.CO_2 \qquad \text{Equation 10}$$

$$CH_4 + 2.O_2 = CO_2 + 2.H_2O \qquad \text{Equation 11}$$

$$2.C_2H_6 + 7.O_2 = 4.CO_2 + 6.H_2O \qquad \text{Equation 12}$$

$$2.H_2 + O_2 = 2.H_2O \qquad \text{Equation 13}$$

## Setpoint and convergence criteria

The sinter plant mass balance is governed primarily by the ore mix mass rate to reach the aim sinter production rate. CaO and MgO %$_{mass}$ targets in the product sinter are achieved by limestone and olivine addition, respectively (See

**Table** 7).

Solid carbonaceous streams' (i.e., breeze and anthracite) input rates are change (manipulated) fields to satisfy the energy balance of the SP (See

**Table** 7) at specified brutt sinter (i.e. averaged sinter bed) temperature and heat losses as specified below.

Table 7. EU SSM Sinter plant in IRMA operational targets and change fields

| Condition | Target field | Accuracy | Unit | Change field | Unit |
|---|---|---|---|---|---|
| 1 | Production rate | 0.1 | tons/hr | Ore mix rate | tons/hr |
| 2 | CaO content | 0.1 | %mass | Limestone rate | tons/hr |
| 3 | MgO content | 0.1 | %mass | Olivine rate | tons/hr |
| 4 | Energy balance | 0.1 | GJ/hr | Anthracite, breeze and mixed fuel gas rate | tons/hr |

Several settings introduced to the SP are;

- Temperature inlet streams, °C:          15
- Temperature brutt sinter, °C:           780
- Temperature fue gas, °C:                150
- Heat loss, %$_{eng.}$:                  5
- Temperature sinter, °C:                 25

Electrical energy and MP steam consumptions of the SP are correlated to sinter productivity as described below:

- Electrical energy input nominal to plant capacity:    136.4 MJ$_{el.}$/t$_{Sinter}$
- MP steam input nominal to plant capacity:             1.6 kg./t$_{Sinter}$

## 3.1.1.2 Pellet Plant

The pellet plant unit operations include the following stages:

- Mixing of ores, solid carbon and fluxes at ambient temperature.
- Drying of wet mix using the mixed fuel gases (from the gas - energy network) and hot flue gas from an induration section.
- Grinding – drying at elevated temperature.
- Balling – addition of binder and balling moisture: Forming of green pellets.
- Strand drying of formed pellets using waste heat from the induration section.
- Induration: Mixed fuel gas and anthracite combustion and pellet heating to target bed temperature (See **Equation 9** - **Equation 13**).
- Oxidation of Wustite and Magnetite to Hematite with the available oxygen (See **Equation 7** and **Equation 8**).
- Pellet cooling and induration gas separation for drying operations.
- Pellet product separation: Pellet to BF and Pellet fines to SP.

Table 8 shows the input – output streams of the PP. Plain pellet is the main product that is used as a charge feed to the BF1 and 2. Pellet fines that are side product of the PP are recycled in the SP.

Table 8. Material input – output streams of the PP

| Input streams | | Output streams |
|---------------|---------------|----------------|
| Fine iron ore | Olivine | Plain pellet |
| Anthracite | Mixed fuel gas | Pellet fines |
| Coke breeze | Air | Flue gas |
| Limestone | Water | |
| Bentonite | MP steam | |

## Setpoint and convergence criteria

The setpoints are implemented in pellet plant to reach target pellet plant capacity and chemistry . The CaO and $SiO_2$ content of the pellet are controlled by the limestone and olivine addition, respectively (See **Table 9**). Necessary limestone and olivine input rates (to reach target pellet chemistry) are influenced by the gangue content - chemistry of the ore and ash content - chemistry of the solid carbonaceous streams (i.e. coke breeze and anthracite).

Target plant productivity is reached, by changing the ore mix mass rate. The energy balance of the pellet plant is solved separately for grinding, drying, induration and cooling zones by change fields: mixed fuel gas, air intake rate, solid carbonaceous stream rate and internal gas circulation to cooling rates, respectively (See **Table 9**).

Table 9. EU SSM Pellet plant in IRMA operational targets and change fields

| Condition | Target field | Accuracy | Unit | Change field | Unit |
|-----------|--------------|----------|------|--------------|------|
| 1 | Production rate | 0.1 | tons/hr | Ore mix rate | tons/hr |
| 2 | CaO content | 0.1 | $\%_{mass}$ | Limestone addition | tons/hr |
| 3 | $SiO_2$ content | 0.1 | $\%_{mass}$ | Olivine addition | tons/hr |
| 4 | Energy balance grinding | 0.1 | GJ/hr | Mixed fuel gas rate | kNm3/hr |
| 5 | Energy balance drying | 0.1 | GJ/hr | Air intake flow rate | kNm3/hr |
| 6 | Energy balance induration | 0.1 | GJ/hr | Carbonaceous solids rate | tons/hr |
| 7 | Energy balance cooling | 0.1 | GJ/hr | Internal gas circulation | $\%_{vol.}$ |

Several settings introduced to the PP are;

- Temperature inlet streams, °C:     15
- Temperature drying, °C:     100
- Temperature flue gas, °C:     95

- Heat loss, %eng.:            5
- Temperature plain pellets, °C:     135

Electrical energy and MP steam consumptions of the PP are correlated to pellet productivity as described below:

- Electrical energy input nominal to plant capacity:     145 MJ$_{el.}$/t$_{Bell\ pellet}$
- MP steam input nominal to plant capacity:     1.2 kg./t$_{Bell\ pellet}$

### 3.1.1.3 Cokes Plant 1 & 2

Coke and COG making operation in the CP 1 and 2 are sub-divided into below given unit operations:

- Coal drying
- Coal heating to final temperature
- Generation of tar and benzole
- Release of light gases
- Water quench

Coal drying, heating, cracking and COG generation operations require input of thermal energy. Necessary thermal energy for the coke making operation is supplied by combustion of mixed fuel gas under the coke batteries in the regeneration furnaces (in-direct heating).

Coking coal goes under chain of decomposition reactions, plasticity initiates and develops forming heavy hydrocarbons (i.e. tar and benzole). Cokes oven gas formation is simplified into the reaction steps as shown in **Equation 14** - **Equation 19**:

$$C_{(s)} + 2H_{2(g)} \rightarrow CH_{4(g)}$$     Equation 14

$$2C_{(s)} + O_{2(g)} \rightarrow 2CO_{(g)}$$     Equation 15

$$H_{2_{volatiles}} \rightarrow H_{2(g)}$$     Equation 16

$$CH_{4(g)} + CO_{2(g)} \rightarrow 2CO + 2H_2$$     Equation 17

$$2H_{2(g)} + O_{2(g)} \rightarrow 2H_2O_{(g)}$$     Equation 18

$$CH_{4(g)} + H_2O_{(g)} \rightarrow CO + 3H_2$$     Equation 19

**Table** 10 shows the input – output streams of the CP1 and 2. Own coke is the main product that is charged to the BF1 and 2 as a reductant and energy source. Coke breeze (i.e. coke fines) are partly/ fully recycled in the SP and PP (See **Table 6** and

**Table** 8) as energy source. Produced tar and benzole are reported as export streams in the EU SSM. COG is an input stream to the gas – energy section. Chemical energy contained in the COG is recycled in the EU SSM to generate thermal and electrical energy for the iron and steel works (See Section **3.2.3**).

Table 10. Material input – output streams of the CP1 and 2

| Input streams | Output streams |
|---|---|
| Coking coal | Own coke |
| Mixed fuel gas | Coke breeze |

| Air | Tar |
|---|---|
| HP steam | Benzole |
| Mixed fuel gas | COG |
| | Fue gas |

**Setpoint and convergence criteria**

The setpoints are implemented in the CP to reach target plant capacity (See **Table 11**). Target CP capacity is reached with changed coking coal input rate. Mass flow and composition of tar and benzole are correlated to volatile matter content of the coking coal, as described in the literature [10].

The energy balance of the CP is satisfied by solving necessary amount of mixed fuel gases combustion in the cokes batteries regeneration furnaces that satisfies the hear reuqirement of the process unit operations. (See **Table 11**).

Table 11. EU SSM Cokes plant in IRMA operational targets and change fields

| Condition | Target field | Accuracy | Unit | Change field | Unit |
|---|---|---|---|---|---|
| 1 | Production rate | 0.1 | tons/hr | Coking coal rate | tons/hr |
| 2 | Energy balance | 0.1 | GJ/hr | Mixed fuel gas rate | tons/hr |

Several settings introduced to the CP 1 and 2 are;

- Temperature inlet streams, °C: 15
- Temperature hot coking coal, °C: 1100
- Temperature flue gas, °C: 150
- Temperature cokes after quench, °C: 25

Electrical energy and HP steam consumptions of the CP' s are correlated to cokes productivity as described below:

- Electrical energy input nominal to plant capacity: $206.5\ MJ_{el.}/t_{Coke}$
- HP steam input nominal to plant capacity: $82\ kg./t_{Coke}$

## 3.1.1.4 Coal grinding line

Coal grinding line is sub – divided into drying-heating and grinding mill subsections as unit operations. Thermal energy required for drying the PCI coal at the target moisture level is achieved by direct heat supply from the combustion of mixed fuel gases (See **Table 13**). Dried and grinded PC is delivered to BF 1 and 2 as an injection coal. **Table 12** shows the input – output streams of the CGL.

Table 12. Material input – output streams of the CGL

| Input streams | Output streams |
|---|---|
| PCI coal | PC |
| Mixed fuel gas | Fue gas |
| Air | Water vapour |

| Nitrogen | |
|----------|--|

Table 13. EU SSM CGL in IRMA operational targets and change fields

| Condition | Target field | Accuracy | Unit | Change field | Unit |
|-----------|-------------|----------|------|--------------|------|
| 1 | Production rate | 0.1 | tons/hr | PCI coal input rate | tons/hr |
| 2 | Energy balance | 0.1 | GJ/hr | Mixed fuel gas rate | tons/hr |

Several settings introduced to the CGL are;

- Temperature inlet streams, °C:          15
- Temperature exhaust mill, °C:           70
- Temperature PC at the outlet of CGL, °C:   50

Electrical energy and Nitrogen consumptions of the CGL are correlated to PCI productivity as described below:

- Electrical energy input nominal to plant capacity:     126.2 $MJ_{el.}/t_{PC}$
- N2 input nominal to plant capacity:                    40 $kg./t_{PC}$

### 3.1.2 Iron and steel making section modelling in IRMA

### 3.1.2.1 Blast Furnaces 1 & 2

Raw materials section including sinter, pellet, cokes and coal grinding IRMA plant models are deployed to deliver input to the BF 1 and 2 for BF hot metal production. Oxygen enriched hot blast is delivered from the hot blast stoves (See Section **3.2.1**). Merchant pellet and lump ore are import streams to the EU SSM IRMA are charged to the BF 1 and 2. Hot metal, slag, BFG and BFG dust are output streams of the BF 1 and 2. Material input and output streams of the BF' s are shown in **Table 14**.

Hot metal is delivered to steel making shop for the liquid steel production. Chemical energy contained in the BFG is recycled in the EU SSM to generate thermal and electrical energy for the iron and steel works  (See Section **3.2.1**). BFG dust is partially/fully recycled in the SP (See Section **3.1.1.1 Sinter Plant**). BF Slag is reported as an export stream of the EU SSM, and mainly used as a feedstock in the cement making industry.

Table 14. Material input – output streams of the BF 1 and 2

| Input streams | Output streams |
|---------------|----------------|
| Coke | Hot metal |
| PC | BF Slag |
| Sinter | BFG |
| Own Pellet | BFG Dust |
| Merchant Pellet | |
| Lump ore | |
| Hot blast | |

Blast furnaces 1 and 2 are integrated to the site model by IRMA user defined process unit that operates the TS RD in-house BF HMB model. Chemical compositions of the charged and injected materials are introduced as fixed values that are imported to BF HMB model from the site wide model-lay out in IRMA. HMB model is invoked with the source code that contains OLE specific compound. Site wide model lay-out material stream chemistries are written to HMB, material stream flow rates are read from the HMB (calculated / fixed) and picked up in the main IRMA flow sheet using scripting and coupling features. In this regard, HMB model is included to every iteration loop for the site wide model convergence. Relevant outputs of the BF process are written as material and energy blocks (e.g. BFG dust, hot metal, BF slag, BFG, heat losses) with calculated (/fixed) chemistries, flow rates, temperature and pressure.

Table 15 shows the selected list of fixed and computed parameters as implemented in the TS RD BF HMB model.

Table 15. BF HMB model setting: Selection of fixed values and computed variables

| Fixed parameters | Unit | Computed parameters | Unit |
|---|---|---|---|
| Hot metal productivity | $t_{HM}/day$ | Pellet rate | $kg_{dry}/t_{HM}$ |
| PCI rate | $kg_{dry}/t_{HM}$ | Slag rate | |
| Sinter rate | | Cokes rate | |
| Lump ore rate | | TGT | °C |
| Air blast $O_2$ | %vol. | TG chemistry | %mass |
| Total heat loss | %eng. | Slag chemistry | |
| Hot metal chemistry ex. Fe | %mass | Gas utilisation | %vol. |
| Humidity blast | $g/Nm^3$ | Heat loss rate | GJ/day |
| Pressure blast | barg | | |
| Temperature blast | °C | | |
| Temperature hot metal | | | |

## 3.1.2.2 Basic oxygen steel plant

Through Cost Model used in IRMA simulation for the MaxH2DR project is a TS in-house development model for the steel making process of OSF2, IJmuiden, and have been used by other steel plants as well. The model covers the process of hot metal desulphurization, converter and secondary steelmaking metallurgy. It is developed upon a static charge balance model for the converter process, and includes many operational aspects of other 3 processes. With the pre-defined target quality and temperature of steel, the model generates output in terms of material consumptions. Hence, it provides an opportunity to make off line calculations to study the effect of various hot metal input on the flow of materials through the steel plant.

In Through Cost Model, the target property of liquid steel is taken from the quality book of steel plant and the target temperature from operational experience. With the targets and input hot metal properties, the model calculates:

•       Input of base materials (scrap, lime, ore, oxygen, etc.)

•       The amount and the contents of steel and slag

The calculations in the model are based upon the idea, that a specific charge is made using a number of pre-set values. The important variables that need to be set are:

• Steel weight after tapping in the ladle

• Temperature and carbon analysis at turndown

• Hot metal composition and temperature

• Scrap menu

For the converter process, the heat and mass balance is calculated using the appropriate rules for flux additions. Metallurgical relations are used to simulate the refining behaviour of converter slag, e.g. FeO generated in slag, Mn,  P and S distributed between the liquid steel bath and slag by oxidation. The relationship are described as a function of other process parameters. In general, in order to use such relations in a simulation model, parameters need to be tuned with process data. The aim values for the converter process, e.g. carbon and temperature of liquid steel at the end of oxygen blow etc, are either calculated with the process rules or defined with input parameters.

For the desulphurisation process, the yield of deS agents, e.g. Mg and CaO, is calculated as a function of other process parameters. For the secondary steelmaking units, e.g. ladle furnace, stirring station etc., the yield of added alloys is calculated as a function of other process parameters.

Dust loss from different inputs through vacuum system, e.g. hot metal loss during tapping and  small particles of lime and other fluxes, is calculated with related mass weight and pre-set loss coefficients. The post combustion phenomenon related with converter offgas is simulated by water-shift reaction and CO oxidation reaction. See **Table 16** for input and output material streams of the BOSP.

Table 16. Material input – output streams of the BOSP

| Input streams | | Output streams |
|---|---|---|
| Hot metal | Burnt dolomite | Liquid steel |
| Lump ore | Miscellaneous | BOS slag |
| Scrap | Oxygen | BOS tap loss |
| Dolomite | Nitrogen | BOSG |
| Burnt lime | Argon | BOSG Dust |

## 3.1.2.3 Casters and Hot strip mill

Casters and Hot strip mill sub-processes are highly simplified black -  box models that operate with script -  coupling feature of the IRMA model, in which below described calculations are implemented:

• Main input / output yield ratios

• Utilities; e.g. thermal, electrical energy, steam, N2, Ar consumption

Using linear equations that take into consideration the plants' capacity and ouputs are reported as text files. Slope functions used in these linear equations are aggrevated values from ULCOS SP9 - WP4 Reference data  [9] and expert opinion in the TS RD.

Table 17. Casters and Hot strip mill model setting: Governing equations as modelled in EU SSM in IRMA

| Parameter | Casters | HSM |
|---|---|---|
| Product yield | 1020.3 kg$_{LS}$/t$_{BOS\ Cast}$ | 1024.7 kg$_{BOS\ Cast}$/t$_{HRC}$ |
| Caster/ HSM Scrap output | 20 kg$_{Caster\ Scrap}$/t$_{BOS\ Cast}$ | 11 kg$_{HSM\ Scrap}$/t$_{HRC}$ |
| Mill scales output | - | 15.1 kg$_{Mill\ Scales}$/t$_{HRC}$ |
| Thermal energy input nominal to plant capacity | 13 MJ/t$_{BOS\ Cast}$ | 1380 MJ/t$_{HRC}$ |
| Electrical energy input nominal to plant capacity | 45 MJ$_{el.}$/t$_{BOS\ Cast}$ | 309.6 MJ$_{el.}$/t$_{HRC}$ |
| MP Steam | 1 kg/t$_{BOS\ Cast}$ | 6 kg/t$_{HRC}$ |
| Argon | 0.5 kg/ t$_{BOS\ Cast}$ | - |
| Nitrogen | - | 0.5 kg/t$_{HRC}$ |

### 3.1.3 Description of the EU SSM Reference Case:

Raw materials, iron and steel making plant productivities are shown in **Table 18**. Plant capacities in the raw materials section, basic oxygen steel plant, casters and hot strip mill are set based on the feedstock to BF and BF hot metal output rates. BF's productivities are established to reach 4 Mt$_{HRC}$pa capacity in the EU SSM.

Table 18. Annual plant capacities and main product names in the EU SSM

| Sub-process | Production rate, tpa | Product Name |
|---|---|---|
| Cokes plant 1 | 453,768 | BF cokes |
| Cokes plant 2 | 691,164 | BF cokes |
| Sinter plant | 3,802,733 | Bell sinter |
| Pellet plant | 1,201,872 | Pellets |
| Coal grinding line | 750,732 | Injectant coal |
| Blast furnace 1 | 1,522,269 | Hot metal |
| Blast furnace 2 | 2,321,400 | Hot metal |
| Desulphurisation; Basic oxygen steel plant; Secondary metallurgy | 4,182,288 | SM liquid steel |
| Casters | 4,098,925 | BOS cast |
| Hot strip mill | 4,000,007 | Hot rolled coil |

EU SSM in the Reference Case operates with own/merchant pellets ratio of 2:1 in mass as described in the **Introduction**. Own and merchant (i.e. purchased) pellet target chemistries are aligned with the BF grade pellet A and B that are sourced by TS in the context of the (H2 enriched) direct reduction trials in the WP1 (See **Table 19**). Sinter chemistry is defined based on a generic EU sinter chemistry and cross-checked with the relevant literature [11], [12] (See **Table 19**). The SP and PP model material – energy balances are solved based on defined target chemistries and plant productivities as explained in Sections **3.1.1.1 Sinter Plant** and

**3.1.1.2 Pellet** Plant.

Table 19. Chemical composition of the Pellet A, B and Bell Sinter in the EU SSM

| | Pellet A (Own) | Pellet B (Merchant) | Bell Sinter |
|---|---|---|---|
| T.Fe (%) | 64.85 | 64.6 | 55.66 |
| Al$_2$O$_3$, %$_{mass}$ | 0.35 | 0.64 | 1.30 |
| CaO | 1.04 | 2.10 | 10.08 |
| Fe$_2$O$_3$ | 92.54 | 92.19 | 72.64 |

| | | | |
|---|---|---|---|
| Fe₃O₄ | 0.16 | 0.15 | 6.25 |
| MgO | 0.41 | 1.34 | 1.67 |
| MnO | 0.19 | 0.27 | 0.20 |
| S | 0.01 | 0.00 | 0.03 |
| SiO₂ | 5.03 | 2.76 | 5.74 |
| Rest | 0.26 | 0.55 | 2.09 |
| Mass rate, ktpa | 1,201.9 | 600.9 | 3,802.7 |

BF 1 and 2 hot metal productivities (See **Table 18**) are set according to agreed EU SSM annual productivity (of 4 $Mt_{HRC}pa$), hot metal output ratios of BF 1/2 and annual availability BF' s as described in **Section 1**. BF' s HMB model operates with fixed and calculated parameters as explained in Section **3.1.2.1 Blast Furnaces 1 & 2.** Fixed parameters of the BF 1 and 2 are defined using as reference ULCOS SP9 - WP4 Reference data [9], other relevant literature [7] and expert opinion in the TS RD (See **Table 20**).

Table 20. BF 1 and 2 HMB model fixed parameters in the EU SSM

| Fixed parameters | Unit | Value | |
|---|---|---|---|
| Hot metal productivity | $t_{HM}$/day | 4170.6 | 6360.0 |
| PCI rate | | 195 | |
| Sinter rate | $kg_{dry}/t_{HM}$ | 992.2 | |
| Lump ore rate | | 150 | |
| Air blast O₂ | %$_{vol.}$ | 28 | |
| Total heat loss | %$_{eng.}$ | 2 | |
| Humidity blast | g/Nm³ | 10 | |
| Pressure blast | barg | 3.4 | |
| Temperature blast | °C | 1140 | |
| Temperature hot metal | | 1490 | |

## 3.2 Gas and Energy Network of the Steelworks Aspen model

The transition of integrated steelworks towards $H_2$-based DRI steelmaking involves significant changes in the offgases, steam and electricity production, demand and management. For this reason, MaxH2DR multipurpose simulation toolkit includes a model area to simulate gas cleaning, processing and distribution, steam production and distribution, and electricity production and distribution. In general, it allows the management of all the energy sources, their processing, conversion, and distribution. The involved models have been developed to be linked with production area models (i.e. IRMA-based models): production area models send data to the gas and energy network area models and these last satisfy the energy demand of production area models considering also some defined constraints in terms of Lower Calorific Values (LCV) and Wobbe Index (WI) as reported in **Table 21**. While indications concerning different gases distribution is provided in Table 22. References for these values are previous projects [13]- [15].

