

CHAPTER II



THEORY

2.1 Minerals of copper ores and concentrates

The main minerals in ores from which copper is extracted are listed in Table 2-1. Normally, ores contain less than 1%Cu. Due to its dilute concentration, it is uneconomic for direct smelting the ores to produce copper as the process would require too high energy and furnace capacity. For this reason, all ores which are destined for pyrometallurgical extraction are concentrated by physical processing prior to smelting. Usually, the copper mines concentrate the copper ores to have more than 25% copper content.

The concentrated product obtained is copper sulfide concentrates typically containing a range of about 25 to 35% Cu, 24 to 30% Fe, 28 to 34%S and 2 to 10% SiO₂, in addition to minor amounts of gangue oxides. Chalcopyrite is the biggest copper source. Sulfide minerals are treated by a pyrometallurgical process. Carbonates, Chlorides, Oxides, Silicates and sulfates are treated by a hydrometallurgical process. It is noted that Chalcocite is able to be treated by both ways.

2.2 Primary smelting process

2.2.1 General description

General process flow diagram of a primary smelting process is represented in Figure 2-1. This process is also known as a fusion conversion for copper concentrates. The objective of the process is to smelt copper concentrate to produce white metal with 73 – 75% Cu and fayalite slag with the following chemical characteristics: 8% Cu, 16 – 20% magnetite and 23 – 28% silica.

Table 2-1: Principal minerals of copper ores (Biswas and Davenport, 1994)

Minerals	Theoretical composition	Theoretical (%Cu)	Specific Gravity
SULFIDES			
Chalcopyrite	CuFeS_2	34.6	4.2
Chalcocite	Cu_2S	79.9	5.7
Bornite	Cu_5FeS_4	63.3	4.2
Covellite	CuS	66.4	4.6
METAL			
Native copper	Cu^0	100	8.8
OXIDES			
Malachite	$\text{CuCO}_3 \cdot \text{Cu}(\text{OH})_2$	57.5	4.0
Azurite	$2\text{CuCO}_3 \cdot \text{Cu}(\text{OH})_2$	55.3	3.8
Cuprite	Cu_2O	88.8	6.0
Tenorite	CuO	79.9	6.0
Chrysocolla	$\text{CuSiO}_3 \cdot 2\text{H}_2\text{O}$	36.2	2.1
Antlerite	$\text{CuSO}_4 \cdot 2\text{Cu}(\text{OH})_2$	53.8	
Brochantite	$\text{CuSO}_4 \cdot 3\text{Cu}(\text{OH})_2$	56.2	

The oxidation reactions in the fusion conversion process are regulated by the control of the ratio between the feed flow of concentrate and the total oxygen flow injected into the Teniente converter. These reactions are exothermic and the rate of heat generation depends on the total oxygen flow. The heat balance can be adjusted by manipulating the following variables: revert mass flow rate and enrichment of air to fix the ratio between the flow rate of copper concentrate and total oxygen. The temperature of this process is close to 1,240 °C.

The oxygen required for the oxidation reactions is fed via tuyeres sunk into the white metal at the pressure of 18 to 20 psig and with an enrichment that varies between 33 to 38% oxygen depending upon the chemical characteristics of the concentrate.