Table 21: LCV and WI constraints for gas usage in main users

| Unit | LCV | WI |
|---|---|---|
| | MJ/Nm3 | |
| Mixing & Enrichment Station | | 4-5 |
| Power Station | 3-4.5 | 3.5-6 |
| Auxiliary Boilers | >3 | |

| Hot Blast Stoves | 3-4 | |
| Hot Rolling Mill | 14-27 | |

Although the gas and energy networks models have been developed by SSSA especially to be linked with IRMA-based process models, they can receive/send data also from/to other data sources/sinks and models. Models are stationary ones, developed using the Aspen Plus simulation software and, at this stage, all the involved units related to gas, steam and energy network of standard integrated steelworks have been included. Indeed, it constitutes the starting point for guiding the transition. In particular, the following sections have been modelled:

- Blast Furnace Gas (BFG) Area
- Basic Oxygen Furnace Gas (BOFG) Area
- Coke Oven Gas (COG) Area
- Mixing and Enrichment Station (M&ES)
- Auxiliary Boilers
- Power Plant

Table 22: Indicative ranges of gases distribution

| Gas | User | % |
|---|---|---|
| BFG | Hot Blast Stoves | 20-35 |
| | Mixing & Enrichment Stations | 60-80 |
| | Others (e.g. coke plants) | 0-5 |
| BOFG | Mixing & Enrichment Stations | 80-90 |
| | Others (e.g. Pellet Plant) | 10-20 |
| COG | Coke Plant | 10-40 |
| | Hot Rolling Mill | 25-55 |
| | Hot Blast Stoves | 5-20 |
| | Power Stations | 0-40 |
| | Mixing & Enrichment Stations | 0-15 |
| | Others (e.g. Pellet Plant, Steel Plant, Boilers) | 0-20 |
| Enriched BOFG | Power Plant | ~65 |
| | Coke Plant | ~20 |
| | Others (e.g. Hot Rolling Mill) | ~15 |

In addition, also Air Separation Unit (ASU) have been modelled for ensuring the request in terms of nitrogen and oxygen.

Models have been developed according to discussions and choices done during the first phases aof the project and summarized in Sections **1** and **2** and considering information and data coming from the MaxH2DR industrial partner, previous projects and literature; main references will be provided in the dedicated subchapters.

As general information that is common for all the models, Peng-Robinson equation of state was used as base property method in the development. Furthermore, a list of chemical compounds have been selected for simulating all the main features and aspects of the involved gas and steam streams (i.e. $C_2H_6$, $CH_4$, $CO$, $CO_2$, $H_2$, $H_2O$, $N_2$, $O_2$, $HCN$, $NH_3$, $SO_2$, $HCl$, $Ar$, $NO$, $NO_2$, $H_2S$, $C_6H_6$, TAR (assumed for simplicity as high carbon chemical compound, i.e. $C_{40}H_{80}$), solid components included in dusts (i.e. $Al_2O_3$, $CaO$, $C$, $Fe$, $FeO$, $Fe_2O_3$, $MgO$, $S$, $SiO_2$, $ZnO$, $K_2O$, $CaCO_3$) and few further auxiliary components (i.e. $H_3O^+$, $OH^-$, $S^{2-}$).

The current version of developed models are described below; however, all the developed models can be improved during all the duration of the project according to the emerging needs.

## 3.2.1 BFG area

BFG area model has been developed according to the following literature and previous projects data and information [13]- [20] and has been used and tested with data coming from the two BFs IRMA-based models.

**Figure 1** depicts the current version of BFG area that includes :

- Primary dedusting system
- Wet cleaning system
  - Secondary dedusting and cleaning system
  - Demister
- Top Recovery Turbine (TRT)
- Hot Blast Stoves (HBS)
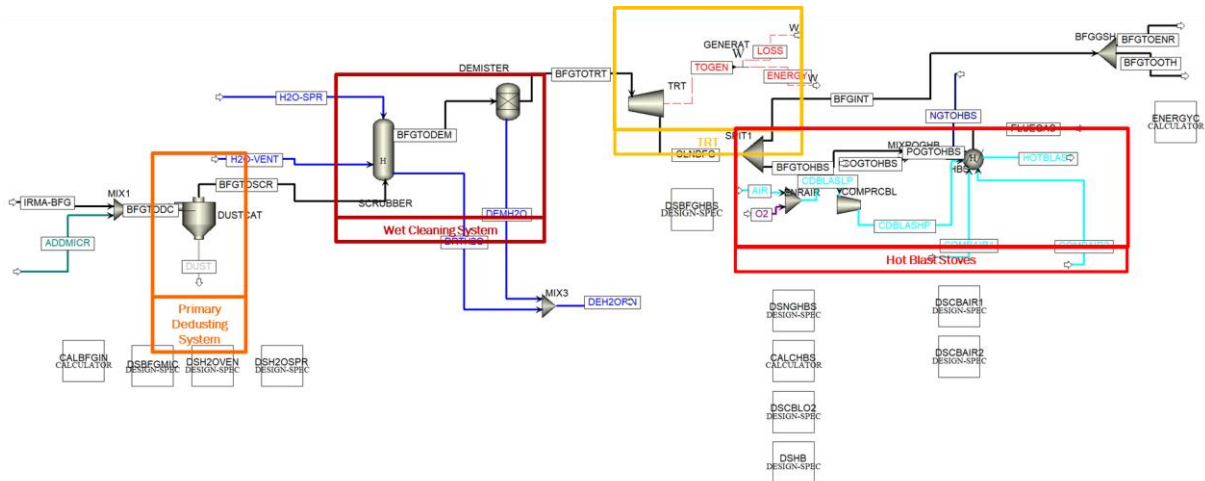


Figure 1 : Flowsheet of BFG area model

The model has been developed to receive the input stream data from IRMA model including both main gas components and dusts. An auxiliary input has been included for considering also microcontaminants (i.e. HCN, $NH_3$, $NO_2$, $SO_2$, HCl) not simulated in IRMA model but whose average data have been obtained from literature and previous projects and that are important in simulating BFG cleaning area. First test simulation data are included in **Table 23**.

Table 23: BFG first test simulation main data

| Variable | UoM | BFG1 | BFG2 |
|----------|-----|------|------|
| CO | %mol | 23.87 | 23.87 |
| $CO_2$ | | 23.82 | 23.85 |
| $H_2$ | | 4.61 | 4.61 |
| $H_2O$ | | 4.30 | 4.31 |
| $N_2$ | | 43.40 | 43.34 |
| HCN | mg/Nm³ | 140 | |
| HCl | | 140 | |
| $NH_3$ | | 0.5 | |
| $SO_2$ | | 5 | |
| $NO_2$ | | 0.5 | |
| Flowrate | kNm³/h | 246.67 | 378.48 |
| | t/h | 339.25 | 509.93 |
| Temperature | °C | 177.1 | 176 |
| Pressure | bara | 2.8 | 2.8 |
| Dust mass | t/h | 4.26 | 6.39 |
| Dust content | g/Nm³ | 17.27 | 16.88 |
| Dust composition | | | |
| $Al_2O_3$ | %wt | 1.27 | |
| CaO | | 1.86 | |

| | | |
|---|---|---|
| C | | 52.81 |
| $Fe_2O_3$ | | 15.14 |
| FeO | | 24.63 |
| $H_2O$ | | 0.29 |
| MgO | | 0.59 |
| S | | 0.34 |
| $SiO_2$ | | 2.27 |
| Other | | 0.8 |

The primary dedusting system includes a dust catcher (DC) for removal of coarse particles; the obtained removal is of about 50% of initial dust. Particle Size Distributions (PSD) of BFG dust before and after the primary dedusting system are reported in **Table 24**

Table 24: PSD of BFG dust before and after primary dedusting system

| PSD | UoM | Before DC | After DC |
|---|---|---|---|
| 0-50 µm | | 69.0 | 98.6 |
| 50-100 µm | | 17.0 | 1.4 |
| 100-200 µm | %wt | 10.0 | trace |
| 200-500 µm | | 3.0 | |
| 500-1000 µm | | 1.0 | |

BFG after the primary dedusting system goes in the wet cleaning system including both a secondary dedusting and cleaning system, and a demister. In particular, the secondary dedusting and cleaning system is reported in **Figure 2** and has been modelled including two sections: a Venturi Annular Gap and a Spray Scrubber. The first has been modelled using the Yung calculation model and:

- specifying gas velocity at throat inlet according to literature and available real data and for fitting removal and pressure drop;
- specifying throat length according to literature and real data and for fitting removal and pressure drop;
- using common industrial L/G ratio of 1.15 L/Nm³.
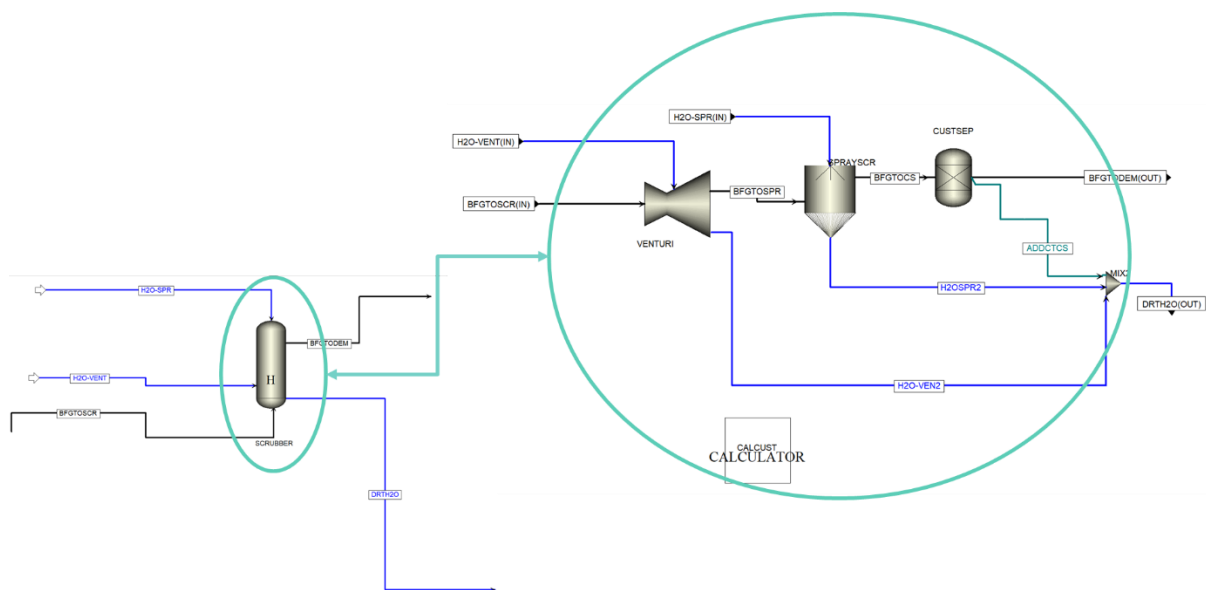


Figure 2 : Internal flowsheet of BFG secondary dedusting and cleaning system model

The spray scrubber has been modelled using the Calvert calculation method and:

- specifying gas velocity according to literature and available real data and for fitting removal and pressure drop;
- specifying Sauter diameter of droplets according to literature and available real data and for fitting removal and pressure drop;
- using common industrial L/G ratio of 1.7 L/Nm³.

It also includes a customized separator for the removal of microcontaminants; it was modelled considering previous projects results and available real data.

Demister is the last part of the wet cleaning system and is used for removing entrained water. The composition and main features of the BFG after the wet cleaning system are included in **Table 25**.

Table 25: BFG features after the wert cleaning system

| Variable | UoM | BFG1 | BFG2 |
|---|---|---|---|
| CO | %mol | 24.93 | 24.94 |
| $CO_2$ | | 24.88 | 24.92 |
| $H_2$ | | 4.81 | 4.82 |
| $H_2O$ | | 0.03 | 0.03 |
| $N_2$ | | 45.33 | 45.28 |
| HCN | mg/Nm³ | 146.12 | 146.13 |
| HCl | | 18.24 | 18.24 |
| $NH_3$ | | 0.06 | 0.06 |
| $SO_2$ | | 3.78 | 3.78 |
| $NO_2$ | | 0.27 | 0.27 |
| Flowrate | kNm³/h | 237.92 | 362.08 |
| | t/h | 326.27 | 496.63 |
| Temperature | °C | 41.7 | 41.6 |
| Pressure | bara | 2.59 | 2.59 |
| Dust content (after DC) | g/ Nm³ | 8.49 | 8.37 |
| Dust content (after Venturi) | mg/ Nm³ | 40.04 | 39.24 |
| Dust content (after spray tower and demister) | mg/ Nm³ | 1.61 | 1.58 |

The cleaned gas was then sent to the TRT that was modelled using the Polytropic ASME calculation method and considering, according to real and literature data:

- a Polytropic Efficiency of 92%
- a Mechanical Efficiency of 99%
- a Generator Efficiency of 95%
- a Pressure drop of 1 bar.

The generated power for the BFG from the two BFs is the following:

- BFG1: 3.1 MW
- BFG2: 4.7 MW

Concerning HBS whose internal flowsheet is reported in **Figure 3**, they were modelled as a combination of reactors (i.e. "Gibbs reactors") for combustion of gases (i.e. BFG, natural gas (NG) and COG), heaters and "design specification" blocks. An excess of combustion air of 18% with respect to the stoichiometric was considered and an efficiency of HBS of 75%. Considering, currently, a fixed amount of COG used in HBS corresponding to 18% of its production, the model computes the amount of BFG and NG necessary to satisfy the request of hot blast in terms of amount and temperature (according to the request by IRMA model); priority is given to the use of BFG. Cold blast, before its heating in HBS and according to the request by IRMA model, is enriched of oxygen (provided by ASU) and compressed in an electrical compressor modelled according to literature data using the Isentropic calculation method and with isentropic and mechanical efficiencies of 90% and 99% respectively. Required compression energy was computed.

Then remaining BFG is shared between M&ES and for other uses. Since in stationary simulation has no sense considering gasholders, currently excess BFG is sent to M&ES. Main outputs of the models are therefore the hot blast, the BFG to be sent for internal uses and then the flue gas from HBS.

Table 26 shows related results where also energetical contributions linked with distributed streams and computed with the models are reported.
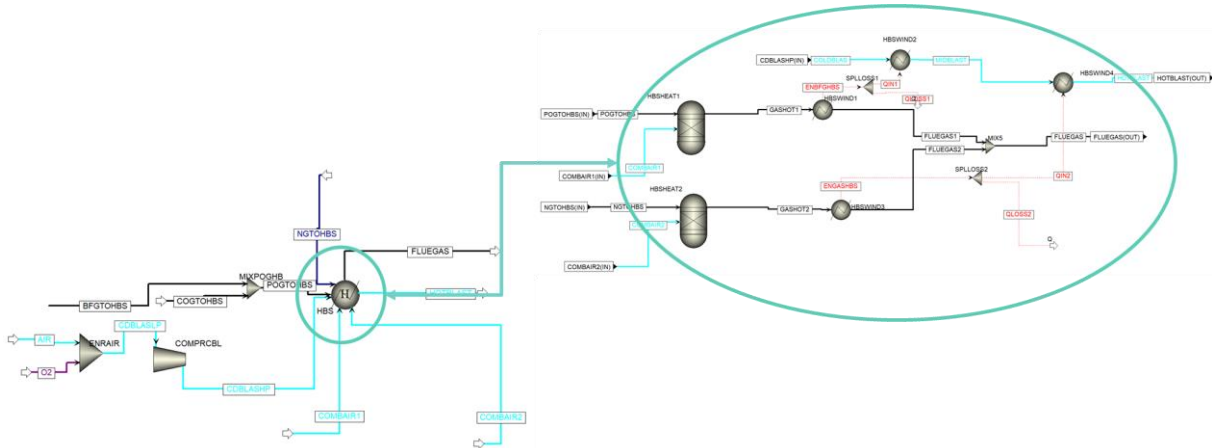


Figure 3 : Internal flowsheet of HBS model

Table 26: Main outputs of BFG area model

| Variable | UoM | BF1 | BF2 |
|---|---|---|---|
| Hot Blast | | | |
| Flowrate | t/h | 189.29 | 289.30 |
| Temperature | °C | 1141 | 1141 |
| Pressure | bara | 4.4 | 4.4 |
| $N_2$ | %mol | 70.76 | 70.76 |
| $O_2$ | | 28.00 | 28.00 |
| $CO_2$ | | 0.04 | 0.04 |
| $H_2O$ | | 1.20 | 1.20 |
| BFG | | | |
| To HBS | % | 21.90 | 21.98 |
| | kNm³/h | 52.11 | 79.58 |
| | t/h | 71.46 | 109.16 |
| | GJ/h | 191.21 | 292.10 |
| To M&ES | % | 73.02 | 72.95 |
| | kNm³/h | 173.73 | 264.14 |
| | t/h | 238.25 | 362.29 |
| | GJ/h | 637.48 | 969.51 |
| Excess BFG | % | 5.08 | 5.07 |
| | kNm³/h | 12.08 | 18.36 |
| | t/h | 16.56 | 25.19 |
| | GJ/h | 44.32 | 67.40 |
| Flue Gas | | | |
| Flowrate | kNm³/h | 112.37 | 171.72 |
| | t/h | 157.31 | 240.41 |
| $CO_2$ | %mol | 24.41 | 24.42 |
| CO | | 0.18 | 0.18 |
| $H_2O$ | | 6.81 | 6.82 |
| $N_2$ | | 66.30 | 66.28 |

| O$_2$ | | 1.78 | 1.78 |
|---|---|---|---|
| NO | mg/Nm$^3$ | 1242.27 | 1243.61 |
| NO$_2$ | | 1.52 | 1.52 |

## 3.2.2 BOFG area

BOFG area model has been developed according to the following literature and previous project data and information [13]- [15], [21]- [23], [33]- [39] and has been used and tested with data coming from the BOF IRMA-based models.

**Figure 4** depicts the current version of BOFG area that includes:

- Heat recovery system
- Dedusting system
- Flare
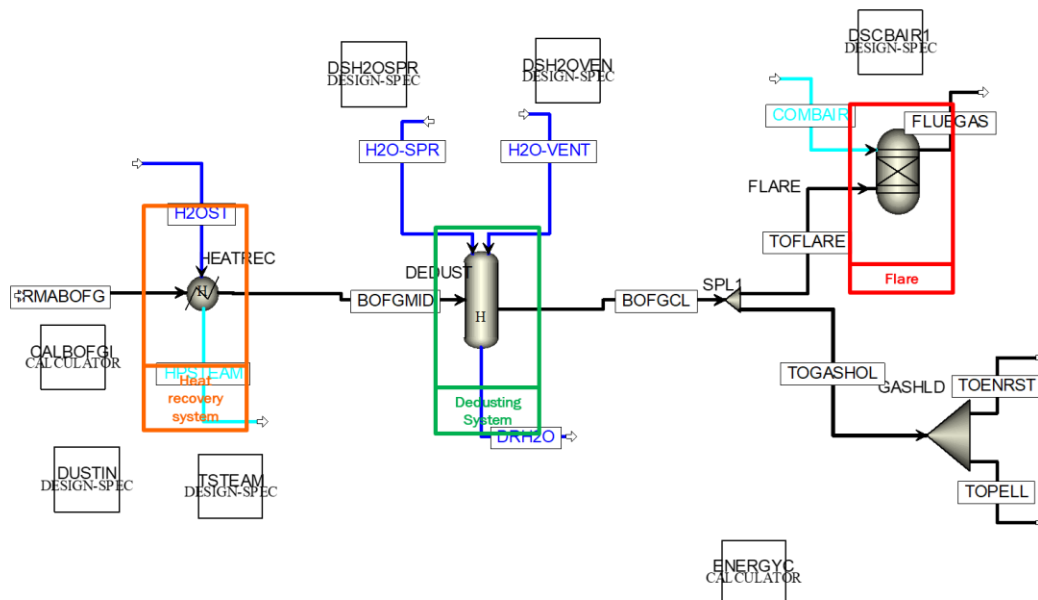


Figure 4 : Flowsheet of BOFG area model

The area was developed assuming the BOFG recovery and cleaning system as suppressed combustion system and having near to atmosphere/slightly negative pressure in the circuit for avoiding leak of CO rich gas. The model has been developed to receive the BOFG input stream data from IRMA model. Received BOFG features are reported in **Table 27**; dust composition, PSD and content currently are data from literature.

The heat recovery system allows decreasing the BOFG temperature until 900°C recovering related heat by producing high pressure steam (HPS) at 44 bar (pressure can be set according to the needs). A combination of heaters units have been used for the modelling as shown in **Figure 5**. In the current simulation, the amount of obtained steam is 20.03 t/h.

The dedusting system was assumed as wet type. It is well known that dry systems are considered in novel plants but for investigating the transition it was chosen the most common system in current integrated steelworks (i.e. wet type) as more representative of current situation. The system considers three subsections (**Figure 6**): first coarse dedusting system, second Venturi based dedusting system and a demister. The parameters of the different sections were configured considering literature and

real data and for fitting common temperature reduction and cleaning efficiencies. BOFG features after first cleaning/recovery stage and the whole dedusting system are reported in **Table 28**.

Table 27: BOFG first test simulation main data

| Variable | UoM | BOFG |
|---|---|---|
| CO | %mol | 64.18 |
| $CO_2$ | | 14.27 |
| $H_2$ | | 3.39 |
| $O_2$ | | 0.59 |
| $N_2$ | | 17.58 |
| Flowrate | $kNm^3/h$ | 42.63 |
| | t/h | 55.99 |
| Temperature | °C | 1650 |
| Pressure | bara | 1 |
| Dust mass | t/h | 3197.25 |
| Dust content | $g/Nm^3$ | 75 |
| **Dust Composition** | | |
| $Al_2O_3$ | %wt | 3.8 |
| CaO | | 1.1 |
| $Fe_2O_3$ | | 9.4 |
| FeO | | 49.3 |
| S | | 0.13 |
| $SiO_2$ | | 1.6 |
| Fe | | 11.6 |
| $CaCO_3$ | | 23.2 |
| **Dust PSD** | | |
| 0-0.5 µm | %wt | 22 |
| 0.5-1 µm | | 16 |
| 1-3 µm | | 23 |
| 3-6 µm | | 16 |
| 6-10 µm | | 12 |
| 10-15 µm | | 11 |
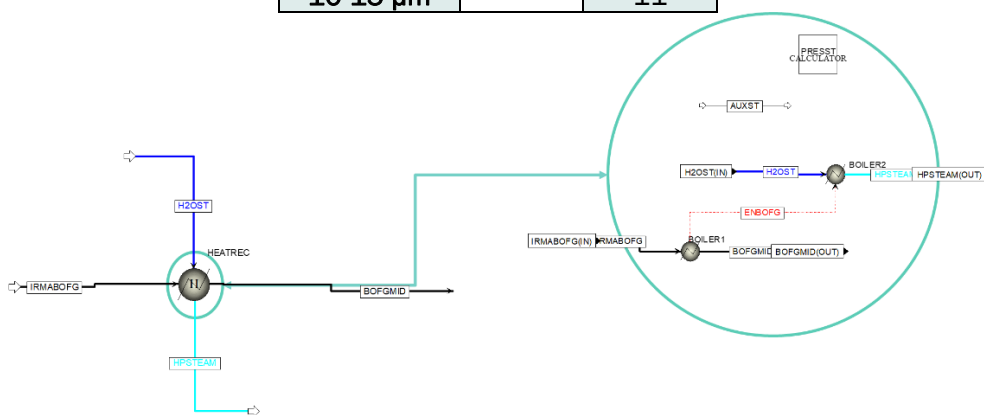


Figure 5 : Internal flowsheet of BOFG heat recovery system
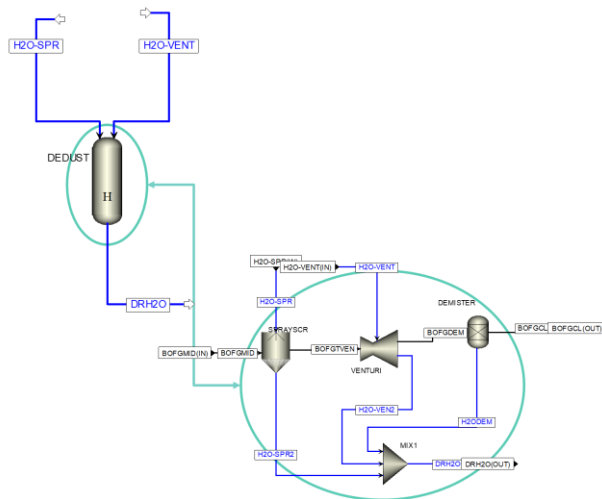
Figure 6 : Internal flowsheet of BOFG dedusting

Table 28: BOFG features after first cleaning/recovery stage and the whole dedusting system

| Variable | UoM | After first section | After the whole dedusting system |
|---|---|---|---|
| Temperature | °C | 75.80 | 65.86 |
| Pressure | bar | 1 | 0.84 |
| Dust Content | mg/Nm³ | 32444.64 | 44.90 |
| Dust PSD | | | |
| 0-0.5 μm | | 32.11 | 93.02 |
| 0.5-1 μm | | 23.34 | 4.68 |
| 1-3 μm | %wt | 30.20 | 1.71 |
| 3-6 μm | | 9.25 | 0.39 |
| 6-10 μm | | 3.16 | 0.12 |
| 10-15 μm | | 1.94 | 0.07 |

Finally, flare was modelled to eventually be used in some investigations (currently no BOFG is sent to flare). It was modelled as a combustion reactor and considering an excess of combustion air of 18% with respect to the stoichiometric. Obtained cleaned BOFG is sent to M&ES and to pellet plant as depicted in **Table 29** where also energetical contributions linked with distributed streams and computed with the models are reported.

Table 29: Main outputs of BOFG area model

| Variable | UoM | BFG1 |
|---|---|---|
| Flowrate | kNm³/h | 42.80 |
| | t/h | 56.12 |
| CO | | 63.93 |
| $CO_2$ | | 14.21 |
| $H_2$ | %mol | 3.38 |
| $H_2O$ | | 0.38 |
| $N_2$ | | 17.51 |
| $O_2$ | | 0.59 |
| BOFG Distribution | | |
| To M&ES | % | 79.79 |
| | kNm³/h | 34.15 |
| | t/h | 44.78 |
| | GJ/h | 287.84 |
| To Pellet Plant | % | 20.21 |
| | kNm³/h | 8.65 |
| | t/h | 11.34 |
| | GJ/h | 72.91 |

### 3.2.3 COG area

COG area model has been developed according to the following literature and previous project data and information [13], [14], [40]- [60] and has been used and tested with data coming from the two coke plants IRMA-based models.

**Figure 7** depicts the current version of COG area that includes:

- Cooling and TAR condensing section
    - flushing and pre-cooling
    - cooling
    - Electrostatic TAR separator
- Exhauster
- Second cleaning stage
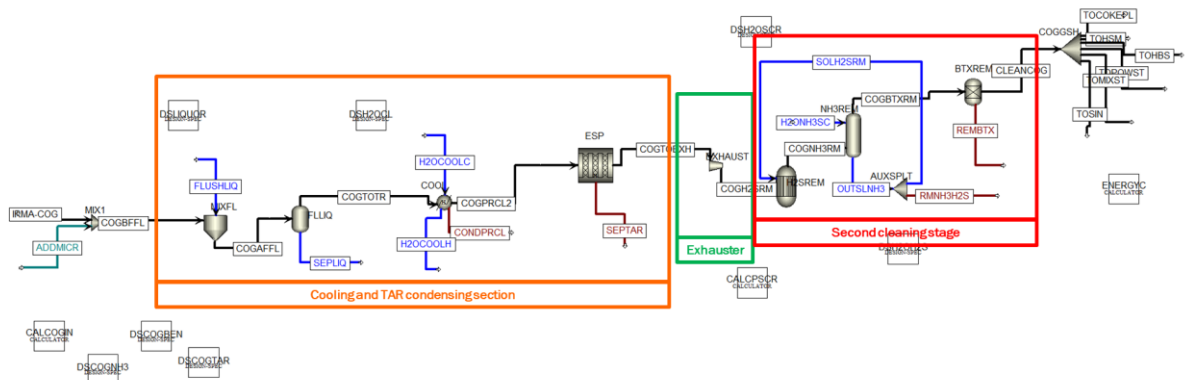


Figure 7 : Flowsheet of COG area model

The model has been developed to receive the COG input stream data from IRMA model. An auxiliary input has been included for also considering contaminants not simulated in IRMA model that are however important for the simulation of COG area; their average data have been obtained from literature and previous projects. First test simulation data are included in **Table 30**

Table 30: COG first test simulation main data

| Variable | UoM | COG1 | COG2 |
|---|---|---|---|
| $C_2H_6$ | %mol | 2.94 | |
| $CH_4$ | | 26.75 | |
| CO | | 4.43 | |
| $CO_2$ | | 0.04 | |
| $H_2$ | | 65.34 | |
| $N_2$ | | 18.55 | |
| Flowrate | kNm³/h | 21.66 | 33.16 |
| | t/h | 7.60 | 11.64 |
| Temperature | °C | 1100 | |
| Pressure | bara | 1 | |

The cooling and TAR condensing section includes three subsections. First COG is pre-cooled to 80°C by spraying a flushing liquor (i.e. low $NH_3$ concentration solution) and condensed compounds are separated. Then cooling is continued indirectly with water until 30°C and further compounds are condensed. Finally, an electrostatic separator (ESP) is used for removing fine tar droplets; for its simulation a tubular model was chosen and "Svarovsky" calculation method was used by fixing dimension and electrical parameters following literature and Aspen Plus suggestions. Two auxiliary

units have been included for allowing managing PSD for liquid particles in Aspen Plus. In this section a removal higher than 99.7% of TAR was obtained.

COG is then sent to the second cleaning stage through exhausters (i.e. suction fans) simulated as simple isentropic compression units with an efficiency of 85%; related required energy was computed. Then two columns constitute the desulphuration and ammonia removal. In particular, $H_2S$ is chemically absorbed using part of the outlet scrubbing water used in the ammonia scrubber where $NH_3$ is removed through water scrubbing. Finally, a simple unit with a fix removal efficiency of 85% was used for the removal of BTX that for simplicity were considered as only benzene. The cleaned COG, whose composition is reported in **Table 31**, is then distributed to the following users: coke plants, hot rolling mill, hot blast stoves, power stations (currently no COG is sent to power plant), M&ES and to sinter plant. The distribution is reported in **Table 31** both in terms of flowrate and energy content as computed by the model.

Table 31: Main outputs of COG area model

| Variable | UoM | COG1 | COG2 |
|---|---|---|---|
| Flowrate | kNm³/h | | 34.24 |
| | t/h | | 12.63 |
| $C_2H_6$ | | | 2.85 |
| $CH_4$ | | | 25.96 |
| CO | | | 3.94 |
| $CO_2$ | | | 0.04 |
| $H_2$ | %mol | | 63.38 |
| $H_2O$ | | | 2.79 |
| $N_2$ | | | 0.18 |
| **COG Distribution** | | | |
| To Coke Plant | % | 25 | |
| | kNm³/h | 5.59 | 8.56 |
| | t/h | 2.06 | 3.16 |
| | GJ/h | 105.36 | 161.30 |
| To Hot Rolling Mill | % | 51 | |
| | kNm³/h | 11.40 | 17.46 |
| | t/h | 4.21 | 6.44 |
| | GJ/h | 214.94 | 329.05 |
| To HBS | % | 18 | |
| | kNm³/h | 4.02 | 6.16 |
| | t/h | 1.49 | 2.27 |
| | GJ/h | 75.86 | 116.14 |
| To Power Station | % | 0 | |
| | kNm³/h | 0 | |
| | t/h | 0 | |
| | GJ/h | 0 | |
| To M&ES | % | 3 | |
| | kNm³/h | 0.67 | 1.03 |
| | t/h | 0.25 | 0.38 |
| | GJ/h | 12.64 | 19.36 |
| To Sinter Plant | % | 3 | |
| | kNm³/h | 0.67 | 1.03 |
| | t/h | 0.25 | 0.38 |
| | GJ/h | 12.64 | 19.36 |
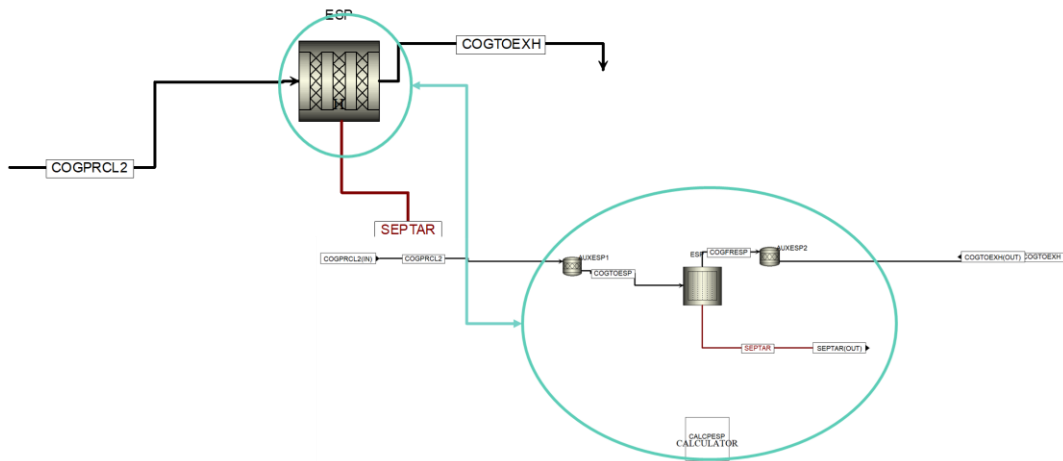
Figure 8 : Internal flowsheet of COG ESP model

### 3.2.4  Mixing and Enrichment Station

This model, whose flowsheet is reported in **Figure 9**, is a simple set of mixer units for allowing mixing the gases coming from the other areas of the gas network. In particular, it allows enriching BFG (the most abundant offgas) for obtaining higher calorific values in the so-called enriched BFG (rBFG). Main references have been previous projects [13], [14].
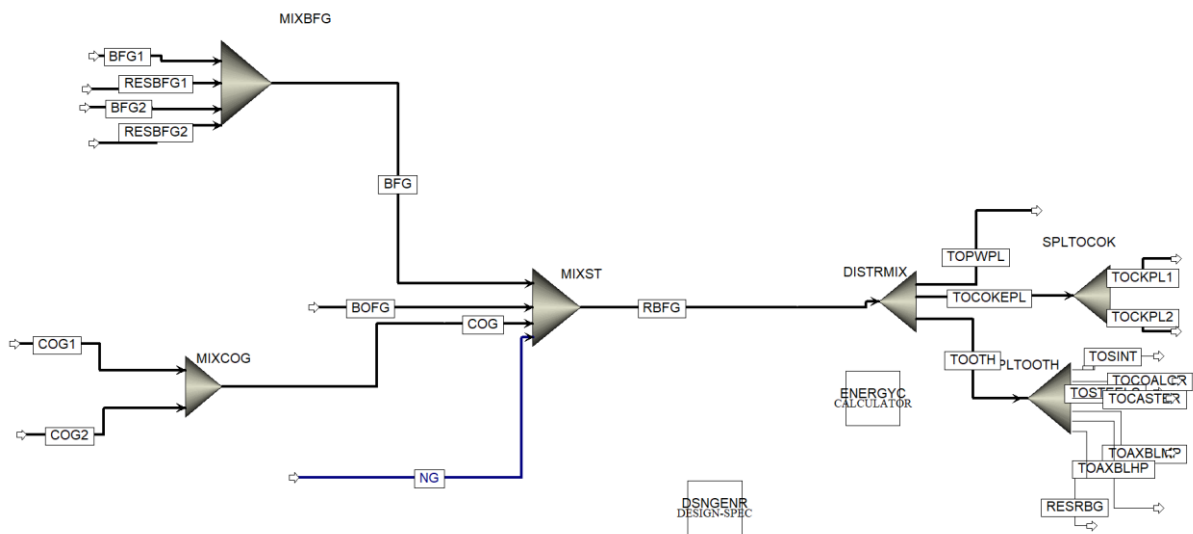


Figure 9 : Flowsheet of M&ES model

WI constraints (see **Table 21**) guide the mixing and especially the addition of NG; currently minimum WI has been set to 4.05 MJ/Nm³. Then gases are distributed to the following users: power plant, coke plants, sinter plant, coal grinding line, steel shop, casters and auxiliary boilers. Due the use of excess BFG in M&ES (due to gasholder absence in stationary mode and to assumption of continuous production), the excess of produced rBFG is sent currently to power plant. The distribution is reported in **Table 32**.

Table 32: Simulated rBFG distribution

| User | UoM | rBFG |
|---|---|---|
| Power Plant | % | 65.00 |
| | kNm³/h | 327.70 |
| | t/h | 446.99 |
| | GJ/h | 1324.55 |
| Coke Plant 1 | % | 5.54 |
| | kNm³/h | 27.92 |
| | t/h | 38.08 |
| | GJ/h | 112.84 |
| Coke Plant 2 | % | 8.39 |
| | kNm³/h | 42.31 |
| | t/h | 57.71 |
| | GJ/h | 171.00 |
| Sinter Plant | % | 0.19 |
| | kNm³/h | 0.94 |
| | t/h | 1.28 |
| | GJ/h | 3.80 |
| Coal Grinding Line | % | 1.38 |
| | kNm³/h | 6.95 |
| | t/h | 9.47 |
| | GJ/h | 28.10 |
| Steelshop | % | 2.83 |
| | kNm³/h | 14.25 |
| | t/h | 19.44 |
| | GJ/h | 57.60 |
| Caster | % | 0.30 |
| | kNm³/h | 1.51 |
| | t/h | 2.06 |
| | GJ/h | 6.10 |
| Auxiliary Boiler (MP steam) | % | 22.15 |
| | kNm³/h | 11.16 |
| | t/h | 15.23 |
| | GJ/h | 45.13 |
| Auxiliary Boiler (HP steam) | % | 0 |
| | kNm³/h | 0 |
| | t/h | 0 |
| | GJ/h | 0 |
| Residual rBFG | % | 14.16 |
| | kNm³/h | 71.41 |
| | t/h | 97.41 |
| | GJ/h | 288.65 |

### 3.2.5  Auxiliary Boilers

The auxiliary boilers are used to produce steam to be used for satisfying plant demand. Two models have been developed for low pressure (LP at 15 bar) and high pressure (HP at 44 bar) steam; however, pressures can be also modified. Main references have been previous projects [13], [14]. They were modelled including isentropic compressors for gas and air compressions having isentropic and mechanical efficiencies of 90% and 99% respectively; related required energy was computed. Then, there is a combustion reactor (i.e. "Gibbs reactor") for combustion of fuel gas (i.e. rBFG, COG and NG) where an excess of combustion air of 18% with respect to the stoichiometric was injected.

Finally, a combination of heaters units allows the heat exchange between water and combustion gases for obtaining the required amount of steam. Currently, the amount of HP steam is satisfied with the steam produced in the BOFG area and in the power plant, while the amount of currently required MP steam of 15.3 t/h is produced by using these boilers and an amount of 11.16 kNm3/h (152.15 t/h) of rBFG. Model flowsheet is shown in **Figure 10**.
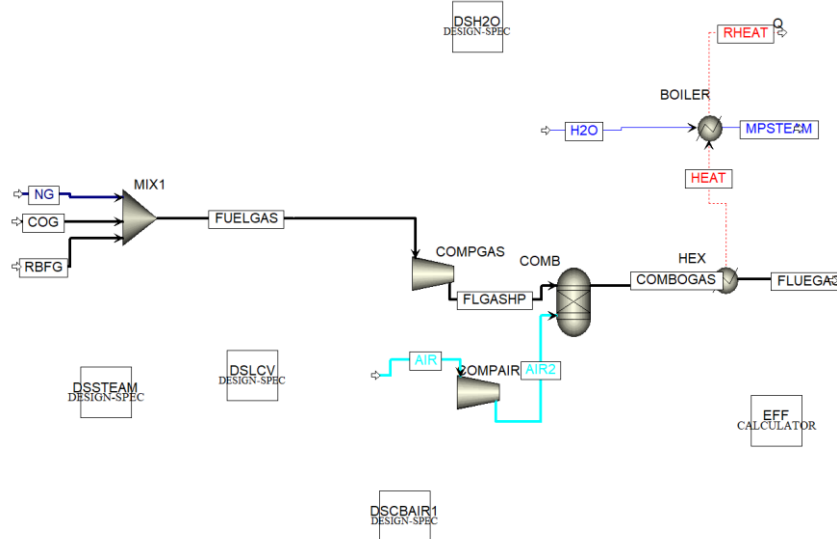


Figure 10 : Flowsheet of Auxiliary Boilers model

## 3.2.6  Power Plant

A Combined Heat and Power (CHP) plant (**Figure 11**) was modelled for allowing a production of about 130 MWe and HP steam. The size of the plant has been chosen for satisfying together with BFG TRTs more than the 90% of the electricity demand of the steelworks. The main references exploited in the modelling are the following:  [13],  [61]- [64].
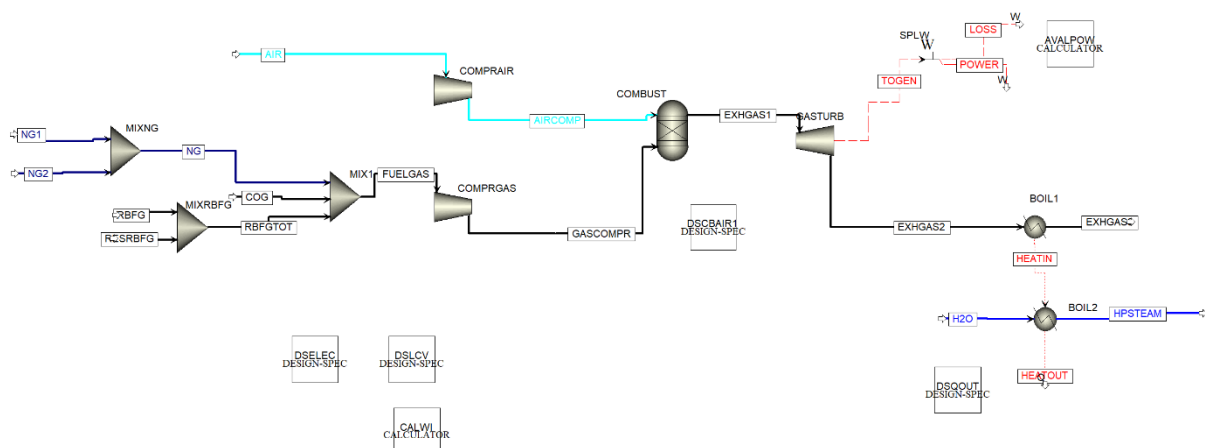


Figure 11 : Flowsheet of Power Plant model

It was fed especially by enriched BFG but there is also the possibility to use COG and/or NG. This last is used for reaching the desired electricity production in case of enriched BFG or COG lack and for reaching desired LCV value (currently set at least 4). Compressors for achieving air and fuel gas pressure of 38 barg were modelled as isentropic compressors having isentropic and mechanical efficiencies of 90% and 99% respectively; related required energy is computed. Then, a "Gibbs reactor" was used for allowing the combustion with an excess of air of 18% with respect to the

stoichiometric. Exhaust gases are sent to the gas turbine modelled using the Polytropic ASME calculation method and considering, according to real and literature data:

- a Polytropic Efficiency of 92%
- a Mechanical Efficiency of 99%
- a discharge pressure of 1.2 barg.

Generator efficiency is then considered of 95%.

Expanded gases are then sent to boilers (modelled as a couple of heaters units) for obtaining HP steam. Produced electricity together with the ones produced in TRT is then distributed to the different users (according to IRMA demands) as shown in Section **4.2.2**. Additional electricity was taken from the grid. Main inputs and outputs of the model are reported in **Table 33**.