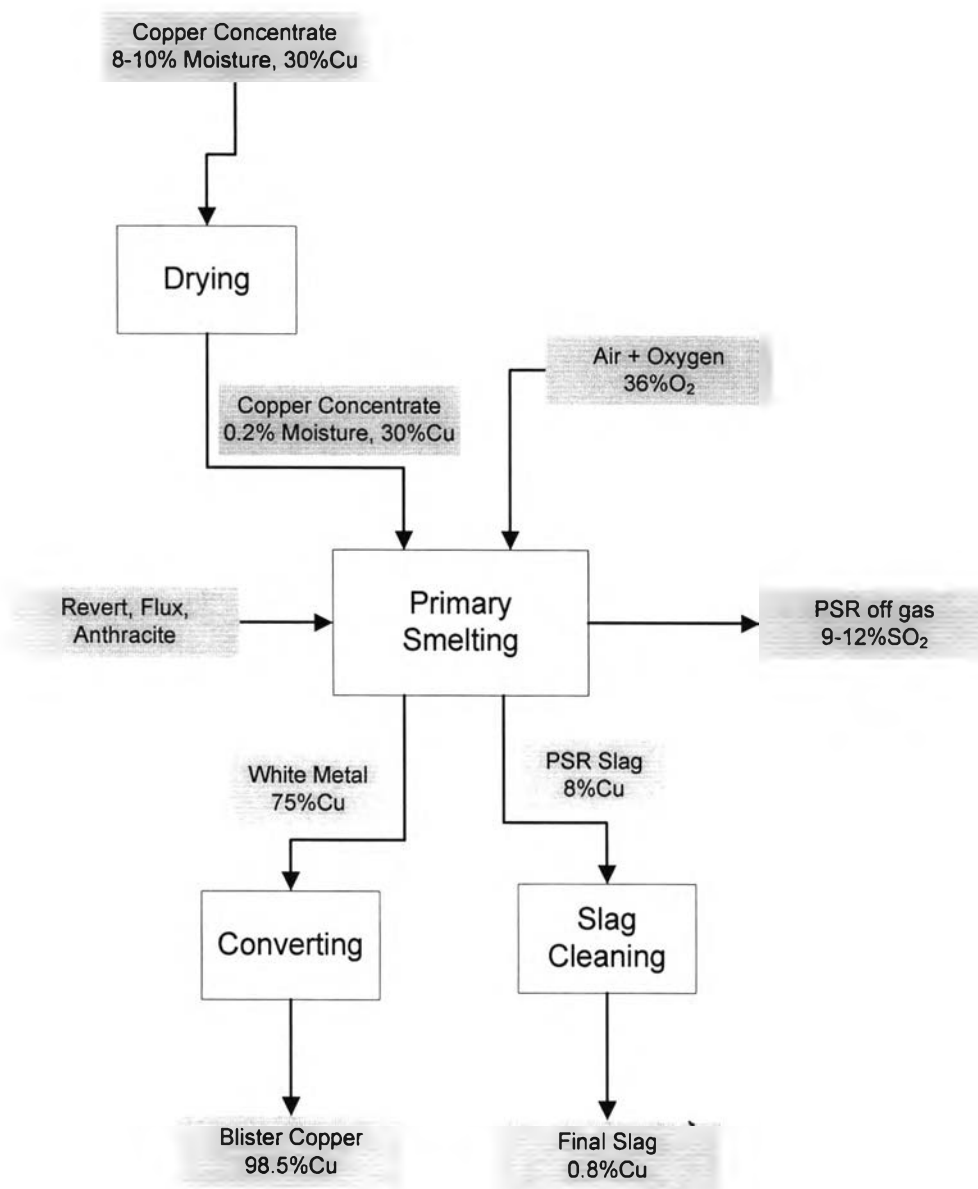


Figure 2-1: Flowsheet of a primary smelting process

Base on the plant design data, a bone dry concentrate blend having 0.2% moisture content with an average copper content of 30% is continuously and directly fed through 4 tuyeres into molten bath at the rate of 78.7 tph, using dry air as conveying fluid. Simultaneously, a blend of silica flux (7.4 tph), solid reverts (10.2 tph) and coke (0.78 tph) are fed into the reactor via a garr gun feeder.

Note that the bone dry concentrate is injected into the Teniente converter by a pair of dense phase pneumatic systems loaded from the bone dry concentrate bin and four feed hoppers. Each system comprises of two feed hoppers and the

interconnecting piping and special valves to operate the hoppers in a continuous manner. Feed hoppers are supplied with dry air from dedicated compressors and air dryers. They operate on a batch regime, one feed hopper receiving the bone dry concentrate while the other is injecting concentrate to the concentrate tuyeres of the reactor. The two systems operate intermittently in sequence.

Solid materials (reverts, silica flux and coke) with different moisture content are stored in independent bins located close to the reactor prior to be charged at the Teniente converter through conveyor belts.