Table 33: Main inputs and outputs of Power Plant model

| Variable | UoM | Value |
|---|---|---|
| rBFG | kNm³/h | 399.11 |
| | t/h | 544.18 |
| NG | kNm³/h | 1.14 |
| | t/h | 0.88 |
| Fuel Gas WI | MJ/Nm³ | 4.38 |
| Produced electric power | MW | 129.82 |
| Produced HP steam | t/h | 351.74 |

### 3.2.7 Air Separation Unit

Oxygen and Nitrogen demands are satisfied through ASU. It was modelled as a cryogenic unit according to [65], [66]. The model flowsheet is depicted in **Figure 12** and it includes the following sections:

- Compression and cooling section
- Low pressure column (LPC)
- High pressure column (HPC)
- Subcoolers
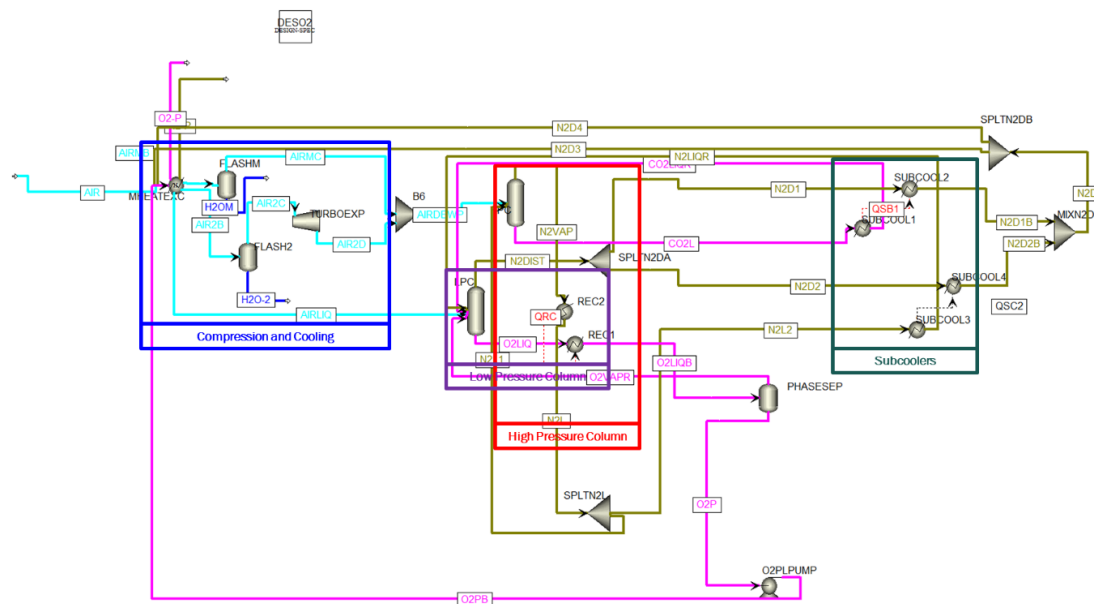


Figure 12 : Flowsheet of ASU model

In the compression and cooling section (**Figure 13**) the desired pressure and temperature for the process are achieved; inlet air stream is first split in three substreams and then is compressed and cooled in a series of compressor and heaters units representing multi-stage centrifugal compressor and air booster compressors with intercoolers. They were modelled using isentropic calculation method and with isentropic and mechanical efficiencies of 90% and 99% respectively; pressure of 5 bar or 35 bar are achieved. While achieved temperature are between -170 and -180°C. Compression and air cooling allows to make air liquefaction thermodynamically feasible operating on Kapitza cycle. Required compression energy is computed. After condensed water separation, an isentropic expansion is then done in a turbine unit with related efficiency of 85% is then used to represent a turbo-expander that leads to a further decrease in air temperature.
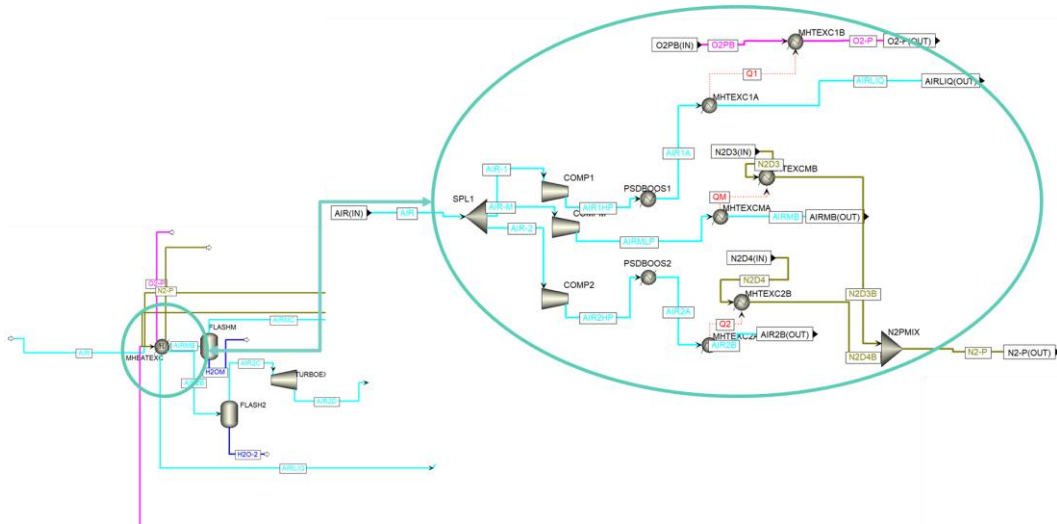


Figure 13. Internal flowsheet of main unit of compression and cooling section of ASU model

The two columns operating at 1.35 bar (LPC) and 5.15 bar (HPC) that generally constitutes a double-column, are modelled as packed columns using the "RadFrac" unit block setting the number of equilibrium stages (i.e. 20 for HPC and 29 for LPC), packing type (i.e. Pall Rings) and features as well as column dimensions. Both columns are integrated with reboiler & condenser units (simulated combining heaters units) that provides $N_2$-enriched liquid reflux both to HPC and LPC and $O_2$-enriched vapor reflux to LPC. The partially evaporated $O_2$ stream is separated in a phase separator simulated as a flash unit. Finally sub-coolers, completing the heat integration in the ASU, are represented as a set of Heaters unit blocks. Since $O_2$ is the "limiting" gas as it is most used than $N_2$, the ASU model has been configured for satisfying $O_2$ demand (e.g. from IRMA models) and consequently producing also $N_2$. Currently the obtained streams are reported in Table 34.

Table 34: Main inputs and outputs of Power Plant model

| Variable | UoM | Value |
|---|---|---|
| $O_2$ | kNm$^3$/h | 57.34 |
| | t/h | 81.15 |
| | %mol (purity) | 95.64 |
| $N_2$ | kNm$^3$/h | 210.26 |
| | t/h | 262.95 |
| | %mol (purity) | 99.57 |

As Argon currently was neglected in Air composition it is not obtained in the ASU and consequent demand is satisfied from external sources. In addition, in the current ASU version, only an $O_2$ quality was obtained. Further improvements will allow obtaining different $O_2$ qualities.

## 3.3  Interaction with IRMA - Aspen model digital toolkit

### 3.3.1  Overview of the MaxH2DR multipurpose simulation toolkit

In order to better understand why interactions are fundamentals within the MaxH2DR multipurpose simulation toolkit, a brief reminder of what is expected in the project is provided in this subsection.

The holistic studies of MaxH2DR will combine three different tools to a multipurpose simulation toolkit by specifically exploiting their individual strengths and avoiding their weaknesses. AAU (ABO) provides an algebraic model-based steelmaking chain superstructure with highly simplified unit models, including tools for multi-objective optimisation. The optimisation will provide rough estimates of promising plant states and layouts, which are further analysed with special focus on gas and energy networks by an Aspen Plus based tool by SSSA and on critical metallurgical aspects by the Iron Making IRMA-based model by TS. **Figure 14** outlines the flow of information between the tools as reported in the MaxH2DR proposal, where dashed lines indicate the exchange of data managed through a server interconnection database, which will thus allow the joint exploitation of the three process chain tools.



Figure 14: Strategy of multipurpose process chain simulation toolkit

### 3.3.2 Communication database design

One of the aims of Task 3.1 is the development of the communication database between adapted tools. Input/output streams among the tools have been defined. AML model will provide configura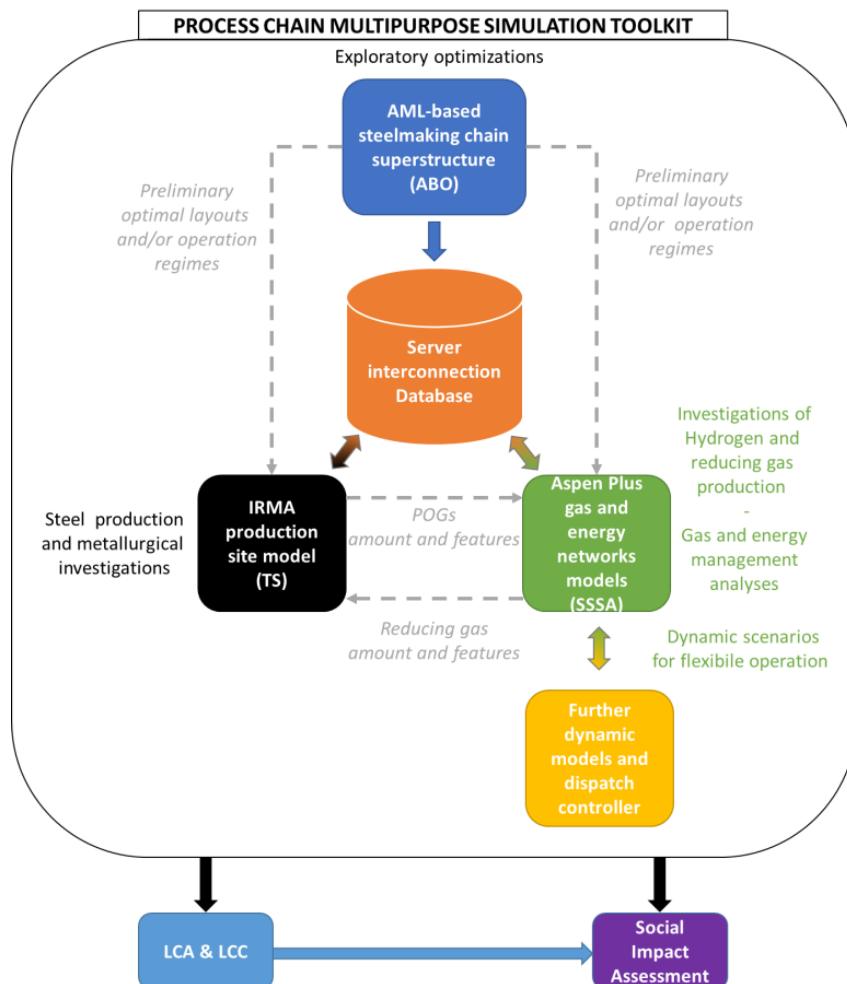tions and operation regimes to IRMA and Aspen Plus models, which will exchange data regarding reducing gas and POGs. An interconnection database has been developed by SSSA and deployed on a server.

In MaxH2DR project, the developed communication database is a PostgreSQL relational database, named maxh2dr. PostgreSQL is a powerful, open-source object-relational database management system. Relational data model is considered a well-suited choice for the project, since data stored is structured and organizing it into tables helps to a better data understanding and management. Moreover, schema flexibility, scalability and high performance are not primary requirements for the project, in which case the focus would have been on No SQL databases that are properly designed to handle very large volumes of data that can be rapidly changing.

#### 3.3.2.1 The relational model

In a relational database, data are structured into relations (tables). A relation is a set of tuples having the same attributes and is commonly described as a table which is organized into rows and columns, where columns correspond to attributes and rows, also called records, correspond to tuples. Generally, each table represents one entity type: a row represents an instance of that type of entity and the columns represent values attributed to that instance.

Relationships between different tables are logical connections based on the interaction among them and are defined in the relational model through integrity constraints, such as primary keys and foreign keys set on tables. A primary key uniquely identifies a tuple within a table and consists of one or more attributes of the table. Foreign keys are used to link different tables. A foreign key is a set of attributes in a table that refers to a primary key of another table. By using integrity rules, the data integrity process is handled by the relational database itself and not by the applications, with the result of having a single, well-controlled and well-defined data-integrity system that increases stability, performance, re-usability and maintainability.

More generally, relationships between two tables can be classified as follows:

- A one-to-one relationship refers to a relationship between two tables A and B, in which one element of A can be linked to one element of B and vice-versa.
- A one-to-many relationship refers to a relationship between two tables A and B, in which one element of A can be linked to many elements of B, but an element of B is linked to only one element of A.
- A many-to-many relationship refers to a relationship between two tables A and B that relate each row in one table to many rows in another table, and vice-versa.

In the relational model, relationships between two tables are defined by means of integrity constraints and can represent either a one-to-one or a one-to-many relationship. However, most relational database resolve many-to-many relationships by creating an additional table (called junction table) containing the primary keys migrated from both the tables you want to relate. Then a relationship (one-to-many) from the primary key columns of each of those two tables to the matching columns in the junction table is created and the two foreign keys are combined in the junction table to form its primary key.

The Entity-Relationship (ER) Diagram is a high-level conceptual data model diagram. The ER Diagram represents the ER model displaying the entities, their attributes and relationships existing between entities using different symbols and connectors. ER diagrams are used to model and design relational databases, by representing the data logical structure.

### 3.3.2.2    Basic idea – Information data of interest

Concerning the MaxH2DR project, the overall system is composed of three different tools that need to exchange data exploiting a server interconnection database, which thus allows the joint exploitation of the three process chain tools. This section deals with an analysis of the information data of interest in our specific domain of knowledge.

In the terminology adopted to define the objects involved in the domain, each tool is assimilated to an area. Each area is composed of different operating units and different materials, with specific properties, are exchanged among these units within the area. Moreover, some materials can be exchanged between units belonging to different areas.

On one side, an area can be considered as a black box, where some inputs enter and some outputs exit. On the other side, while running a model concerning the area, it is also important to take into account the streams of materials among the single units within the area, as materials flow from upstream units to downstream units (after the box has been fed by charging the global input), as shown in **Figure 15**.
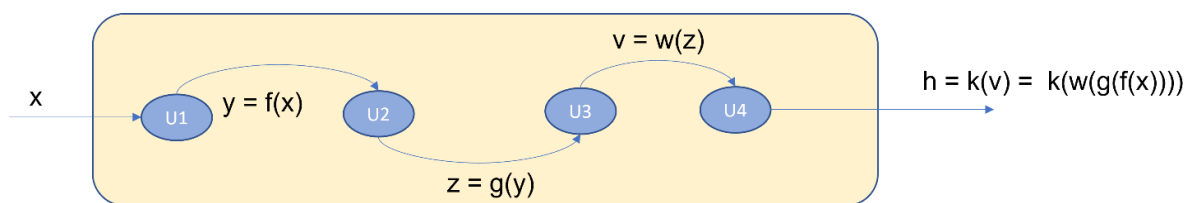


Figure 15: Streams of materials between single units within an area

A suitable approach to model the data is based on the concept of stream. A stream is an entity that represents a flow of a specific material from a source unit to a destination unit within the same area or among different areas. During the execution of a model concerning an area, some specific properties of the flowing material are defined such as the flow rate, pressure, chemical composition etc. These properties, also called material parameters, are depending on the material class.

A graphical representation of the basic idea of this approach is shown in **Figure 16**. In both sides of the figure, the area is represented as a graph where the nodes (named $Unit_i$) are the units that are active in the area, while the edges (named $e_j$) represent the streams of materials between units and are labelled with the name of the material ($m_k$). On the right side of the figure, as an example, edges are enriched with a single valued parameter associated to the material. More generally, for each active edge, the values of all varying parameters associated to the material, labelled on the edge, will be calculated at running time, during the execution of the model. In addition, streams of materials entering the area but coming from a different area or exiting the area but directed to a subsequent area are displayed, together with all streams of materials coming from auxiliary sources or directed to them.
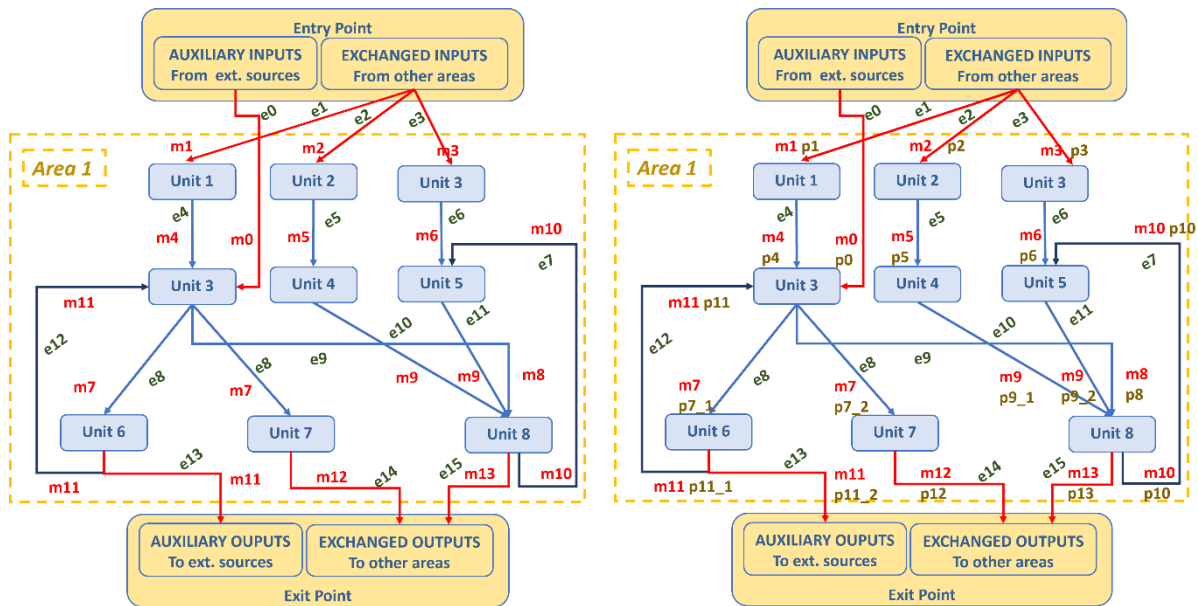
Figure 16:Graphical representation of active units and material streams within an area

In the end, the information of interest to be associated to the execution of a model is the set of the active units and active streams within the area the model belongs to, together with all parameter values associated to the material related to each stream.

During the project, the operating units that are active in an area can be changed: for instance, in the steelworks area the Blast Furnace and Blast Oxygen Furnace will be replaced by the Direct Reduction Shaft Furnace and Electric Arc Furnace at a later stage of the project. Therefore, it is useful to introduce the scenario concept, representing the actual operating units that are active in an area, together with the active streams of interest. New scenarios will be introduced and managed during the evolution of the project. Therefore, the executions of models concerning the area must be related to a specific scenario of that area.

Different areas may exchange some materials each other and therefore the execution of a model, that simulates a certain behaviour in one area, may depend on some input materials produced by the execution of another model in another area. In this way, the executions of two different models must be performed in sequence and the execution of the first model should cause the execution of the second one. Moreover, the linked execution must be able to extract and use some of the output materials produced by the triggering execution.

### 3.3.2.3    The Data Model (ERD)

In the light of the considerations discussed in the previous paragraph, a relational database has been designed to collect and manage any information of interest above-mentioned. The information data handled by the database can be summarized as follows:

- Areas and units concerning the areas.
- Material classes and properties (parameters with respective default unit of measure) for each material class.
- Allowed materials and associated material classes.
- Constant parameters values for some materials expecting fixed chemical composition.
- Scenarios of an area, each defining the active units and material streams between units within that area and eventually towards other areas.
- Tracing data about the executions of models (simulations) and their result sets.

- Interrelated simulations, i.e. executions of different models performed in sequence with an exchange of data between them.

An ER Diagram of the maxh2dr database is shown in **Figure 17**, where tables are displayed with their attributes (columns) and relationships among them are depicted. maxh2dr is also the name of the relation schema all tables belong to. In this diagram, tables used to manage the global convergence of models in different areas are omitted for space reasons and will be discussed later in paragraph 3.3.3.2.2 and represented in **Figure 21**.
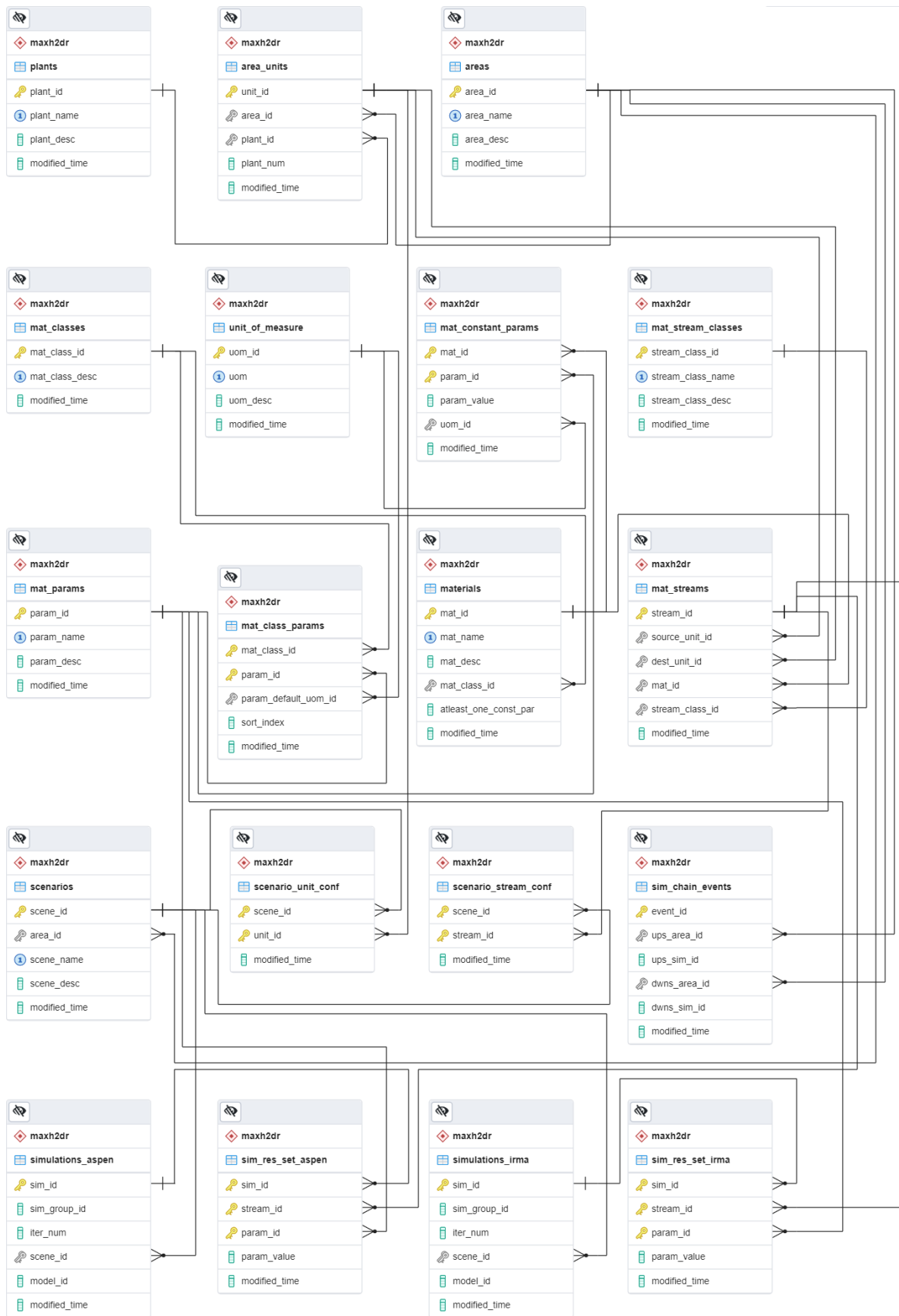
Figure 17: Entity Relationship Diagram of maxh2dr database

### 3.3.2.4 Database population and data storage layer enhancements

In the first phases of the project, a data gathering process was carried out by project partners to exactly identify the operating units involved in standard real plants of different areas and to distinguish which flows of material between units (within the same area or different areas) to consider. Moreover, some specific material classes were defined, together with parameters of each flowing material (such as the flow rate, pressure, chemical composition etc), depending on the material class, and corresponding default units of measure. Afterwards, this primary data collection was exploited to develop ad-hoc stored procedures used to populate the matching tables of the database.

A database trigger is a procedure that is automatically executed in response to certain events on a particular table. During a second phase of the design, some triggers were defined on several tables of the database mainly to prevent unwanted changes to data by users belonging to a different area, to ensure data integrity.

- Triggers on Scenarios table to make scenarios private to users, avoiding possible changes of a scenario of an area from a user not pertinent to that area (since scenario tables area shared between different areas).
- Triggers on Simulations tables to check that the simulation scenario belongs to the expected area (since simulations tables are distinct per area).
- Triggers on Interrelated simulations table to forbid changing some critical fields after a chained simulation process has started.

In addition, several database views were introduced into the database to help data retrieve, avoiding tedious join among tables. On top of tables and views, a big set of PostgreSQL stored procedures and functions was developed in the data storage layer to provide a simplified handling of the following entities:

- Plants
- Area units and streams
- Scenarios
- Simulations and results
- Interrelated simulations

Multiple users and programs can perform operations on underlying database objects by using these stored procedures and functions that control the activities performed and protect the database objects. Some benefits deriving from this approach are a stronger security, a reduction of network traffic between client and server and an improved performance. Moreover, keeping database operations separated in the data layer promotes an easier maintenance, since only the procedures must be updated for any changes in the underlying database, and a reuse of code too.

### 3.3.2.5 Deployment on the server

The designed database was deployed on a server at SSSA. Access to the database is provided through SSH (Secure Shell) tunnel using dedicated accounts supplied to WP3 partners. SSH tunnelling is a method of transporting arbitrary networking data over an encrypted SSH connection. Therefore, SSH is used to create a secure channel between a local and a remote computer, so that application data traffic cannot be eavesdropped or intercepted while it is in transit. The server at SSSA has been accurately configured as an SSH server listening for connections from the clients.