Molten bath agitation and iron and sulfur oxidation is performed through the continuous blowing into the molten bath of a gaseous mixture formed by low pressure compressed air and industrial oxygen through a maximum of 46 blowing tuyeres. The blowing air and oxygen average flow are controlled at 37,700 – 42,100 Nm³/hr and 10,000 – 10,700 Nm³/hr respectively to reach a total nominal blowing flow of 51,200 – 55,800 Nm³/hr with an enrichment of 36 – 37 %O₂. Enriched air blowing is interrupted only for maintenance purposes.

The liquid products of the fusion-conversion process are white metal and slag. White metal containing about 75% copper is intermittently tapped every hour through water cooled copper taphole, located at the endplate close to the garr gun, and poured into ladles of 7 m³ capacity. The white metal is transferred to the Hoboken Syphon Converters, where it continues the copper blister conversion process. Molten slag formed by iron oxide (FeO) and silica is tapped at the opposite endplate of the furnace to be transported through a transfer launder to the Electric Furnace where it is processed to recover its copper content.

The white metal is a mixture of Cu₂S (copper sulfide) and FeS (iron sulfide) where the composition of the latter component regulates the grade of copper. Its average chemical composition is 75 %Cu, 3 %Fe and 21 %S.

The slag is mainly formed from fayalite (2FeO.SiO₂), Magnetite (Fe₃O₄) and white metal. The characteristic chemical composition is as follows: 6–8 %Cu, 16–20 %magnetite and 23–28 %silica. The magnetite content is controlled by adjusting a silica flux feed rate among others.

Molten slag and white metal are tapped at temperatures from 1,240 – 1,260 °C and 1,220 – 1,240 °C respectively. In case of necessity, slag could be extracted through the off gas mouth but the normal process is to make it through the slag taphole.

Sulfur dioxide and other gases generated within the converter together with the water steam coming from process air and solid charge moisture are collected. The total average volume is about 52,500 – 56,800 Nm³/hr that are continuously extracted through the off gas mouth at 1,220 °C.

The sulfur dioxide gases (more than 10 %SO₂) whose concentration depends on the hood dilution level and on the gas handling facilities are collected through a water cooled panel hood before sending to the cooling and cleaning systems to produce sulfuric acid at the sulfuric acid plant.

2.2.2 Density of white metal and slag

The principle phenomenon that makes the efficiency of fusion-conversion process being possible is the low solubility of white metal in the slag and its relative density difference:

Density of White Metal	=	4.8 (FeS) to 5.6 (Cu ₂ S) g/cm ³
Density of Slag	=	2.8 to 3.8 g/cm ³

When two liquids, white metal and slag, are produced, the separation between them is possible and relatively rapid even if they are mixed. The white metal which is, heavier, goes to the bottom, while the slag maintains itself in the upper part of the bath. The phenomenon is similar to that occurs when water and oil are mixed; the liquid mixture is always separated into two layers or phases.

If the separation is maintained at constant temperature and mass balance, it is possible to work indefinitely with a stable rate of production. The thermal balance is reached when in the period of determined time; the heat generated by the fusion conversion process reactions is equivalent to the heat necessary to smelt the feed concentrate, to heat the products and to compensate for heat losses and permits the operation at a stable temperature. On the other hand, the mass equilibrium is obtained when all of the materials that enter reactor are the same as those that exit during a certain amount of time. According to the mass equilibrium condition, the level of white metal and slag in reactor has to be stable and consistent.

It should be noted that the chemical composition of white metal is handled through the ratio between the flow of the copper concentrate and the total flow of

oxygen whereas the chemical composition of the slag depends on the level of the phases, white metal copper grade and the amount of silica added.

2.2.3 Fusion-conversion process

In the fusion-conversion process, the following phenomena occur;

2.2.3.1 *Drying of moisture in feed material*

The elimination of humidity by drying has impact on the control of the process temperature because of the large consumption of heat required. As a result, a high humidity in the feed of the copper concentrate for lowers the bath temperature.