A client wishing to connect to the maxh2dr database can create a SSH tunnel using the PuTTy Client User Interface, after properly configure this open-source tool and by exploiting the right account

supplied for connecting to the SSH server. A small guide explaining how to configure and use the PuTTY client on Windows was provided by SSSA to WP3 partners.

The security of maxh2dr database is handled by creating proper <u>roles</u> that allow access to the server resources and then granting <u>privileges</u> to database objects suitably. Each user account is associated to a role and has only proper and expected grants on database objects, according to the Principle of Least Privilege, stating that users should only be granted to access to the least amount of information needed to perform their task. For example, write privilege on simulations and result set tables (*simulations_aspen* and *sim_res_set_aspen* for example) are granted only to specific user (ASPEN area user), while read privilege on all database tables is given to all users having an access account to the database, as well as write privilege on scenario tables, which are shared between different areas users. As previously discussed in section **3.3.2.4**, data are also protected through proper triggers introduced to guarantee data integrity.

### 3.3.3 Interaction between system tools through the database

In a more general context, the models/simulators belonging to different areas interact with each other by exchanging data and simulations are run in cascade alternately in respective area until a certain global convergence condition is achieved causing the process to stop. However, in some cases convergence does not occur and therefore a maximum number of iterations forces the end of the process.

#### 3.3.3.1 System areas operating modes

Two modes of operation of the system must be envisaged:

**Simple mode (stand-alone)**: the areas are considered as independent. Each model, simulating a certain behaviour in one area, is stand-alone and independent from other models. This operating mode, depicted in **Figure 18**, can be useful especially in the initial phase of the project to run simulations in a total independent way.

**Automatic mode**: areas and concerning models are dependent and connected within a global process where upstream and downstream areas operate in series, with some upstream area units feeding other downstream area units. Running an upstream model automatically causes a downstream model to be run, with an exchange of data between them. The process repeats until a certain global convergence condition of the system is reached or the maximum limit of iterations allowed is exceeded. This operating mode, depicted in **Figure 19**, corresponds to a realistic interaction between model simulations of different areas.
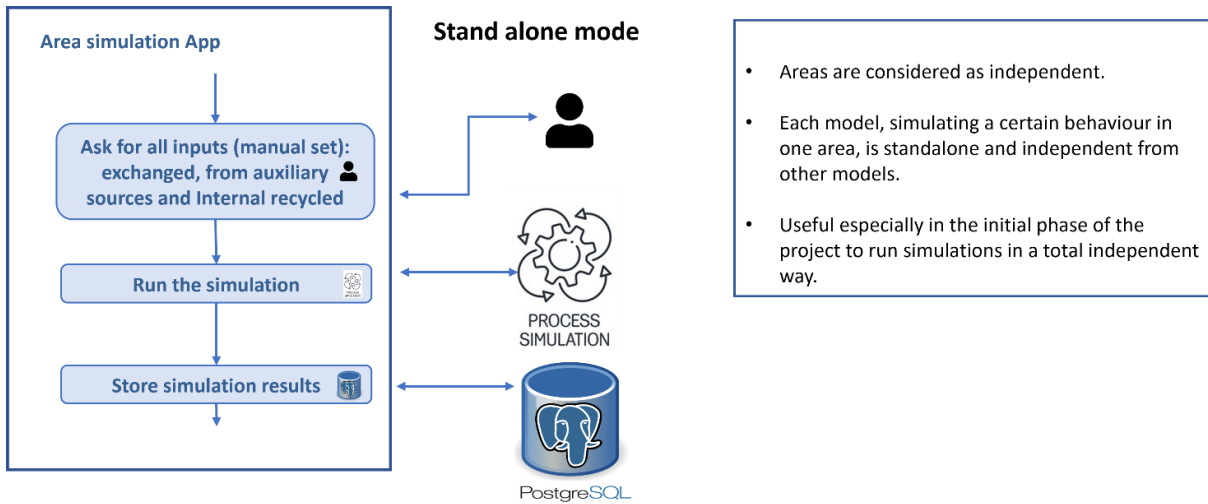
Figure 18: Stand-alone operative mode
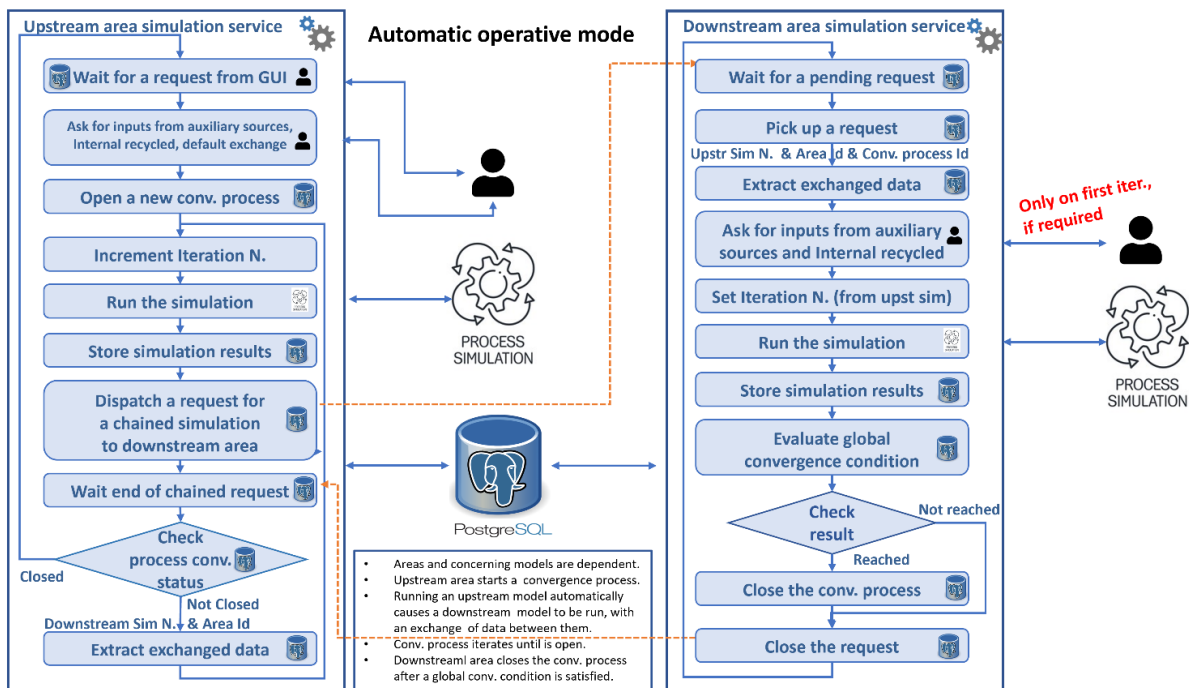


Figure 19: Automatic operative mode

### 3.3.3.2 Automatic operative mode design

In the automatic operating mode of the system, each area provides a service to manage the automatic running of models pertinent to the area. The interaction of simulations of different areas is supervised according to a master-slave like approach. The upstream area (the master) starts the global simulation process and, at each process iteration, executes a simulation on its own side and afterwards asks the downstream area (the slave) to execute a correlated simulation. At each iteration both area simulations exploit data fed from the other side area and furthermore the downstream area verifies the achievement of the global convergence condition and closes the simulation process whenever the condition is satisfied.

As depicted on the left side of Figure 19, the main functions of the upstream area simulation service can be summarized as follows:

- to wait for a simulation request from the application and ask for related inputs
- to open a new convergence process when a new simulation request arrives from the application
- to repeat the process until convergence is reached.

    Specifically at each process iteration main actions performed are as follows:
    - to extract data exchanged with the downstream simulation (only on iterations next to the first)
    - to manage the automatic running of simulation
    - to store the simulation results on the database
    - to dispatch a new request for a simulation to the downstream area only if convergence process is still open and wait until the request is fulfilled on the downstream side
    - to go back waiting for a new simulation request from the application only if convergence process has been closed.

As depicted on the right side of **Figure 19**, the main functions performed by the downstream area simulation service are the following:

- to pick up the pending requests coming from the upstream area
- Specifically processing each request consists of the following actions:
    - to extract data exchanged with the upstream simulation
    - to ask for other eventual inputs needed on first iteration
    - to manage the automatic running of requested simulation
    - to store the simulation results on the database
    - to evaluate the global convergence condition
    - to close the convergence process, when convergence condition is reached, by updating its status and adding the convergence result (convergence successfully reached or limit of iterations exceeded)
    - to notify the end of the request dispatched from the upstream area.

Obviously, the convergence process must be closed on upstream or downstream side if respectively upstream or downstream simulation fails, to avoid infinite waits.

The designed automatic operative mode will be used to implement the interaction between IRMA and ASPEN areas, respectively as upstream and downstream areas.

### 3.3.3.2.1    Requirements for an effective IRMA-ASPEN interaction

This section focuses the attention on some aspects to be considered in the interaction between IRMA and ASPEN, such as which convergence condition to adopt and how to handle possible material and energy demands asked from IRMA tool.

More generally, besides depending on material/energy streams from a different area, the execution of a model in an area may depend also on other input materials/energy provided by external auxiliary sources (e.g. raw material sources) or even on recycled materials coming from the same area. **Figure 20** depicts in a simple flow diagram the interaction of IRMA and ASPEN in terms of input and outputs both exchanged with each other (green edges) and from or to external auxiliary sources.
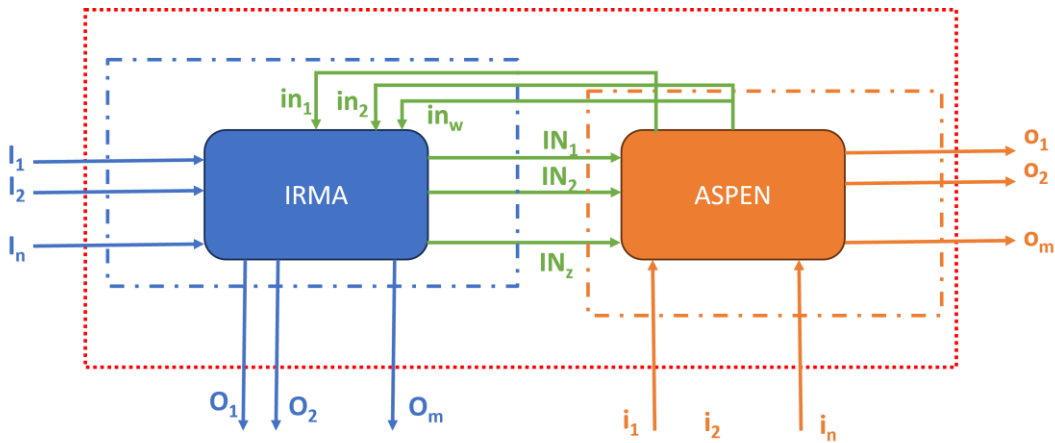
Figure 20: General IRMA - ASPEN interaction

A plausible global convergence condition can be the Mass and Energy Balance, stating no matter is never created nor destroyed only transformed, evaluated on the whole system both on IRMA and ASPEN side. As depicted in formula (1) , describing this condition, only input and output material/energy streams entering or exiting the whole system (according to pointed red boundaries) are accounted for.

$$\left| \sum_{a=1}^{n} I_a + \sum_{a=1}^{w} i_a - \sum_{a=1}^{m} O_a - \sum_{a=1}^{z} o_a \right| \leq threshold, \ threshold \sim 0 \quad (1)$$

Concerning the nature of expected material/energy streams from the upstream area, two different types of demand must be envisaged:

- Direct demand: the same material of the received stream is requested. Different requirements for associated parameters can be asked (e.g. temperature, flowrate, composition). In this case, normally no constraint on the demand should be expected.
- Indirect demand: a different item from the material directly received on streams is requested. In this case the request can be satisfied in terms of multiple streaming materials and specific constraints on streams to be received must be satisfied. An example can be heat provided by gases.

Referring to a realistic interaction between IRMA and ASPEN, Hot Blast represents an example of direct demand since it is a material stream demand received from the Blast Furnace unit at IRMA area and produced and provided by the Hot Blast stoves unit at ASPEN area.

Instead, a demand of heat by fuel gases represents an example of indirect demand since it can be provided to a certain unit of IRMA area as a mixture of different types of gas streams supplied by specific units at ASPEN area. For example, the Coke Plant can receive COG or rBFG from respective ASPEN area (i.e. COG Area and M&ES), as long as certain constraints on their percentages are respected.

### 3.3.3.2.2 Automatic operative mode support in the database

The existing database has been extended with additional tables to support the automatic operative mode, considering both global convergence achievement and possible demands coming from the upstream area. The additional information data handled by the database can be summarized as follows:

- Global scenarios, each identifying a couple of upstream and downstream scenario.
- Convergence processes with concerning control information such as status (open/close) and process outcome.

  Each convergence process is related to a global scenario, to a global convergence condition, to a demand and finally to the group of simulations (upstream/downstream) executed during the process.

- Global convergence conditions with associated threshold and included streams.

Focusing on possible material or energy demands of the upstream area to be satisfied within correlated simulation requests to the downstream area, the supplementary information data to be handled by the database for this aim can be summarized as follows:

- Material unit requests, each identifying a possible material requested by a unit. Only these requests are allowed to be associated to demands.
- Demands, each defining a set of requests (in terms of units and requested materials).

  A demand, with requests and constraints, is related to a global scenario and can be reused for multiple convergence processes.

- Demand constraints, defining allowed ranges for parameters of other combined materials that will be used to satisfy the material requests (absolute or %) associated to the demand.
- Demand instances specifying actual values of requests associated to the demand. Specifically actual request values define dynamic values for parameters of the material assigned to a request and are set by the upstream area in an instance of the demand when the convergence process is opened.

During the convergence process, the demand representing the set of requested material/energy values and possible constraints is retrieved by the downstream area and translated in terms of input streams (to be processed) or unit setup before running the downstream simulation.

An ER Diagram of all the tables in the database used to manage the interaction and global convergence of models of different areas is shown in **Figure 21**, where tables are displayed with their attributes (columns) and relationships among them are depicted.
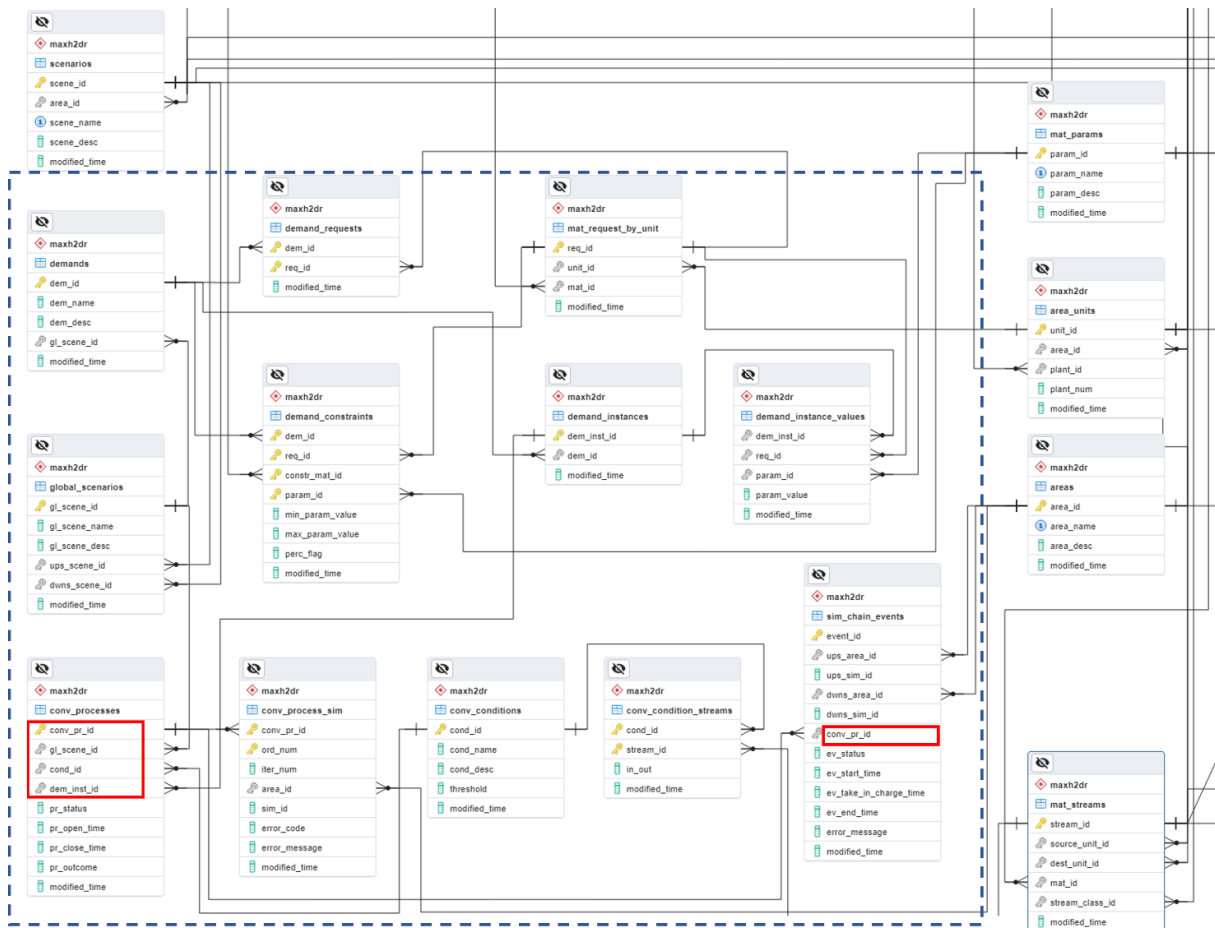
Figure 21: Entity Relationship Diagram of maxh2dr tables used to support automatic mode

During the interaction between model simulations, requests of simulations dispatched from the upstream area to the downstream area and communications of responses by the downstream area are managed through event entities stored in a table named *sim_chain_events*, which behaves as an event queue. After finishing the execution of the upstream model and storing of results, the upstream area automatic service starts a new event to trigger the execution of the downstream model. On the other side, the downstream area automatic service checks if there are any pending model execution requests through a polling mechanism on the event table (e.g., every minute), looking for not completed events. When the service receives a request, after finishing the execution of the downstream model and storing of results, it signals the completion of the request by ending the event. The interrelation between the two executions is traced in the event itself by means of simulation and respective area identifiers on both sides (upstream/downstream), so that the exchanged data resulting from the execution of the upstream/downstream model simulation can be automatically retrieved by the downstream /upstream area service before running corresponding model next execution.

All events started by the downstream area within a convergence process refer the same convergence process identifier, provided as a field of the event entity. Moreover, dedicated tables are employed to handle all the information involved in a convergence process, from global convergence condition to be reached and material or energy demand by the upstream area and expected to be satisfied from the requested downstream area simulation.

### 3.3.4  Application architecture design in the gas, steam and energy area

The architecture design of the application that manages simulations in the gas, steam and energy area is depicted in **Figure 22**.
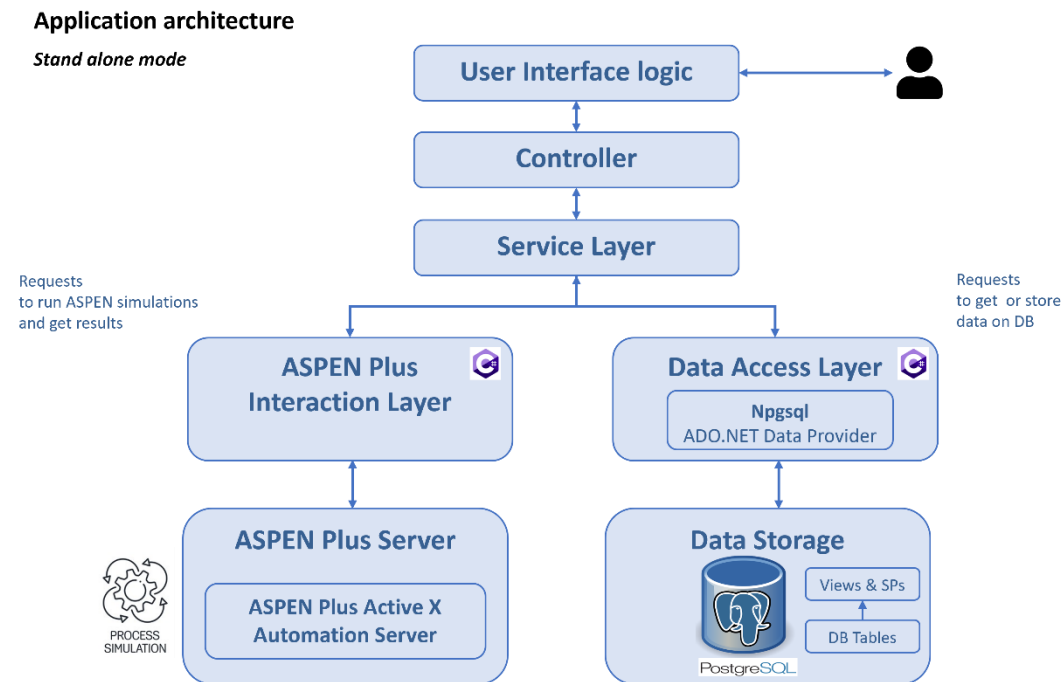


Figure 22: Architecture design of the application managing simulations in the gas, steam and energy area

The application is made of functional units or modules, each performing a specific task, that can communicate with each other. The modular approach used to design the application makes the development, test and maintenance easier and allows the reuse of modules for other applications. The stand-alone mode application is represented in **Figure 22**, but the same modules will be extended and employed for the development of the automatic ASPEN simulation service.

The User interface logic module represents the user interface layer, containing all user interface components used to display the application data and to serve as the primary point of user interaction.

The Controller receives the request from the user interface and pass it straight to the service layer, that will process it, and then returns the response given back from the service layer.

The Service Layer handles the business logic and performs the operations needed to satisfy the requests and returns the responses to the controller. Practically, it mainly receives the requests to run simulations of ASPEN models, after the user has set the proper input data. For this purpose, on one side the service layer takes advantage of the ASPEN Plus Interaction Layer to properly execute the process simulation on the ASPEN Plus Server (where ASPEN Plus software is installed) and to obtain the ASPEN simulation results; on the other side, it exploits the Data Access Layer to store or read the results of simulations into or from the database.

The Data Access Layer provides an easy and simplified access to the data stored in the persistent database by creating an abstraction of the logical data model so that other layers are agnostic of it. The Data Access Layer is built on top of the Data Storage Layer that contains the actual database engine where the maxh2dr PostgreSQL database is stored: here on top of tables and views, a big set of PostgreSQL stored procedures and functions was firstly developed to simplify the access to the entities, as previously explained in Section **3.3.2.4**.

The Data Access Layer in turn encapsulates calls to the provided database stored procedures and functions in suitable methods and was developed in C# programming language by exploiting Npgsql, an open source ADO.NET Data Provider for PostgreSQL that allows C# programs to access the PostgreSQL database server.