2.2.3.2 *Pyrite decomposition*

As the temperature is increased, the feed charge follows a series of thermal decompositions (endothermic reactions) generating solid phases and gases. In practice, the disassociations of Covellite (CuS), Bornite (Cu₅FeS₄), Chalcopyrite (CuFeS₂) and Pyrite (FeS₂) by the following reactions are of interest.

Reactions of pyrite decomposition	Temperature (°C)	
$4\text{CuS(s)} \Rightarrow 2\text{Cu}_2\text{S(s)} + \text{S}_2\text{(g)}$	502	(2-1)
$4\text{Cu}_5\text{FeS}_4\text{(s)} \Rightarrow 10\text{Cu}_2\text{S(s)} + 4\text{FeS(s)} + \text{S}_2\text{(g)}$	927	(2-2)
$4\text{CuFeS}_2\text{(s)} \Rightarrow 2\text{Cu}_2\text{S(s)} + 4\text{FeS(s)} + \text{S}_2\text{(g)}$	949	(2-3)
$2\text{FeS}_2\text{(s)} \Rightarrow 2\text{FeS(s)} + \text{S}_2\text{(g)}$	626	(2-4)

From the above reactions, Cu₂S, FeS and pyritic S₂ are considered to be principle components, independent of concentrate chemical and mineralogical composition. The other components such as some of metal oxide (SiO₂, Al₂O₃, CaO etc.), which called gangue composition, will go the slag.

2.2.3.3 Smelt and dissolutions

The mineral decomposition produces pyritic S_2 , Cu_2S , FeS and gangue. However, at operating temperature of the Teniente converter (1250 °C), the pyritic S_2 generated is in vapor form and goes to the gas phase.

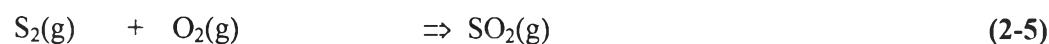
The formation process of the two liquid phases, white metal and slag, begins with the fusion and dissolution of the FeS and Cu_2S (digestion) in the liquid bath. The white metal found inside the reactor is a homogenous solution formed by two components Cu_2S and FeS , which have the same type of chemical link (covalent link) and being soluble. In general, the mixture of Cu_2S and FeS will always come from only one liquid phase called “the metal phase”.

On the other hand, slag starts to form after the reactions of silica flux and the oxides generated by blowing of oxygen.

2.2.3.4 Principle chemical reaction

The principle oxidation reactions that occur as a consequence of the blowing air in the matte phase are shown in Equations (2-5) and (2-6).

Pyritic sulfur oxidation



FeS oxidation



The oxygen injected through the tuyeres oxidizes the pyritic sulfur and the FeS while the heat generated by these oxidations melts the solid charge. Depending on the amount of FeS oxidized, the copper grade in white metal can vary so that the extent of reaction in Equation (2-6) is used to calculate %Cu in the white metal.

2.2.3.5 Secondary chemical reaction

The formation of fayalite slag is the reaction of FeO and silica as FeO is very reactive liquid, particularly with regards to oxygen and the refractory bricks. This

means that in the presence of oxygen it must react and continue its extent of oxidation. FeO is a basic oxide partially soluble in bath that has a range of fusion close to 1,380°C when pure.

In order to reduce the chemical activity of this oxide which can cause the formation of magnetite by reacting further with oxygen, silica is added to form the ferrous ortho-silicate, $2\text{FeO}\cdot\text{SiO}_2$, which is known in solid state as fayalite, by the corresponding reaction;

FeO oxidation



FeO which is not reacted with SiO_2 will over oxidizes with the presence of oxygen as:

Magnetite formation



This reaction is very favorable if the condition inside the Teniente converter is highly oxidizing from enriched air injection. Magnetite has a fusion point at 1,597 °C and consequently is maintained solid, thus complicating the liquid bath with a heterogeneous and viscous mixture.

The intermediate densities of the metal, slag and magnetite are

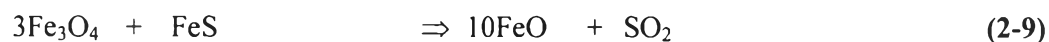
- Metal phase density about 4.8 – 5.6 ton/m³ (from 100%FeS to 100%Cu₂S)
- Slag phase density about 2.8 – 3.8 ton/m³
- Magnetite density about 5.2 ton/m³

Consequently, the solid magnetite has limited solubility in the slag at around 13 – 20% for temperatures of 1,200 – 1,240 °c. The difference in its density and high Cu₂S in metal can constitute a layer that floats between the slag and the matte forming a false floor.

2.2.3.6 Other reactions

- Reaction between the magnetite and iron sulfide

Due to the agitation in the bath, the iron sulfide attack action over the magnetite present in the bath is favored. Upon generating SO₂ gas, bubbling is produced from the reaction which allows dragging of particles of White Metal (Cu₂S) in the slag by floatation. The reaction between the magnetite and iron sulfide as followings;

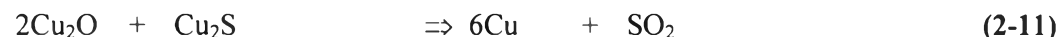


A high ratio of Fe/SiO₂ in the slag promotes the formation of magnetite, which increases slag viscosity and dragging of white metal particles in the slag, resulting in the higher loss of copper in the final slag. On the other hand, the magnetite upon reacting with the refractory lining of the reactor forms a solid layer of protection that allows protection of infiltrations of liquid metal thus preserving the physical integrity of the reactor shell.

As previous mentioned, a large amount of magnetite content in the slag increase copper losses but low magnetite content damages the reactor.

- Reaction between copper oxide and iron sulfide

Occasionally, reaction occur at normal working temperature in a Teniente converter between the copper oxide (Cu₂O) that can be present in a from of revert from Anode Furnace or over blown copper.



These reactions easily occur spontaneously allowing a rapid generation of SO₂ in the inter-phase of the liquid-liquid reaction. This could cause a harmful foaming phenomenon. The formation of gas (SO₂) in the bulk of the liquid produces a gas emulsion (foam) that overwhelms reactor volume causing the explosive emptying of the furnace. Consequently, materials losses and the danger of serious accident could

happen. To prevent this phenomenon, reheating and over-oxidation of the bath are avoided and rapid charging of oxidized slag with metal should also be avoided.

2.2.4 Generation of gases in the fusion-conversion process

In the fusion-conversion process, the gaseous phase emitted by the reactor, is trapped by the hood at TC and is conducted to the gas cleaning plant where it is treated to produce sulfuric acid to recover of its sulfur content. These emissions are composed of Gases and Vapor which consist of:

Nitrogen : coming principally from the air injected through the tuyeres and air infiltration.

Oxygen : coming from the air injected by the garr gun, from the oxygen injected by tuyeres that didn't react in the bath, as well as infiltrated air.

Sulfur dioxide : coming from the oxidation of the pyretic sulfur and from the oxidation of FeS.

Water Vapor : coming from the evaporation of the water in the charge.

CO₂ and CO : in those cases in which a fossil fuel (Anthracite) is burned.

2.2.4.1 Smoke and particulates

The smoke and particulates are liquid or solids finely dispersed that tend to agglomerate. The biggest particle sediment quickly fall in the ducts; those of moderate size deposit themselves farther and smallest particles maintain in suspension and are transported by the gases which can be recovered as a dust from PSR and off gas handling unit.

Some of the particulates corresponds to solid or liquid material generated from the reactor especially when the Garr-gun is loaded or the molten metal addition through the mouth because of the agitation of the bath. Particulate material is also formed from the sublimated material coming from the interior of the reactor and that because of the effect of the dropping of the temperature, the materials solidifies in the duct, reaching sizes larger that 0.01 microns.

2.3 Process control in a primary smelting reactor

The process variables are those that indicate if the process is under operational control. For the Teniente Converter the following are the fundamental process variables:

2.3.1 Phase level

2.3.1.1 *White metal level*

The conversion grade obtained and the quality of the white metal are largely related to the height of the phase present in the reactor. The height of this phase influences the resident time of the oxygen (time that oxygen stays in the bath) which reacts with the sulfur present.