Before speaking about the ASPEN Plus Interaction Layer, it is worth to spend a few words on ASPEN Plus ActiveX Automation Server. The ASPEN Plus ActiveX Automation Server, by means of the ActiveX technology, enables an external Windows application to interact with Aspen Plus through a proper interface (IHapp object) using a language such as Visual Basic or C++. The server exposes objects through the COM object model. In general terms, with the Automation interface, it is possible for an external application to set the inputs of an Aspen Plus simulation, run the simulation and finally get the results of the simulation without using the Aspen Plus user interface.

Within the gas, steam and energy area application, the ASPEN Plus Automation Interaction Layer takes advantage of the Aspen Plus ActiveX Automation Server and was designed as a wrapper layer for useful methods that allow to interact with ASPEN Plus Automation Server, in order to run automatically the preliminary models provided by this area. This layer is developed in C# programming language and is under finalization according to the developed models' needs.

By now, a simple C# test application was developed as an Automation Client and real models of gas, steam and energy area were successfully executed on the server by the client application after setting the inputs and finally results were acquired and saved to file.

In next developments, the Service Layer will implement the mapping between ASPEN simulations outputs/inputs and the corresponding database streams and will store the mapped results of the simulation in the database by means of the Data Access Layer.

### 3.3.5 Database client development in IRMA

For the steel mill side wide model calculations in the Tata Steel (TS) proprietary software package IRMA, some process input information is generated by SSSA using ASPEN. For this, a database is developed by SSSA and hosted at SSSA facilities. This database act as a bridge in between IRMA and ASPEN for exchanging process information at a central place with a generic interface. The knowledge gained in the development stage could be used in future European projects.

This section describes the design of the database client for IRMA at TS, the work done during the development stage and the work to be done after this report.

### 3.3.5.1 System Description

Before starting with the description of the work executed, a better understanding of the components and it's place in the complete system is necessary, with particular focus on IRMA side. The following section describes the hole system and it's components.

The overview of the complete system is shown in Figure 23.
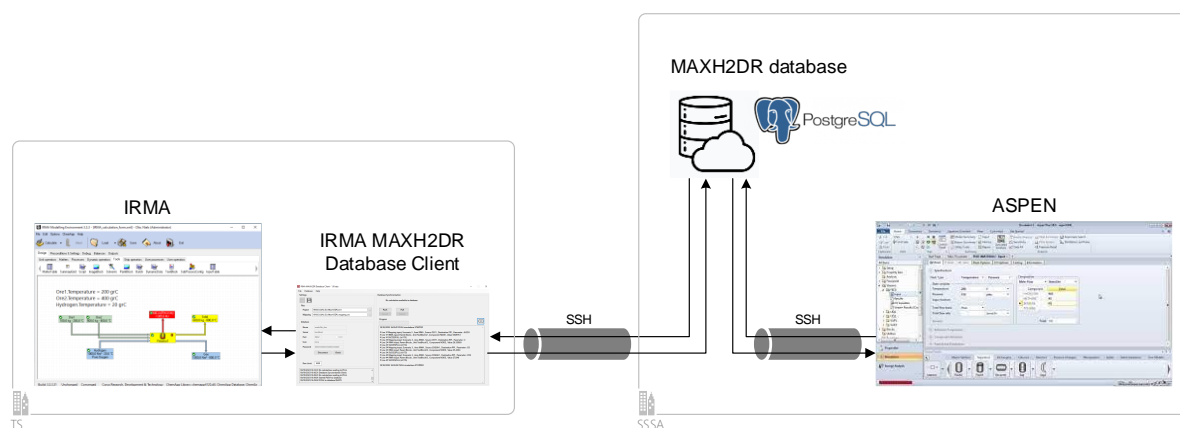


Figure 23: System overview (left TS and right SSSA parts)

The main parts of this system are

- IRMA is a flow sheeting software package developed by TS RD and integrated with a thermodynamical database for chemical reactions and equilibria calculations. This software package is used for the iron and steel making process flow sheet modelling and integrated steel mill site wide model development. In the MAXH2DR project gas and energy related process parameters are exchanged with ASPEN.

- MAXH2DR database has been developed by SSSA to act as a bridge between the IRMA and ASPEN Plus-based models (details are provided in Section **3.3.1**). The design of the database is based on the required parameters exchange between in IRMA and ASPEN. The content is agreed between TS and SSSA. To avoid problems reading and writing parameters from multiple database tables, SSSA included stored procedures to be executed. The results of the stored procedures are based on the application rights in the database. The needed stored procedures are implemented in the IRMA MAXH2DR database client (IMDBC) by TS.

- IRMA MAXH2DR database client (IMDBC) has been developed at TS to support the development and the calculations made with the steel mill side wide model in IRMA. The database client act as a bridge between IRMA and the MAXH2DB database.

### 3.3.5.2 Software

For the development of the IRMA MAXH2DR database client (IMDBC) the decision has been made to develop the software in C#, as it's better to maintain and the necessary tools and knowledge that is available as open source.

The build-up of the IMDBC is shown in Figure 24 that consists of

- a User Interface for the interaction with the user.
- a Controller acting as an interface between the UI and the Data Access Layer and the IRMA Interaction Layer.
- a Data Access Layer for the communication with the MAXH2DR database over a SSH tunnel.
- an IRMA Interaction Layer for parsing the IRMA project file with a custom XML parser, and for loading the mapping between units in the MAXH2DB database and the IRMA project file.
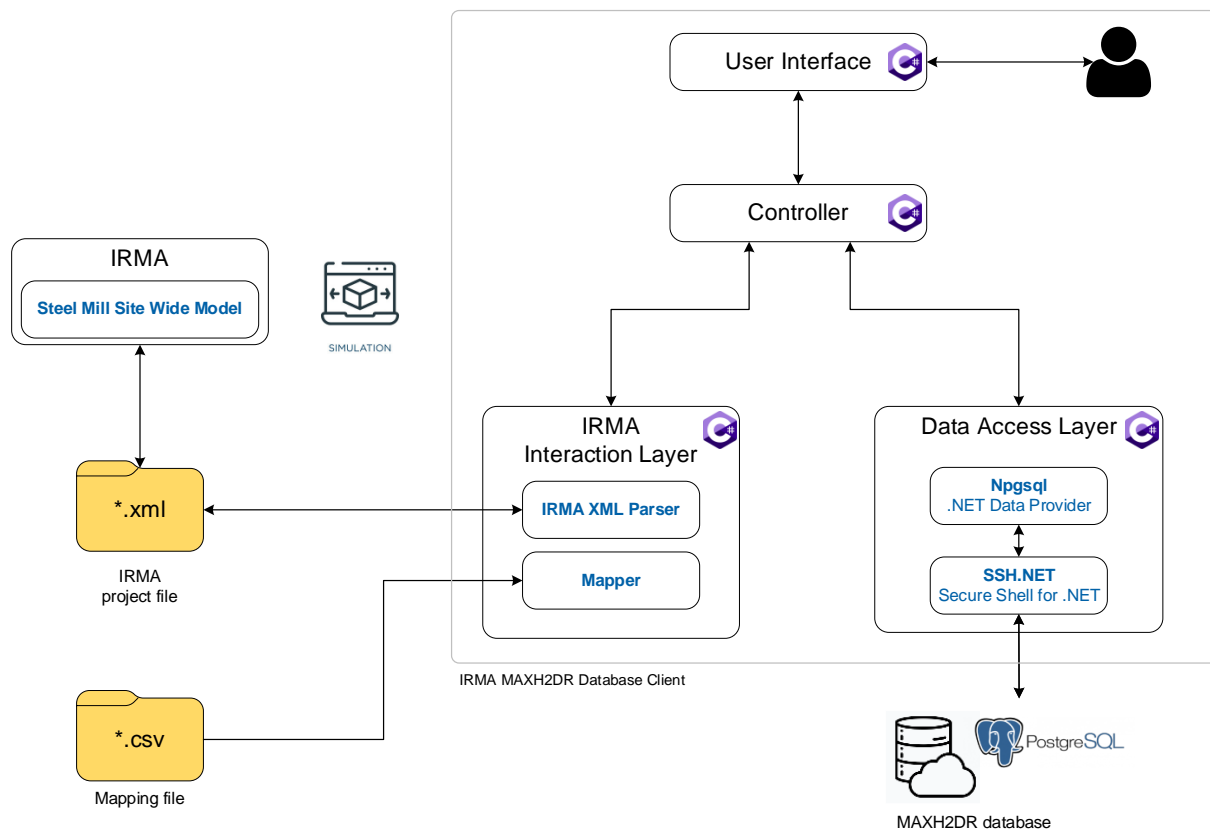


Figure 24: IRMA MAXH2DR Database Client build-up

The MAXH2DR database is hosted on a PostgreSQL[2] relational database server, developed and hosted at SSSA. For the exchange of data in the Data Access Layer of the IMDBC the open source package npgsql[3] is used. For support of creating SSH tunnelling in the IMDBC, the open source package SSH.NET[4] is used. For overall logging purposes the open source package Log4Net[5] is used.

### 3.3.5.3 Development

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[2] https://www.postgresql.org/
[3] https://www.npgsql.org/
[4] https://github.com/sshnet/SSH.NET
[5] https://logging.apache.org/log4net/

The development of the IMDBC can be separated in two different stages, a preparation stage where all the information and knowledge needed has been collected, and the development stage where the actual software code is written and tested.

In the preparation stage work has been carried out to collect the necessary information before starting the development stage of the IMDBC.

- At TS a Security Assessment has to be carried out. Goal of this Security Assessment is to get the business impact and the risks when there's a data loss due to system errors and unauthorised access to the stored data on internal and external systems. The input of SSSA as a cloud provider was needed because the data about the steel mill site wide model is stored in their systems. The outcome of the Security Assessment describes if the applied security measurements are sufficient or that other security mitigations are needed. As the data used in this project are highly anonymized and generic plant model is implemented, no further security mitigations where needed next to the usage of the SSH tunnelling.

- The IRMA software package uses a XML file structure to store flow sheet settings and the process parameter output data from the calculations. The structure of this file is not 100% compliant to the XML Document Object Model[6] used in the C# XML parser. To extract and insert process parameters knowledge for a custom XML parser was needed and tested before usage in the IMDBC, next to get knowledge of where process parameter values where stored in the IRMA XML file.

- During the development of the IMDBC, a local database server exact to the SSSA database server was setup at TS.

- Knowledge of available procedures and functions in the MAXH2DR database was needed to implement and the use the stored procedures and functions developed by SSSA.

The following work has been done during the development stage of the IMDBC.

- Creating a User Interface with the possibilities to select the IRMA project file and the corresponding mapping file needed for the exchange of process parameter values. For the user it has to be clear what's the status of the actions executed by the IMDBC and the status of the exchanged process parameter values (successful or not).

- Creating a mapping file in CSV format so that a user can create a mapping between the parameter sources in IRMA and it's corresponding parameter source in the database.

- Storing the program and the database access security settings provided by the user. The storage of the user security information has to be encrypted to avoid unauthorised access.

- Creating a Data Access Layer with automated access to the MAXH2DR database via SSH tunnelling with the proper security settings provided by the user.

- Inserting process parameter values in the MAXH2DR database in a stand alone matter to prove that the IMDBC is communicating properly with the MAXH2DR database.

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[6] https://learn.microsoft.com/en-us/dotnet/standard/data/xml/xml-document-object-model-dom

### 3.3.5.4 Current status

At the moment of writing this report, the IRMA MAXH2DR Database Client can be used for storing process parameters from a steel mill site wide model in IRMA to the MAXH2DR database in a stand alone situation. In Figure 25 screenshots are shown of process parameter which are processed from the IRMA model through the client into the MAXH2DR database based on the settings in the mapping file showed in Table 35.

For more clarifications, Table 35 acts only as an example. Indeed, the process parameters are not the actual values but values chosen as an indication. In addition, source and destination areas are not specified (e.g. for COGGH, it is not specified that it belongs to ASPEN area). Furthermore, also the stream material (e.g. ore, COG) is not specified in the table; only parameters are shown in Table 35. However, this proves that reading process parameter values as defined functions.

Table 35. Mapping file content

| | | | | | | | | | MAXH2DR database related fields | | IRMA related fields | | |
|---|---|---|---|---|---|---|---|---|---|---|---|---|---|
| LineNumber | ScenarioId | AreaName | SourcePlantName | SourcePlantNumber | DestinationPlantName | DestinationPlantNumber | ParameterName | ParameterValue | IrmaParent | IrmaUnit | IrmaComponent | IrmaAttributeName |
| 1 | 3 | IRMA | OSY | 1 | PP | 1 | Al2O3 | 0 | Blocks | TextBlock1 | NODE | DisplayText[0] |
| 2 | 3 | IRMA | OSY | 1 | PP | 1 | C | 0 | Blocks | TextBlock1 | NODE | DisplayText[1] |
| 3 | 3 | IRMA | COGGH | 1 | PP | 1 | CO | 0 | Blocks | TextBlock1 | NODE | DisplayText[2] |
| 4 | 3 | IRMA | COGGH | 1 | PP | 1 | CO2 | 0 | Blocks | TextBlock1 | NODE | DisplayText[3] |
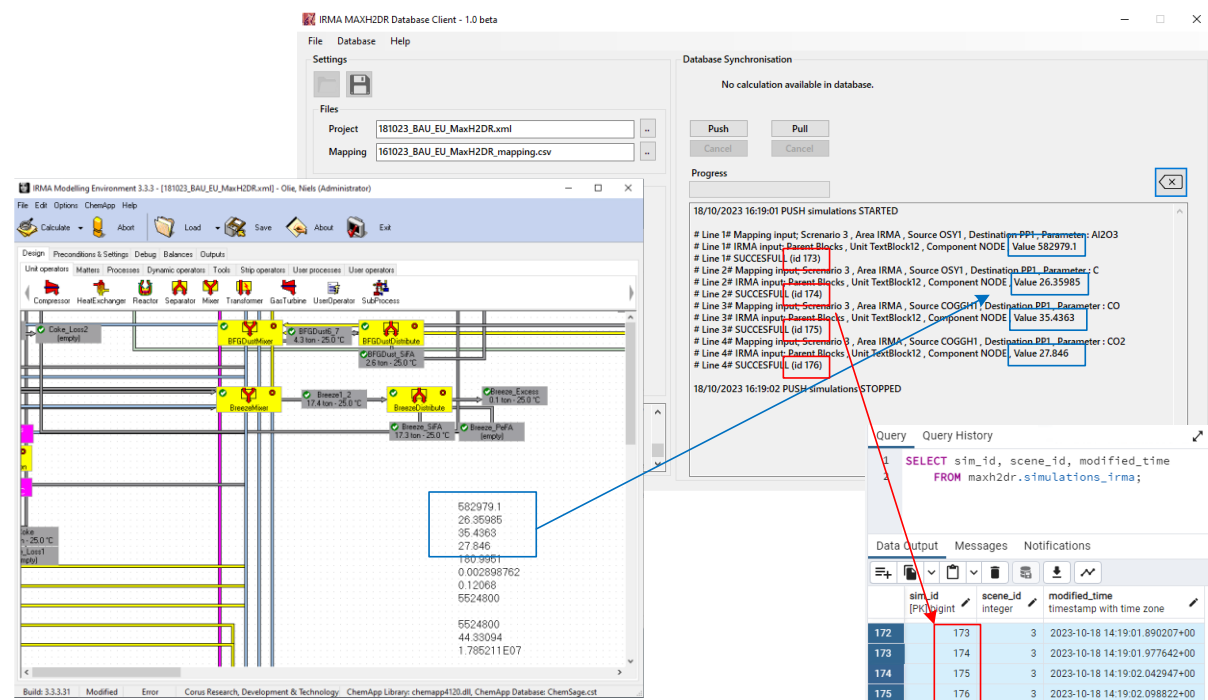


Figure 25: Process parameter values from IRMA to MAXH2DR database

### 3.3.6 Ongoing development and future implementations

Although all approaches have been defined for allowing model interactions and most of the related work has been concluded, at SSSA, the finalization of the Data Storage Layer and Data Access Layer is still ongoing. In the Data Storage Layer new stored procedures and functions are under development aimed at easily manage the global convergence processes and their associated convergence condition and material demands. Therefore, the Data Access Layer will be extended with C# methods incapsulating calls to these new databases stored procedures and functions.

On both areas, IRMA and ASPEN, the respective Automatic Simulation Service is under development according to the flow diagram designed for automatic interaction and depicted in Figure 19 of section 3.3.3.1.

More in details, in the next step each area service has to retrieve process parameter values from ASPEN through the MAXH2DB into the IRMA flowchart of the integrated steel mill site wide model, and viceversa. Therefore scenarios has to be agreed by TS and SSSA users and added into the MAXH2DR database. Then, convergence flow will be implemented on both side services.

Afterwards, a proper User Interface will be designed to facilitate the insertion of simulation inputs and simulation results visualization.

In particular, the amount of features that has to be added to the IMDBC so a user can execute the parameter exchange and can keep an overview about the convergence and the multiple simulations available for a scenario, forces a redesign of the user interface of the IMDBC by TS. The redesign has to be executed while implementing the parameter exchange flow as it is unknown at this moment which information is relevant for the user.

In a secondary step, the database will be adapted or extended to support the case of dynamic (non-stationary) models.

## 3.4 Standard Integrated Steelworks AML model

The integrated steel plant was modelled using the Python Pyomo AML as a system model built of interconnected simplified unit models. The model is used to simulate different system configurations and operational schemes in different stages of a transition towards hydrogen-based steelmaking, reflecting both different initial configurations and different possible options for future development.

Units included in the model are shown schematically in Figure 26. Coke plants, air separation units, combined heat and power plants, blast furnaces, hot stoves, basic oxygen furnaces, ladle treatment, continuous casting and rolling mills comprise units in the traditional BF-BOF route, and pellet plants, electrolyzers, shaft furnaces and electric arc furnaces are included as potential units for the hydrogen reduction route. The model can include several of the main units, such as blast furnaces, shaft furnaces and electric arc furnaces, and capacities of other units are variable as well.

Model variables are mainly flows of materials and energy between the system units, and from external sources, as well as binary variables representing decisions and logical relations. Flows included in the model are presented in Figure 27. System integration during a transition phase may involve connections between old and new units, and new units and connections can be introduced to the model flexibly.
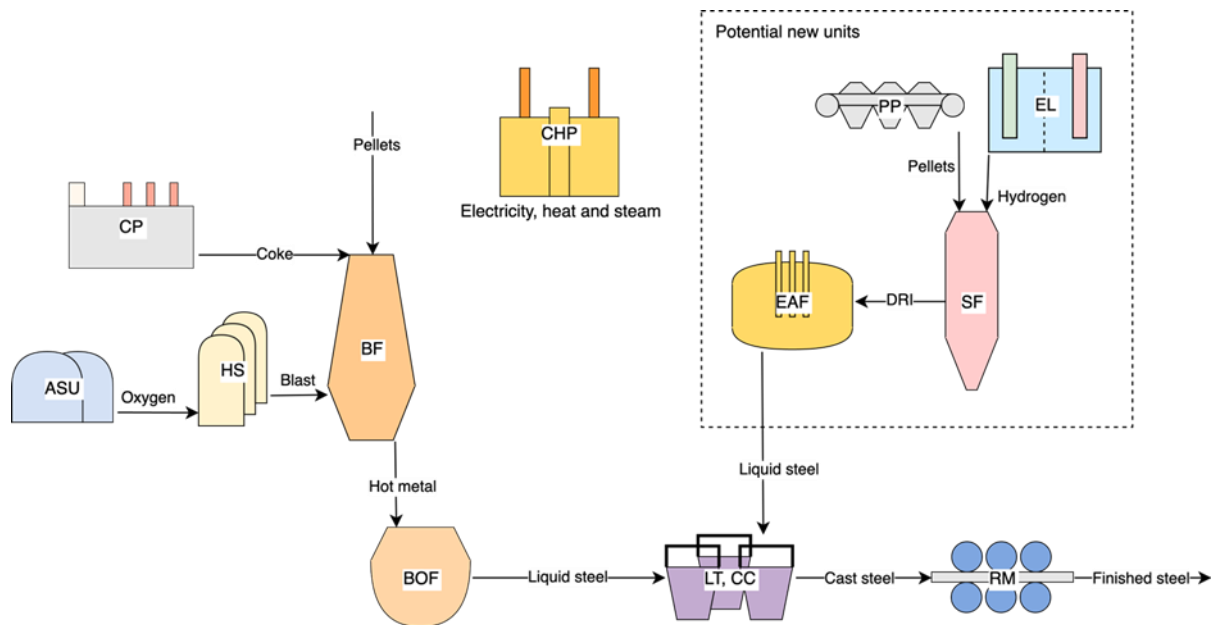
Figure 26. Simplified schematic of the units included in the system model.
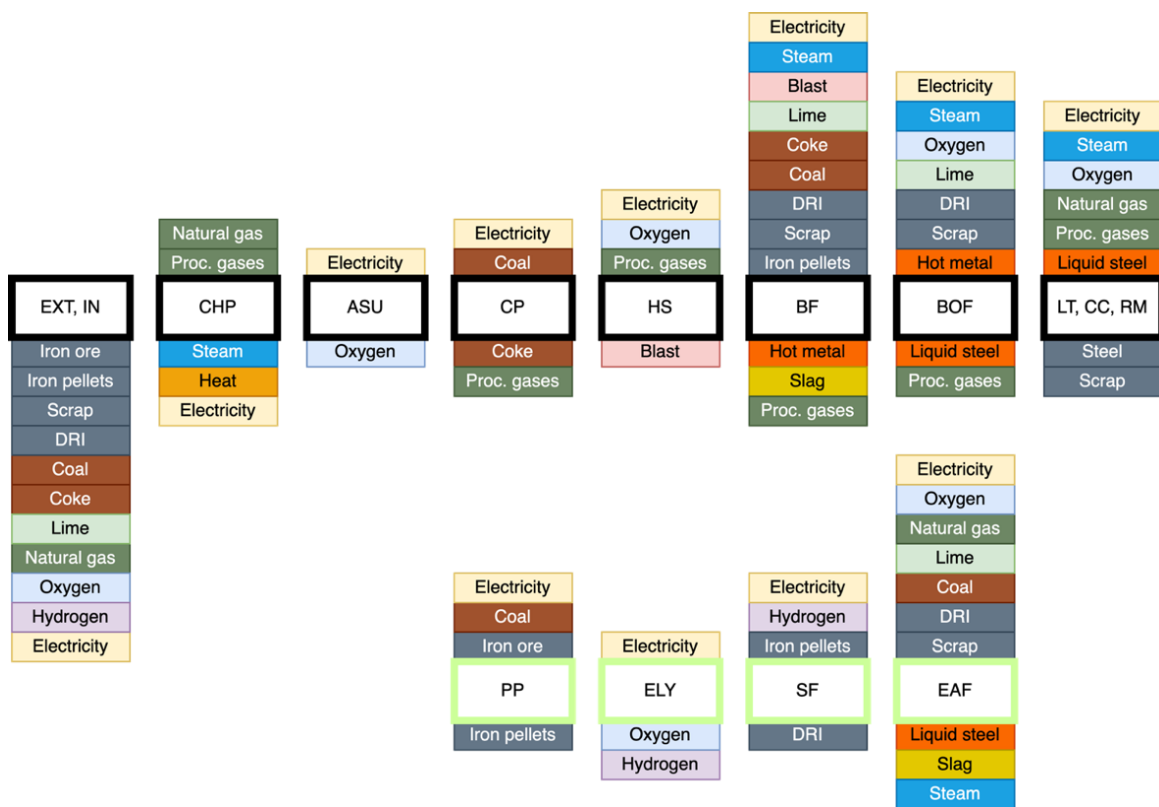


Figure 27. In- and outputs of system units in the model. Inputs are above the units and outputs below. Abbreviations: EXT, IN – External imports; CHP – Combined heat and power plant; ASU – Air separation unit; CP – Coke plant; HS – Hot stoves; BF – Blast furnace; BOF – Basic oxygen furnace; LT, CC, RM – Ladle treatment, continuous casting and rolling mills; PP – Pellet plant; ELY – Electrolyzer; SF – Shaft furnace; EAF – Electric arc furnace.