Conversely, a low level of white metal can have the consequence where the air injected into the reactor that is close to the slag phase, would over oxidize the slag and causes the risk of producing foam.

2.3.1.2 *Slag level*

The fayalite slag formation is complex. To generate the slag requires that the silica flux is digested in bath. The digestion depends largely on the level of the slag, where a low slag level can cause silica contamination during metal tapping.

On the other side, the continuous slag generation, increases the slag level inside the furnace. At a higher slag level (because of effects for more resistance time), the slag is more likely to over-oxidize result in generating magnetite, and will likely increase the copper losses. Another consequence of a high level of slag is overblowing and risks of foaming. High level of slag could also cause the obstruction of the Garr Gun from splashes of the melt.

To summarize, the level of metal- slag phase has a great influence in the grade of copper in the metal, the temperature and the quality of the slag which are very crucial in the operation of the PSR.

2.3.2 Copper content in white metal

The white metal is principally a solution of copper and iron sulfide in variable proportions, including other sulfurous metals dissolved in the charge like nickel, cobalt, bismuth, lead and zinc sulfides.

In this sulfides solution, selenides and tellurides are also dissolved, together with arsenides, antimonides, sulfiarsenides and sulfiantimonides of copper, and almost all of the precious metals that accompany copper minerals. Finally small quantities of oxygen can also be found dissolved as traces of oxide such as Al_2O_3 and SiO_2 .

The critical copper grade is defined as the maximum copper grade that white metal would have, when all the iron content is oxidized, it can be calculated by the following method.

The proportion of metallic copper in the copper sulfide can be calculated as shown in the following example:

- In a molecule of Cu_2S , the weight of Copper is $= 2 \times 63.5 = 127$
- In a molecule of Cu_2S , the weight of Sulfur is $= 32.1$
- The total weight of the molecule of Cu_2S is $= 159.1$

Then the proportion of metallic copper in the Cu_2S is $= 127 / 159.1 = 0.798$.

As such, the critical copper grade in white metal is 79.8%

A lower copper grade will produce operational problem in the Hoboken Syphon converters because the white metal in this case will contain a large quantity of iron sulfide (FeS) which will consequently produce a large quantity of oxidized slag with a high fusion point (mazamorra). This slag that is normally returned to the Teniente converter will produce some interference in the process.

On the other hand, a higher copper grade in the white metal indicates that the conversion grade in the reactor is much more advanced. However, with the presence of oxides and iron according to equation 2-6, then there will be a larger quantity of white metal retained in the slag.

Additionally, the consumption of revert necessary to maintain the thermal balance in the reactor will depend largely on the extent of the white metal grade

because of the higher exothermic heat generated. As a consequence, there will be a higher consumption of reverts.

2.3.3 Slag quality

The slag obtained in the smelting of concentrates have compositions that vary considerable from in one smelter to another according to the nature of the minerals, concentrates, fluxes, operational condition and other diverse factors. The principal oxides are CaO, SiO₂, Al₂O₃ and the iron oxides FeO and Fe₃O₄. Occasionally, levels of MgO and Cr₂O₃ rise, with the appearance of sulfur suspensions and trapped gas.

2.3.3.1 Presence of copper in the slag by physical entrapment

The primary cause for the entrapment of copper in the slag phase is the blowing on the tuyeres and agitation of the bath that causes the segregation of the matte in small drops. These get trapped in the slag, because of the slag viscosity. This situation is enhanced if the droplets are small in size because they do not have sufficient time to detain and return the white metal phase. The copper droplets could be dragged out with the slag, during the slag tapping.

The viscosity of the slag increases when the temperature drops, so colder slag has a greater physical capacity to trap copper than a hot slag.

Slag with a high magnetite content, as well as a high free silica content are viscous slag so these types of slag also will have a high physical drag of white metal. The correct silica content in the PSR slag will be defined according to the total input of iron into the system.

Normally, the chemical quality of the good slag should have the following properties:

- The average relation (Fe in slag) / (SiO₂ in slag) should be 1.5 – 1.7 while the theoretical ratio is 1.858 which is calculated from pure fayalite slag (2FeO.SiO₂)
- Copper content : lower than 7%
- Magnetite content : between 16% to 20%
- Silica content : between 24% to 28%

2.3.3.2 Presence of copper in the slag by chemical entrapment

The chemical losses of copper are primarily because of the formation of copper oxides which are very reactive and combine themselves easily with the magnetite to form either copper ferrite, $\text{Cu}_2\text{O}\cdot\text{Fe}_3\text{O}_4$ or copper magnetite, CuFe_2O_4 . It also combines easily with the silica to form copper silicate. The only way to recover this copper is the destruction of these components in the slag cleaning furnaces, SCF. It would require magnetite contents lower than 1%, which makes its recovery not economical.

The free copper oxides contained in the slag are easily reduced and can be recovered. To decrease the chemical loss of copper the formation of copper oxides must be minimized.

2.3.4 Temperature

The temperature inside the converter will have a direct effect on the kinetics of the reactions of oxidation, as well as on the viscosity of the slag.

A high temperature will have a higher conversion and digestion grade of the flux, as well as lower slag viscosity, which when combined with lower magnetite content, can cause liquid filtration towards the shell. On the other hand, a low temperature will have the opposite effect, low conversion, high slag viscosity, making cold slag with higher metal contents and over blowing with the danger of foaming.

2.3.5 Adjusted variables (manipulated variables)

The control variables are those that relates with the output and input variables whether directly or indirectly by the way of formulas and algorithms.

2.3.5.1 Tapping products

The balance between the product output and tapping of the slag and white metal, will maintain the phase levels inside the furnace. This variable is adjusted by the decision of the operator through the measurement of each phase level.

2.3.5.2 Oxygen coefficient

The oxygen coefficient is a parameter that relates with the air flow, the enrichment of oxygen, air injection, air annular, with the concentrate injected, meaning the overall relationship of the concentrate smelted with all the oxygen fed into the reactor. This parameter is simulated and calculated. It is indicated in the control screen of the PSR and should be used as a reference for the operation and control of the copper grade in the white metal. This parameter will depend on the chemical composition of the concentrate and the grade of the copper in the planned metal.

In practice, the oxygen coefficient is expressed as the ratio between the total flow rate of pure oxygen that is fed into PSR in Nm^3/h and the flow of concentrate that is smelted in dry tons/hour. For the oxygen flow is composed of the flow of oxygen injected in the air flowing into the tuyeres, the oxygen flow from the tuyeres and the flow of injected air and the oxygen in the air annular flow. This parameter is calculated for each type of concentrate or blended concentrates and is indicated on the control screen of the Teniente Converters for used as a reference for the operation

2.4 Others technology

There are different technologies such as the flash smelting and bath smelting. Flash smelting employs oxygenated air to promote autogenous conditions while bath smelting is dependent upon the roasting and smelting steps occurring within a molten pool containing both matte and slag phases.

2.4.1 Flash smelting

Outokumpu flash smelting is currently the most dominant copper smelting technology. The other is Inco (International Nickel Company of Canada) flash process which is different in design and oxidizing environment (Fakheha, Wagialla and El-Dahshan, 1990). In “flash smelting” reactions primarily occur in a gas phase system between oxygen bearing gas and concentrate particles dispersed within. With flash smelting technology, the increase in furnace throughput with simultaneous extension of smelting vessel campaign has occurred due to a) high oxygen enrichment b)

improved feed system and burner design c) protection of furnace integrity by external cooling d) improved settler metallurgy and e) mathematical modeling and process control. High oxygen enrichment-adopted by Outokumpu is now a common practice. It has been the most economic means of increasing furnace capacity without increasing its physical dimensions and its gas cooling and cleaning system.