## 3.4.1 Unit models

This section describes the different unit models constituting the present overall system model.

Blast furnace (BF)

The blast furnace process has previously been modeled at ÅAU as a two-zone model that has been used, e.g., in optimization studies of integrated steelworks. For the present system model, a surrogate model of the two-zone blast furnace model was built by regression, with a select choice of input and output variables related by linear or quadratic functions. In this way, inputs of coke, pellets, lime and blast as well as slag output, top gas temperature, volume and composition and flame temperature were related to hot metal output, pulverized coal input, blast oxygen rate, blast temperature and DRI input. Additionally, scrap input, steam requirement and potential district heat output were defined as proportional to hot metal output. Within common operational limits for the furnace parameters, the surrogate model was found to adequately mimic the performance of the two-zone model.

Blast furnace operation is restricted in the model by upper and lower limits for top gas temperatures, adiabatic flame temperatures, blast oxygen rates, blast temperatures and hot metal outputs. The model has been run with up to two blast furnaces operating simultaneously, but the number could be increased when analyzing larger steelworks.

Hot stoves (HS)

Air and added oxygen injected into blast furnaces are first compressed and blown through hot stoves where they are pre-heated using blast furnace top gas. Models of hot stoves were included in the two-zone blast furnace models, and they were simplified for the present system model by linear regression. This resulted in expressions for compressor electricity demand, heat transfer in the stoves, hot gas temperature and blast furnace gas demand as functions of air volume flow, blast temperature and blast furnace gas composition. These variables relate hot stoves operation to blast furnace operation as well as the rest of the system.

Basic oxygen furnace (BOF)

Hot metal from the blast furnaces is converted to liquid steel in basic oxygen furnaces. Part of the charge can also be scrap or DRI, with a specified limit of this so-called cold charge. A conversion rate for hot metal is based on a carbon balance, while scrap and DRI are assumed to be fully converted to steel. BOF operation additionally requires inputs of oxygen, lime, steam and electricity, while BOF gas can be utilized by other system units and released heat can be used for district heating.

Coke plant (CP)

The coke needed in the blast furnace for the reduction of iron ores can be produced in on-site coke plants. This requires coal as raw material, and additional inputs of process gases and electricity. The

coke oven gas can in turn be utilized in other system units, as can steam produced in coke dry quenching.

Air separation unit (ASU)

Air separation units produce pure oxygen from air through cryogenic separation, which requires electricity. These are simply modelled by a linear relation between the oxygen output and the required amount of electricity.

Combined heat and power plant (CHP)

The CHP model relates inputs of energy as fuels (e.g., natural gas) and process gases (coke oven gas, BF gas, BOF gas) to outputs of heat, electricity and steam. Different assumptions regarding CHP operation can be implemented, with the present model assuming tapping of process steam at high, medium and low pressures, with different requirements of each. Lower and higher limits of steam flow are imposed, reflecting an operating range in which the turbine can function reliably.

Pellet plant (PP)

A pellet plant is included as a new system unit in the model, as direct reduction in a shaft furnace may require iron pellets of different grades than those charged into blast furnaces. The plant model simply constitutes linear relations between pellet production rate and demands of iron ore, coal and electricity.

Electrolyzer (ELY)

Hydrogen for the shaft furnace reduction process can in the model be externally bought or produced in electrolysis units using electricity to split water into hydrogen and oxygen. Efficiencies are selected to reflect reported values for commercial alkaline electrolyzers. Oxygen produced as a by-product can partly be utilized at the steelworks or exported.

Shaft furnace (SF)

The hydrogen-based reduction of iron oxides takes place in shaft furnaces where iron pellets are charged at the top and hydrogen gas enters in the lower part. The iron is reduced during its descent and extracted at the bottom while top gas largely consisting of water and unreacted hydrogen exits at the top. The SF model is based on a previously developed one-dimensional model considering heat and mass transfer and main chemical reactions occurring in the furnace. Similar to the BF model development, the previous SF model was used to generate data points used for determining a surrogate regression model implemented in the system model. DRI output, metallization degree, top gas temperature and hydrogen content, and gas injection pressures are here calculated as functions of pellet and hydrogen inputs, furnace diameter, pellet iron content and gas injection temperature, estimating the corresponding behavior of the more complex model.

As the top gas can contain significant amounts of unreacted hydrogen, part of it can be recycled and re-injected into the furnace. The total amount of hydrogen needed for the process may be higher than the theoretical minimum. Values for both the total required hydrogen and the required rate of fresh hydrogen were estimated based on the original SF model and values from the literature. Energy requirements of heating hydrogen to the desired injection temperature is treated as an additional electricity requirement.

Electric arc furnace (EAF)

EAFs commonly melt recycled steel scrap, but in the hydrogen-based steelmaking route they are also charged with DRI. In the unit model, the ratio of DRI in the charge affects the electricity requirement and the metal yield of the furnaces. Inputs of carbon, lime and oxygen are also included as they contribute to achieving desired steel and slag properties. Electrode consumption, furnace refractory wear and natural gas injection are not considered in the present model. Excess heat from the EAFs can be used for district heating or to produce process steam.

Ladle treatment, continuous casting and rolling mills (LT, CC and RM)

Processes after BOFs and EAFs are modelled with a constant rate of material loss, as well as demands of electricity, steam and oxygen linearly depending on the production rate. Additionally, it is assumed that rolling mills can deliver some heat for district heating and a specified rate of scrap that can be reused in the other parts of the steel plant.

## 3.4.2 Steelworks AML model performance

The system model can be used to evaluate steelworks operation with different configurations built of various system units. Table 36 compares the operational variables in two configurations, both operating at a 260 t/h production rate. The first configuration uses the traditional BF-BOF route, with two BFs and one BOF, while the second configuration utilizes hydrogen-based reduction in a shaft furnace, with further processing in two EAFs. In this second configuration, just below half of the charge to the EAFs is DRI from the shaft furnace, while the rest is recycled scrap iron. Alternative configurations could also feature more varied combinations of processing units and material streams.

$CO_2$ emissions are evaluated considering direct emissions from the steelworks and emissions related to grid electricity generation as well as other upstream emissions related to imported resources. Direct emissions are assessed through carbon balance calculations and grid emissions depend on estimated grid emission intensities, which have a significant impact considering the large electricity requirements of electrolyzers and EAFs as seen in Table 36.

From the type of operational points shown in Table 36, some main differences in the two routes can be seen, such as the shift in primary energy input from coke in the BF-BOF route to electricity in the hydrogen route. The $CO_2$ emissions are lower in the hydrogen route example, but this value is highly dependent on the assumed value for grid emission intensity and the assumed emissions related to scrap recycling.

The developed AML model can flexibly be adapted to different operational schemes, and with estimated costs and emissions factors for raw material and energy imports, it can form a basis for a wide range of analyses of integrated steelworks at different transition stages.

Table 36. Example operational points with different system configurations.

| | Configuration 1 2 BFs, 1 BOF | Configuration 2 1 SF, 2 EAFs |
|---|---|---|
| Production rate, t/h | 260 | 260 |
| BF pellet rate, t/h | 355 | |
| Coke rate, $kg/t_{hm}$ | 311 | |
| PCI rate, $kg/t_{hm}$ | 200 | |
| Blast $O_2$ rate, % | 24.2 | |
| Blast volume, kNm3/h | 303 | |
| BF hot metal output, t/h | 252 | |
| BOF scrap input, t/h | 63 | |
| BOF liquid steel output, t/h | 277 | |
| SF pellet rate, t/h | | 204 |
| SF hydrogen input, kNm3/h | | 133 |
| SF DRI output, t/h | | 147 |
| EAF scrap input, t/h | | 151 |
| EAF liquid steel output, t/h | | 277 |
| Electrolyzer power input, MW | | 534 |
| EAF power input, MW | | 148 |
| CHP power output, MW | 93 | |
| $CO_2$ emissions, $t_{CO2}/t_{hm}$ | 1.95 | 0.67 |

$CO_2$ emissions are calculated with a grid emissions factor of 89 $kg_{CO2}/MWh$

# 4. Results

## 4.1 Material – Energy balance results of the sub-processes

### 4.1.1 Raw material section

Results, raw materials section described material and energy balance results of the sinter, pellet and cokes plants in the EU SSM IRMA Model Reference Case.

### 4.1.1.1 Sinter Plant

Material – energy balance of the SP is shown in **Table 37**. Accordingly, 3.8 Mt$_{sinter}$pa is produced from the SP that uses as feestock the fine iron ore, pellet fines, mill scales, limestone, burnt lime, olivine and BFG dust, at 413.3, 2.4, 6.9, 76.4, 5.4 . Coke breeze, anthracite and mixed fuel gases are input energy streams to satisfy the thermal energy balance of the SP. MP steam, thermal energy (via mixed fuel gases) and electricity consumption rates in the SP are 700 kg/hr, 35.8 GJ/hr and 59.2 GJ/hr, respectively (See **Table 37**).

Table 37. Material – energy balance of the Sinter plant in the EU SSM IRMA Model

| Stream Type | | | Sinter plant | | |
|---|---|---|---|---|---|
| | | | unit output | 1 | t of sinter |
| | | | output | 3,802,716 | t sinter/year |
| | | | unit rate | flow per year | flow per hr |
| | | | unit*1000/workshop output unit | unit/year | unit/hr |
| iron bearing | | | | | |
| | Fine iron ore | t | 952.2 | 3620916.0 | 413.3 |
| | Pellet fines | t | 5.6 | 21407.4 | 2.4 |
| | Sinter | t | -1000.0 | -3802716.0 | -434.1 |
| | Mill scales | t | 15.9 | 60421.4 | 6.9 |
| carbon bearing | | | | | |
| | Anthracite | t | 12.2 | 46319.0 | 5.3 |
| | Coke breeze | t | 40.2 | 152967.4 | 17.5 |
| | Limestone | t | 175.9 | 668892.7 | 76.4 |
| | BFG dust | t | 6.0 | 22995.0 | 2.6 |
| fluxes (non C - bearing) | | | | | |
| | Burnt lime | t | 12.4 | 47029.8 | 5.4 |
| | Olivine | t | 4.1 | 15491.6 | 1.8 |
| Energy & utilities | | | | | |
| | Mixed fuel gas + Air | t | 907.9 | 3452409.0 | 394.1 |
| | Flue Gas | | -1132.4 | -4306133.0 | -491.6 |
| | Mass Balance | | | 0.3 | 0.0 |

| demand | MP Steam 15 bars | t | 1.6 | 6202.8 | 0.7 |
| demand | Mixed fuel gas | GJ | 82.4 | 313381.8 | 35.8 |
| demand | Electricity | GJ | 136.4 | 518601.1 | 59.2 |

### 4.1.1.2 Pellet Plant

Material – energy balance of the PP is shown in **Table 38**. Accordingly, 1.2 Mt$_{pellet}$pa is produced from a single SP that uses as feestock the fine iron ore, limestone, bentonite, olivine. Coke breeze, anthracite and mixed fuel gases are input energy streams to satisfy the thermal energy balance of the PP. Pellet fines are produced as by-product, recycled in the SP (See **Table 37**). MP steam, thermal energy (via mixed fuel gases) and electricity consumption rates in the PP are 200 kg/hr, 72.9 GJ/hr and 19.9 GJ/hr, respectively (See **Table 38**).

Table 38. Material – energy balance of the Pellet plant in the EU SSM IRMA Model

| Stream Type | | | Pellet Plant | | |
|---|---|---|---|---|---|
| | | | unit output | 1 | t of pellet |
| | | | output | 1,201,872 | t pellets/year |
| | | | unit rate | flow per year | flow per hr |
| | | | unit*1000/workshop output unit | unit/year | unit/hr |
| iron bearing | | | | | |
| | Fine iron ore | t | 1061.6 | 1275956.0 | 145.7 |
| | Pellets | t | -1000.0 | -1201872.0 | -137.2 |
| | Pellet fines | t | -17.8 | -21407.4 | -2.4 |
| carbon bearing | | | | | |
| | Anthracite | t | 7.8 | 9332.0 | 1.1 |
| | Coke breeze | t | 5.1 | 6123.4 | 0.7 |
| | Limestone | t | 13.0 | 15604.4 | 1.8 |
| | Bentonite | t | 7.7 | 9209.0 | 1.1 |
| fluxes (non C - bearing) | | | 0.0 | | 0.0 |
| | Olivine | t | 2.3 | 2819.7 | 0.3 |
| | Mixed fuel gas + Air | t | 2128.4 | 2558051.0 | 292.0 |
| Energy & utilities | | | | | |
| | Flue Gas | | -2301.6 | -2766185.0 | -315.8 |
| | Water | t | 93.5 | 112369.5 | 12.8 |
| | Mass Balance | | | 0.6 | 0.0 |
| demand | MP Steam 15 bars | t | 1.2 | 1463.2 | 0.2 |
| demand | Mixed fuel gas | GJ | 531.5 | 638808.5 | 72.9 |
| demand | Electricity | GJ | 145.0 | 174292.6 | 19.9 |

## 4.1.1.3 Cokes Plant 1 & 2

Material – energy balance of the CP 1 and 2 are shown in **Table 39** and **Table 40**. As can be viewed in the unit/workshop output unit columns in these tables, CP1 and 2 are near identical plants with varying capacities to supply cokes to BF 1 and 2 respectively.

Accordingly, 454 and 691 $kt_{Cokes}$pa is produced from CP 1 and 2 that uses as main feestock the coking coal. Coke breeze, tar, benzole and COG are produced as side products. Coke breeze is recyled (as energy carrier), the SP and PP (See **Table 37** and **Table 38**). Tar and benzole are export streams in the EU SSM. Chemical energy contained in the COG is recycled in the EU SSM to generate thermal and electrical energy for the iron and steel works (See Section **3.2.3**).

HP steam, thermal energy (via mixed fuel gases) and electricity consumption rates in the CP 1 are 4.2 t/hr, 218.2 GJ/hr and 10.7 GJ/hr, respectively. HP steam, thermal energy (via mixed fuel gases) and electricity consumption rates in the CP 2 are 6.5 t/hr, 332.3 GJ/hr and 16.3 GJ/hr, respectively (See **Table 39**).

Table 39. Material – energy balance of the Cokes plant 1 in the EU SSM IRMA Model

| Stream Type | | | Cokes plant 1 | | |
|---|---|---|---|---|---|
| | | | unit output | 1 | t of coke |
| | | | output | 453,768 | t coke/ year |
| | | | unit rate | flow per year | flow per hr |
| | | | unit*1000/workshop output unit | unit/year | unit/hr |
| carbon bearing | | | | | |
| | Coking coal | t | 1362.0 | 618024.6 | 70.6 |
| | Home coke | t | -1000.0 | -453768.0 | -51.8 |
| | Coke breeze | t | -139.0 | -63052.1 | -7.2 |
| | Tar | t | -30.4 | -13811.1 | -1.6 |
| | Benzole | t | -7.7 | -3509.7 | -0.4 |
| Energy & utilities | | | | | |
| | Mixed fuel gas + Air | t | 2708.8 | 1229161.0 | 140.3 |
| | Flue Gas | | -2708.8 | -1229161.0 | -140.3 |
| | Water | t | -34.1 | -15457.4 | -1.8 |
| | Mass Balance | | 0.0 | 0.0 | 0.0 |
| demand | HP Steam 44 bars | t | 82.0 | 37209.0 | 4.2 |
| | COG | GJ | -7972.2 | -3617535.0 | -413.0 |
| demand | Mixed fuel gas | GJ | 4211.6 | 1911084.0 | 218.2 |
| demand | Electricity | GJ | 206.5 | 93703.1 | 10.7 |

Table 40. Material – energy balance of the Cokes plant 2 in the EU SSM IRMA Model

| Stream Type | | | | Cokes plant 2 | |
|---|---|---|---|---|---|
| | | | unit output | 1 | t of coke |
| | | | output | 691,164 | t coke/ year |
| | | | unit rate | flow per year | flow per hr |
| | | | unit*1000/workshop output unit | unit/year | unit/hr |
| carbon bearing | | | | | |
| | Coking coal | t | 1362.0 | 941354.1 | 107.5 |
| | Home coke | t | -1000.0 | -691164.0 | -78.9 |
| | Coke breeze | t | -139.0 | -96038.7 | -11.0 |
| | Tar | t | -30.4 | -21036.5 | -2.4 |
| | Benzole | t | -7.7 | -5345.8 | -0.6 |
| Energy & utilities | | | | | |
| | Mixed fuel gas + Air | t | 1678.6 | 1160211.0 | 132.4 |
| | Flue Gas | | -1678.6 | -1160211.0 | -132.4 |
| | Water | t | -34.1 | -23544.2 | -2.7 |
| | Mass Balance | | 0.0 | 0.0 | 0.0 |
| demand | HP Steam 44 bars | t | 82.0 | 56675.5 | 6.5 |
| | COG | GJ | -8012.7 | -5538077.0 | -632.2 |
| demand | Mixed fuel gas | GJ | 4211.6 | 2910899.0 | 332.3 |
| demand | Electricity | GJ | 206.5 | 142725.4 | 16.3 |

## 4.1.1.4 Coal Grinding Line

Material – energy balance of the CGL is shown in **Table 41**. Accordingly, 751 $kt_{PCI}$pa is produced from the CGL that uses as feestock the PCI coal (with moisture content as received). Thermal energy (via mixed fuel gases) and electricity consumption rates in the CGL are 28.1 GJ/hr and 10.8 GJ/hr, respectively (See **Table 41**).

Table 41. Material – energy balance of the Coal grinfing line in the EU SSM IRMA Model

| Stream Type | | | Coal Grinding Line | | |
|---|---|---|---|---|---|
| | | | unit output | 1 | t of PC |
| | | | output | 750,732 | t PC/ year |
| | | | unit rate | flow per year | flow per hr |
| | | | unit*1000/workshop output unit | unit/year | unit/hr |
| carbon bearing | | | | | |
| | PCI coal | | 1111.1 | 834146.7 | 95.2 |
| | PC | t | -1000.0 | -750732.0 | -85.7 |
| Energy & utilities | | | | | |
| | Mixed fuel gas + Air | t | 142.2 | 106771.1 | 12.2 |
| | Flue Gas | | -283.2 | -212631.9 | -24.3 |
| | Nitrogen | t | 40.0 | 30029.3 | 3.4 |
| | Water | t | -10.1 | -7583.2 | -0.9 |
| | Mass Balance | | 0.0 | 0.0 | 0.0 |
| demand | Mixed fuel gas | GJ | 328.4 | 246519.9 | 28.1 |
| demand | Electricity | GJ | 126.2 | 94716.9 | 10.8 |

## 4.1.2 Iron and steel making section

### 4.1.2.1 Blast furnace 1 & 2

Material – energy balance of the BF 1 and 2 are shown in **Table 42** and **Table 43**. As can be viewed in the unit/workshop output unit columns in these tables, BF1 and 2 are near identical furnaces with varying HM capacities to reach target HRC productivity (of 4 Mtpa) in the EU SSM.

BF 1 and 2 uses as ferrous burden sinter, pellet and lump ore at 992.2, 473.3 and 150 kg/$t_{HM}$ rates, respectively (See **Table 42** and **Table 43**). Charged coke and injected PC at the rates of 297.5 and 197.7 kg/ $t_{HM}$ (averaged in BF1 and 2), are used as reductant and energy source in the BF iron - making process (See **Table 42** and **Table 43**). Oxygen enriched hot blast is injected at the rate of 1090.5 kg/ $t_{HM}$ (averaged in BF1 and 2) at the tuyeres to gasify PCI and cokes in the BF raceway to supply necessary heat and reducing gases.

1.5 and 2.3 $Mt_{HM}pa$ is produced from the BF 1 and 2, delivered to the BOSP to produce liquid steel. BF slag, BFG dust and BFG are produced as side products from the BF1 and 2, at the rates of 265.5 kg/$t_{HM}$, 10 kg/$t_{HM}$ and 5024.1 MJ/$t_{HM}$, respectively (See **Table 42**). BF slag is an export stream in the EU SSM. Chemical energy contained in the BFG is recycled in the EU SSM to generate thermal and electrical energy for the iron and steel works. BFG dust is partly/fully recycled in the EU SSM as a feed stream to the SP (See **Table 37**), excess BFG dust is an export stream in the EU SSM.

Electrical and thermal energy requirement in the BF1 and 2 are mainly attributed to the hot blast stove process (See Section **3.2.1**). 267.1 and 408.2 GJ/hr, equivalent to 1536.9 ans 1540.5 MJ/$t_{HM}$ thermal energy is supplied by the mixed fuel gases to the hot blast stoves operation of the BF 1 and 2, respectively. 33.4 and 51.1 $GJ_{el.}$/hr, equivalent to 192.3 and 192.7 $MJ_{el.}$/$t_{HM}$ electrical energy is supplied to the gas compression duty of the hot blast stoves operation of the BF1 and 2, respectively.

See Section **3.2.1**, for detailed description of hot blast stoves operation as developed by SSSA in AspenPlus.