2.4.2 Bath smelting

During the last 30 years, considerable progress has been made in bath smelting of copper concentrates. In year 2000, about 30% of the world's copper production will be produced by this technology. In bath smelting, the concentrate feed is enveloped and reacted in a turbulent bath of matte (Mackey and Campos, 2001). Five major technologies using this smelting technology are: a) Mitsubishi Continuous Smelting b) El Teniente Converter (TC) c) Noranda Technology and d) Top Submerged Lance Technology (TSL) -Isasmelt and Ausmelt. The advantage of this important smelting method is the high intensity mode of smelting which enables the added charge to quickly reach smelting temperatures and the chemical reactions to rapidly proceed to completion; this feature translates to smaller sized furnaces per unit capacity and a high overall efficiency.

Of the smelters surveyed, about 35% use flash smelting, 35% use bath smelting; rest of the technologies cover the balance of 30%.

Other technologies used, however are not on a large scale. These are the reverberatory furnace, blast furnace, and electric furnace. It is believed that most of them would have changed to either flash or bath smelting by the time the next survey of copper smelters is done.

2.5 Simulation of metallurgical process

Metallurgical process simulations track elemental, compound and energy components of a process. Material and energy balance calculations in integrated metallurgical processes can be very complex. The calculations are frequently encountered in base metal operations and in process developments that consist of multiple unit operations. The process simulation by using METSIM program can support plant operations by providing reference for parameter adjustment and material

and energy balance technical support. Figure 2-3 illustrates the user interface of METSIM program.

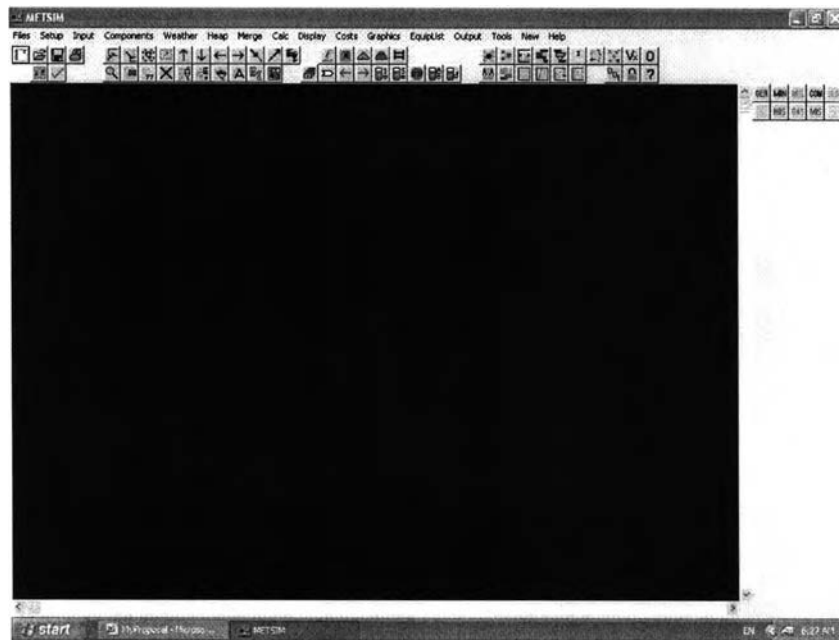


Figure 2-3: User interface of METSIM

2.5.4 METSIM® simulations modules

The modules which are frequently used are as follow;

Base Mass Balance - This module performs mass balance calculations around each unit operation and includes Chemical, Mineral Beneficiation and Hydrometallurgical models.

Heat Balance Module - In this module, heat losses, heats of reaction, stream temperatures, and heat contents are calculated and reported around each unit operation.

However, many parameters influence the design of a process plant. It is important for the design or auditing engineer to realize limitations of the simulated model, for examples:

- Side reactions have not been considered in the above model. Trace contaminates are possible to react.

- The heat generated by the reactions is extremely high. Novel processes employing sulfide oxidation and metal dissolution require detailed energy balances to support the process design and the due-diligence review.
- The laboratory, pilot plant or operating plant data must support the process model. The above chemistry is “assumed” and may not take place in the “real” world.
- Process design parameters such as reactor residence time, absorption / precipitation reactions, and solid-liquid separation parameters should also be developed from laboratory and pilot plant data.

Process simulations do have limitations. Realistic solutions must be supported by engineering and operational judgment, careful examination of input parameters and assumptions, and laboratory, pilot-plant or operating data.