Table 42. Material – energy balance of the Blast Furnace 1 in the EU SSM IRMA Model

| Stream Type | | | Blast furnace 1 | | |
|---|---|---|---|---|---|
| | | | unit output | 1 | t of hot metal |
| | | | output | 1,522,269 | t hm/ year |
| | | | unit rate | flow per year | flow per hr |
| | | | unit*1000/workshop output unit | unit/year | unit/hr |
| iron bearing | | | | | |
| | Lump ore | t | 150.0 | 228340.4 | 26.1 |
| | Pellets | t | 473.3 | 720508.3 | 82.2 |
| | Sinter | t | 992.2 | 1510395.0 | 172.4 |
| carbon bearing | | | | | |
| | BF Hot metal | t | -1000.0 | -1522269.0 | -173.8 |
| | Home coke | t | 297.7 | 453164.0 | 51.7 |
| | PC | t | 197.0 | 299887.0 | 34.2 |
| | BFG dust | t | -10.0 | -15218.7 | -1.7 |
| Slag | | | | | |
| | BF slag | t | -265.5 | -404178.3 | -46.1 |
| Energy & utilities | | | | | |
| | BFG | t | -1927.6 | -2934349.0 | -335.0 |
| | Hot Blast | t | 1089.3 | 1658222.0 | 189.3 |
| | Conveying air | t | 16.3 | 24852.7 | 2.8 |
| | Mass Balance | | 12.7 | 19354.7 | 2.2 |
| demand | MP Steam  15 bars | t | 6.0 | 9133.6 | 1.0 |
| | BFG | GJ | -5024.1 | -7648081.0 | -873.1 |
| demand | Mixed fuel gas | GJ | 1536.9 | 2339533.2 | 267.07 |
| demand | Electricity | GJ | 192.3 | 292759.2 | 33.4 |

Table 43. Material – energy balance of the Blast Furnace 2 in the EU SSM IRMA Model

| Stream Type | | | Blast furnace 2 | | |
|---|---|---|---|---|---|
| | | | unit output | 1 | t of hot metal |
| | | | output | 2,321,400 | thm/year |
| | | | unit rate | flow per year | flow per hr |
| | | | unit*1000/workshop output unit | unit/year | unit/hr |
| iron bearing | | | | | |

| | | | | | |
|---|---|---|---|---|---|
| | Lump ore | t | 150.0 | 348210.0 | 39.8 |
| | Pellets | t | 473.4 | 1098867.0 | 125.4 |
| | Sinter | t | 992.2 | 2303293.0 | 262.9 |
| carbon bearing | | | | | |
| | BF Hot metal | t | -1000.0 | -2321400.0 | -265.0 |
| | Home coke | t | 297.3 | 690064.9 | 78.8 |
| | PC | t | 197.0 | 457315.8 | 52.2 |
| | BFG dust | t | -10.0 | -23207.9 | -2.6 |
| Slag | | | | | |
| | BF slag | t | -265.5 | -616253.9 | -70.3 |
| Energy & utilities | | | | | |
| | BFG | t | -1924.0 | -4466456.0 | -509.9 |
| | Hot Blast | t | 1091.7 | 2534237.0 | 289.3 |
| | Conveying air | t | 10.7 | 24852.7 | 2.8 |
| | Mass Balance | | 12.7 | 29522.9 | 3.4 |
| demand | MP Steam  15 bars | t | 6.0 | 13928.4 | 1.6 |
| | BFG | GJ | -5017.7 | -11648120.0 | -1329.7 |
| demand | Mixed fuel gas | GJ | 1540.5 | 3576182.4 | 408.24 |
| demand | Electricity | GJ | 192.7 | 447373.2 | 51.1 |

## 4.1.2.2 Basic oxygen steel plant

Material – energy balance of the BOSP is shown in **Table 44**. Steel making shop model material and energy balance incorporate hot metal desulphurization, converter and secondary steelmaking metallurgy as described in Section **3.1.2.2 Basic oxygen steel plant**. HM from BF 1 and 2 is delivered to BOSP at the rate of 438.8 $t_{HM}$/hr, equivalent to 919 $kg_{HM}/t_{LS}$ (See **Table 44**). Scrap and lump ore are charged to BOSP at the rates of 89.5 and 4.7 tons/hr, equivalent to 187.5 and 9.9 kg/$t_{LS}$, respectively. Dolomite, burnt dolomite, burnt lime and miscellaneous are the fluxing streams in the de-sulphurisation and oxi-steel making operations, at the rates of 1.5, 31.5, 10.6 and 5.3 kg/ $t_{LS}$, respectively. Oxygen, Nitrogen and Argon gases are used in the BOSP, at the rates of 61.9, 0.4, 0.3 kg/$t_{LS}$, respectively. Air and water are the leakage streams at the rates of 25.2 and 0.3 kg/$t_{LS}$ in the BOSP (See **Table 44**). 4.7 t/hr eq. to 0.7 $\%_{rel.}$ mass balance error has been noticed in the BOSP model. In the course of development of this report, experts in the field are deployed to minimize the identified mass balance incosistency.

4.2 $Mt_{LS}$pa is produced from the BOSP, delivered to the steel Casters to produce the BOS cast. BOF slag, BOSG dust and BOSG are produced as side products from the BOSP at the rates of 52.2 t/hr, 4.6 t/hr and 56 GJ/hr, respectively. BOS slag and BOSG dust are export streams in the EU SSM. Chemical energy of the BOSG is recycled in the EU SSM to generate thermal and electrical energy for the iron and steel works (See Section **3.2.2**). MP steam, thermal energy (via mixed fuel gases) and electricity consumption rates in the BOSP are 8.6 t/hr, 57.6 GJ/hr and 63.9 GJ/hr, respectively (See **Table 44**).

Table 44. Material – energy balance of the BOSP in the EU SSM IRMA Model

| Stream Type | | | Basic oxygen steel plant | | |
|---|---|---|---|---|---|
| | | | unit output | 1 | t of liquid steel |
| | | | output | 4,182,288 | t liq.steel /year |
| | | | unit rate | flow per year | flow per hr |
| | | | unit*1000/workshop output unit | unit/year | unit/hr |
| iron bearing | | | | | |
| | Lump ore | t | 9.9 | 41445.7 | 4.7 |
| | Scrap | t | 187.5 | 784294.9 | 89.5 |
| | Liquid Steel | t | -1000.0 | -4182288.0 | -477.4 |
| | BOS tap loss | t | -7.5 | -31417.3 | -3.6 |
| carbon bearing | | | | | |
| | BF Hot metal | t | 919.0 | 3843669.0 | 438.8 |
| | Dolomite | t | 1.5 | 6472.0 | 0.7 |
| | BOFG dust | t | -9.6 | -40342.5 | -4.6 |
| fluxes (non C - bearing) | | | | | |
| | Burnt lime | t | 31.5 | 131653.2 | 15.0 |
| | Burnt dolomite | t | 10.6 | 44254.2 | 5.1 |
| | Miscellaneous | t | 5.3 | 22361.8 | 2.6 |
| Slag | | | 0.0 | | |
| | BOF slag | t | -109.4 | -457349.0 | -52.2 |
| Energy & utilities | | | | | |
| | BOFG | t | -117.3 | -490426.5 | -56.0 |
| | High purity oxygen | t | 61.9 | 258869.1 | 29.6 |
| | Nitrogen | t | 0.4 | 1819.7 | 0.2 |
| | Argon | t | 0.3 | 1202.7 | 0.1 |
| | Water | t | 0.3 | 1202.7 | 0.1 |
| | Air | t | 25.2 | 105545.2 | 12.0 |
| | Mass Balance | | 9.8 | 40966.8 | 4.7 |
| demand | MP Steam 15 bars | t | 18.0 | 75281.2 | 8.6 |
| | BOFG | GJ | -756.1 | -3162378.0 | -361.0 |
| demand | Mixed fuel gas | GJ | 120.7 | 504718.5 | 57.6 |
| demand | Electricity | GJ | 133.8 | 559579.0 | 63.9 |

## 4.1.2.3 Casters and Hot strip mill

Material and energy balance of the Casters is shown in **Table 45.** Accordingly, 4.1 Mt$_{BOS\ Cast}$pa is produced in the Casters using 4.2 Mt$_{LS}$pa. 9.4 t/hr caster scrap is produced as a side product. Casters require 6.1 GJ/hr, 21.1 GJ/hr and 6.1 t/hr thermal energy (via mixed fuel gases), electricity and MP steam for the works (See **Table 45**).

Table 45. Material – energy balance of the Casters in the EU SSM IRMA Model

| | | | Casters | | |
|---|---|---|---|---|---|
| | | | unit output | 1 | t of BOS cast |
| | | | output | 4,098,925 | t BOS cast/year |
| | | | unit rate | flow per year | flow per hr |
| | | | unit*1000/workshop output unit | unit/year | unit/hr |
| iron bearing | | | | | |
| | Caster scrap | t | -20.0 | -81978.5 | -9.4 |
| | Liquid Steel | | 1020.3 | 4182288.0 | 477.4 |
| | BOS Cast | | -1000.0 | -4098925.0 | -467.9 |
| Energy & utilities | | | | | |
| | Mixed fuel gas + Air | t | 5.2 | 21458.8 | 2.4 |
| | Flue Gas | | -5.7 | -23508.2 | -2.7 |
| | Argon | t | 0.5 | 2049.5 | 0.2 |
| | Mass Balance | | 0.3 | 1384.5 | 0.2 |
| demand | MP Steam  15 bars | t | 1.0 | 4098.9 | 0.5 |
| demand | Mixed fuel gas | GJ | 13.0 | 53274.5 | 6.1 |
| demand | Electricity | GJ | 45.0 | 184451.6 | 21.1 |

Material and energy balance of the HSM is shown in **Table 46**. Accordingly, 4 Mt$_{HRC}$pa is produced in the HSM using 4.1 Mt$_{BOS\ Cast}$pa. 6.9 and 5 tons/hr mill scales and HSM scrap are produced as side products of the HSM. HSM require 630.1 GJ/hr, 141.4 GJ/hr and 6.0 t/hr thermal energy (via mixed fuel gases), electricity and MP steam for the works (See **Table 46**).

Table 46. Material – energy balance of the HSM in the EU SSM IRMA Model

| | | | Hot Strip Mill | | |
|---|---|---|---|---|---|
| | | | unit output | 1 | t of hot rolled coil |
| | | | output | 4,000,007 | t hot rolled coil/year |
| | | | unit rate | flow per year | flow per hr |
| | | | unit/workshop output unit | unit/year | unit/hr |
| iron bearing | | | | | |
| | HSM scrap | t | -10.7 | -44000.1 | -5.0 |
| | Mill scales | t | -15.1 | -60480.1 | -6.9 |
| | BOS Cast | | 1024.7 | 4098925.0 | 467.9 |
| | Hot rolled coil | | -1000.0 | -4000007.0 | -456.6 |
| Energy & utilities | | | | | |
| | Mixed fuel gas + Air | t | 376.4 | 1505447.0 | 171.9 |
| | Flue Gas | | -376.9 | -1507447.0 | -172.1 |
| | Nitrogen | t | 0.5 | 2000.0 | 0.2 |
| | Mass Balance | | -1.3 | -5562.2 | -0.6 |
| demand | MP Steam 15 bars | t | 6.0 | 24000.0 | 2.7 |
| demand | Mixed fuel gas | GJ | 1380.0 | 5520009.0 | 630.1 |
| demand | Electricity | GJ | 309.6 | 1238402.0 | 141.4 |

## 4.2 Global Material – Energy balance results

### 4.2.1 Global Carbon (CO₂) input

Global material over Carbon was established to determine CO2 eq. material flow rates as input and output streams of the EU SSM Reference case. In this analyis, CO2 eq. is not regarded as global warming potential (GWP) of the components but simply a molecular mass based conversion as expressed below:

$$\dot{N}_{Carbon} * M_{A_{CO_2}} = \dot{M}_{CO_2,eq.} \, (tons \, CO_2 \, eq. \, hr^{-1})$$

Equation 20

Table 47 shows the carbon bearing input material streams annual mass flow rates in ktons CO2 eq. Shows the percentile share of the streams in regards to their carbon intensities in the EU SSM. Annual carbon input in the EU SSM Reference case is 7.4 Mt$_{CO2eq.}$pa. The most carbon intensive streams on site are coking coal and PCI coal, constituting 62.8 and 30.2 % of overall CO2eq. input to the EU SSM Reference case.

Table 47. Annual carbon input by streams in the EU SSM Reference case

| Input streams | kt CO2eq/ annum |
|---|---|
| Coking coal | 4649.92 |
| PCI coal | 2237.23 |
| Anthracite | 155.80 |
| Natural gas | 63.53 |
| Limestone | 271.66 |
| Miscellaneous | 26.84 |
| Total | **7405.0** |

Figure 28. Carbon intensities of the streams in the EU SSM Reference case
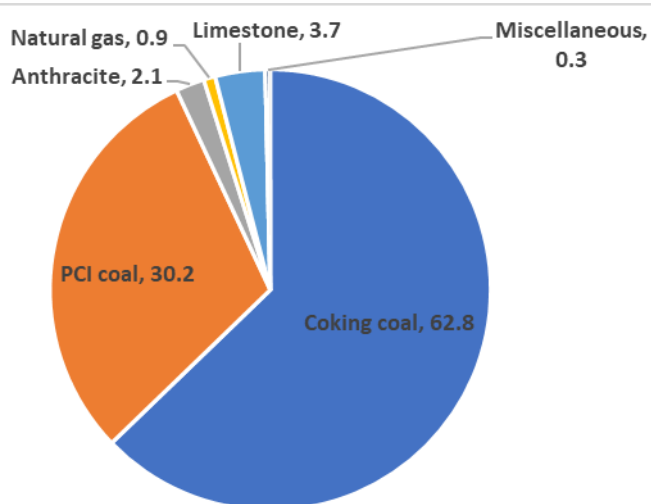


In the normal operation, input carbon streams leave the system in the form of export streams (excess coke breeze, dust, tar, benzole, etc.), steel and waste (flue gas). Latter is dispersed to the sub-

processes on site ,e.g. power plants, boiler units, raw materials section, hot blast stoves, steel making shop, flares, etc.

In the couse of development of this deliverable, finalization steps were still ongoing for the automatic DB interactions of the IRMA and Aspen tools, that limits the reporting of the output carbon streams on site specific to each sub-process.

### 4.2.2 Meeting heat and energy demand

As described in Section **3.3**, an IT infrastructure has been developed for allowing the models from IRMA (production) and Aspen (gas and energy) side to interact automatically. In addition, as described in Section **3.2** anf **3.3** the models have been developed to allow this interaction. Since finalization steps are still ongoing for the automatic interactions as described in Section **3.3.3.2**, currently production and gas & energy models have been simulated in cascade (not automatically). However, their suitability to interact and to satisfy balances has been proved: the demands from production side (IRMA) can be satisfied from gas and energy side (Aspen) as highlighted in the following table. Indeed, **Table 48**,

**Table** 49, **Table 50** and **Table 51** show how heat, electricity and steam demands are satisfied by showing results of cascade simulations aggregating data already shown in tables of Section **3.2** and related to gas and energy models.

Table 48: Heat Demand and related gas distribution

| User | Heat Demand by gas | Gas distribution | | | | |
|---|---|---|---|---|---|---|
| | GJ/h | BFG | rBFG | BOFG | COG | NG |
| | | GJ/h (t/h) | | | | |
| Coke Plant 1 | 218.20 | | 112.84 (38.08) | | 105.36 (2.06) | |
| Coke Plant 2 | 332.30 | | 171.00 (57.71) | | 161.30 (3.16) | |
| Sinter Plant | 35.80 | | 3.80 (1.28) | | 32 (0.63) | |
| Pellet Plant | 72.90 | | | 72.91 (11.34) | | |
| Coal Grinding Line | 28.10 | | 28.10 (9.47) | | | |
| Blast Furnace 1 (for HBS) | 267.07 | 191.21 (71.46) | | | 75.86 (1.49) | |
| Blast Furnace 2 (for HBS) | 408.24 | 292.10 (109.16) | | | 116.14 (2.27) | |
| Steelmaking Shop | 57.60 | | 57.60 (19.44) | | | |
| Casters | 6.10 | | 6.10 (2.06) | | | |
| Hot Rolling Mill | 630.10 | | | | 543.99 (10.65) | 86.11 (1.86) |
| Power Plant | 1653.94 | | 1613.2 (544.4) | | | 40.74 (0.88) |
| Auxiliary Boilers (MP+HP) | 45.13 | | 45.13 (15.23) | | | |

| User | Electricity Demand | Total Electricity Demand | Electricity distribution | | |
|---|---|---|---|---|---|
| | | | Power Plant | TRT | External Grid |
| | GJ/h | | GJ/h (%) | | |
| Coke Plant 1 + exhauster | 10.70+0.83 | | | | |
| Coke Plant 2 + exhauster | 16.30 + 1.27 | | | | |
| Sinter Plant | 59.20 | | | | |
| Pellet Plant | 19.90 | | | | |
| Coal Grinding Line | 10.80 | | | | |
| Blast Furnace 1 (cold blast compressor) | 33.42 | 542.51 | 467.34 (86.14) | 28.08 (5.17) | 45.98 (8.69) |
| Blast Furnace 2 (cold blast compressor) | 51.07 | | | | |
| Steelmaking Shop | 63.90 | | | | |
| Casters | 21.10 | | | | |
| Hot Rolling Mill | 141.41 | | | | |
| Auxiliary Boilers (MP+HP) | 0.73 | | | | |
| ASU | 111.880 | | | | |

Table 50: Steam Demand

| User | Steam Demand | | Total Steam Demand | | Steam Distribution | |
|---|---|---|---|---|---|---|
| | HP | MP | HP | MP | HP | MP |
| | | | | | BOFG Area + Power Plant + Auxiliary Boilers | Auxiliary Boiler |
| | t/h | | | | t/h (t/h of residual steam) | |
| Coke Plant 1 | 4.2 | 0 | | | | |
| Coke Plant 2 | 6.5 | 0 | | | | |
| Sinter Plant | 0 | 0.7 | | | | |
| Pellet Plant | 0 | 0.2 | | | | |
| Coal Grinding Line | 0 | 0 | | | | |
| Blast Furnace 1 | 0 | 1.0 | 10.7 | 15.3 | 10.7 (361.07) | 15.3 |
| Blast Furnace 2 | 0 | 1.6 | | | | |
| Steelmaking Shop | 0 | 8.6 | | | | |
| Casters | 0 | 0.5 | | | | |
| Hot Rolling Mill | 0 | 2.7 | | | | |

Table 51: Oxygen and Nitrogen Demand

| User | Demand | | Total Demand | | Distribution | |
|---|---|---|---|---|---|---|
| | O$_2$ | N$_2$ | O$_2$ | N$_2$ | O$_2$ (from ASU) | N$_2$ (from ASU) |
| | t/h | | | | t/h (t/h of residual) | |
| Coal Grinding Line | | 3.40 | | | 81.15 (0) | 3.80 (259.15) |
| Blast Furnace 1 (for cold blast O$_2$ enrichment) | 20.39 | | | | | |
| Blast Furnace 2 (for cold blast O$_2$ enrichment) | 31.16 | | | | | |
| Steelmaking Shop | 29.60 | 0.20 | | | | |
| Hot Rolling Mill | | 0.20 | | | | |

# 5. Discussion - Conclusion

In this report, models and complex material – energy balance network of a European integrated standardized steel mill (EU SSM) with 4 $Mt_{HRC}$pa productivity has been developed and elucidated. In the context of the MaxH2DR project Task 3.1: Adaptation and extension of available models and interconnection development, this work includes, development and integration of the sub-processes models in the:

- Raw materials section (TS):
    - Sinter Plant
    - Pellet Plant
    - Cokes Plant 1 & 2
    - Coal Grinding Line
- Iron and steel making section (TS):
    - Blast furnace 1 & 2
    - Basic oxygen steel plant
    - Casters and Hot strip Mill
- Gas – Energy section (SSSA):
    - BFG treatment area
    - BOFG treatment area
    - COG treatment area
    - Mixing and Enrichment Station
    - Auxiliary Boilers
    - Power Plant
    - Air Separation Unit

Material balance of the sub-processes in the steel mill have been converged for target production rates and product chemistries. Thermal, electrical energy and steam demands of the sub-processes are communicated to the gas – energy section. Generated process off-gases; i.e. COG, BFG and BOFG are used as input streams in the gas – energy section and delivered as mixed fuel gases to satisfy the demand for the works. Annual carbon input in the EU SSM Reference case is 7.4 $Mt_{CO2eq.}$pa, that is mainly comprised of coking and PCI coal: 62.8 and 30.2 %, respectively.

As requested in **Task 3.1**, SSSA developed a PostgreSQL relational database to allow the communication between the adapted tools. The database is deployed on a server at SSSA and is accessible through SSH (Secure Shell) tunnel using dedicated accounts supplied to WP3 partners.

The database allows defining scenarios each representing the active units in an area and material streams between units (in the same area or in different areas) and to store the result sets of model simulations related to specific scenarios, that will be changing during the project. A big set of PostgreSQL stored procedures and functions was developed in the data storage layer to provide a simplified handling of the stored entities.

In the expected system automatic mode, different area models interact with each other by exchanging data and simulations are run in cascade alternately until a global convergence condition is achieved causing the process to stop.  To manage the interaction of simulations within a convergence process, two services, one in each area (upstream/downstream), were designed and are under implementation, to allow the IRMA-ASPEN interaction, respectively as upstream and downstream areas. In addition, the existing database was extended with additional tables to support the automatic operative mode, considering interrelated simulations, global convergence achievement and possible demands (energy or material) coming from the upstream area. In the Data Storage Layer, new stored procedures and functions, aimed at easily manage the global convergence processes, convergence conditions and material demands, are under development.

An AML steel mill model has been developed, featuring simplified unit models included in the reference BF-BOF route as well as in possible alternative routes including hydrogen-based reduction of iron ores. Blast furnace and shaft furnace models have been implemented as regression-based surrogates of more complex models. The AML model has shown to provide efficient calculation of overall steel mill operation based on a variety of system configurations and input parameters and can thus function as a tool for analysis of possible transition routes and stages when considering hydrogen-based steelmaking.

Accordingly, in Task 3.2: Stationary scenario analyses for transitional pathways, the most promising alternative future steel mill scenarios will be investigated using the developed linked IRMA/Aspen process chain tool as a reference lay-out. Analysis of the impact both on production and gas and energy handling of changed operating conditions, feedstock properties and stepwise replacement of BF-BOF with H2 enriched DRI – EAF route, will be enabled by customizing of the EU SSM IRMA model as well as of related Aspen Plus based gas and energy area model.

Therefore, once all the tools involved in the expected system automatic mode will be finalized, the investigations on scenarios foreseen in Task 3.2 can be carried out exploiting the effective interaction between the steelworks and the energy network, going through gradual transition stages from the reference integrated steelmaking route towards novel routes with $H_2$-enriched DR.

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## Acronyms and Abbreviations

| | |
|---|---|
| EU SSM | European Standardized Steel Mill (See **Section 1**) |
| SP | Sinter plant |
| PP | Pellet plant |
| CP | Cokes plant |
| CGL | Coal grinding line |
| BF | Blast furnace |
| BOF | Basic oxygen furnace |
| HSM | Hot strip mill |
| BFG | Blast furnace gas |
| BOFG | Basic oxygen furnace gas |
| COG | Cokes oven gas |
| NG | Natural gas |
| HM | Hot metal; i.e. pig iron |
| PC | Pulverized coal; i.e. BF injection coal |
| HMB | Heat and mass balance |
| TGT | Top gas temperature |
| ASU | Air Sepration Unit |
| BTX | Benzene Toluene Xilene |
| CHP | Combined Heat and Power |
| DC | Dust Catcher |
| DR | Direct Reduction |
| ERD | Entity Relationship Diagram |
| ESP | Electrostatic Separator |
| HBS | Hot Blast Stove |
| HPC | High Pressure Column |
| IT | Information Technology |
| L/G | Liquid Gas Ratio |
| LCV | Lower Calorific Value |
| LPC | Low Pressure Column |
| M&ES | Mixing and Enrichment Station |
| NG | Natural Gas |
| POG | Process Off Gas |
| PSD | Particle Size Distribution |
| rBFG | Enriched Blast Furnace Gas |
| SSH | Secure Shell |
| SSSA | Scuola Superiore Sant'Anna |
| TRT | Top Recovery Turbine |
| WI | Wobbe Index |
| TS | Tata Steel |