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APPENDICES

APPENDIX A

BUILDING A PSR MODEL IN METSIM

The steps for building a PSR model using METSIM software can be described as follows:

(1) Select the elements and compounds to be included in the database (Figure A-1). The principle elements to be considered are Cu, Fe, S, O, Si and N. Main compounds are Cu₂S, FeS, FeO, Fe₃O₄, Fe₂SiO₄, Cu₂O, SiO₂, SO₂, and N₂. Others elements and compounds are included in this model to describe the impurity distribution from the raw material.

(2) Specify the amounts (flow rates) and compositions of input streams and humidity in the first column (Figure A-2). Adjust the mineralogical composition of a copper concentrate to be compatible with the chemical assays in the second column. It is noted that the first column needs to be filled in before the user can fill in other columns. The last column shows the elemental composition which the program calculates automatically from the second column.

	0.0			Ê	
ELEMENTS	SOLIDS	LIQUIDS	MELTS	GASES	
3 N 7	63 CaSiO3(W) SI	211 H2O(a) LI	248 Bi(m) M1	335 N2(g) G0	с
408	64 Cu(s) SI	212 Ag2SO4(a) LI	249 Bi2O3(m) M1	336 Ag(g) G(с
5 Na 11	65 Cu(s)RE-A SI	213 AgCI(a) LI	250 B12S3(m) M1	337 Ag2S(g) G(С
6 Mg 12	66 Cu(s)RE-B SI	214 CaCO3(a) LI	251 Ca(OH)2(m M1	338 Ag2Se(g) G(С
7 Al 13	67 Cu(s)RE-C SI	215 CaSO4(a) LI	252 CaCO3(m) M1	339 AgC1(g) G0	С
8 Si 14	68 Cu(FCC)(s SI	216 CuSO4(a) LI	253 CaSO4(m) M1	340 AgS(g) G(С
9 S 16	69 Cu(OH)2(s SI	217 Fe2(SO4)3 LI	254 Cu(m) M1	341 A1203(g) G	С
10 Cl 17	70 Cull(AsSb SI	1218 FeO(a) L	255 CuO(m) M1	342 As(g) G(С
11 K 19	71 Cu20(s) SI	219 FeO(a) LI	256 Cu20(m) M1	343 As203(g) G	С
12 Ca 20	72 Cu25(C)(s SI	220 FeSO4(a) LI	257 Cu2S(m) M1	344 As2S3(g) G	С
13 Ti 22	73 Cu2S(s) SI	221 H2SO4(a) LI	258 Fe(m) M1	345 As4(g) G	С
14 Fe 26	74 Cu2S(s) SI	222 H3AsO4(a) ∐	259 FeO(dm) M1	346 As406(g) G	С
15 N1 28	75 Cu2S(s) SI	223 HAsO2(a) LI	260 Fe304(dm) M1	347 As454(g) G	С
16 Cu 29	76 Cu2Se(s) SI	224 HSbO2(a) LI	261 MgCO3(m) M1	348 Au(g) G	С
17 Zn 30	77 Cu2Se(s) SI	225 MgCO3(a) LI	262 Mo(m) M1	349 Bi(g) G	С
18 As 33	78 Cu3(As04) SI	226 NH4HSO4(a LI	263 MoS2(m) M1	350 Bi2O3(g) G	С
19 Se 34	79 Cu3As(s) SI	227 Na2SO4(a) LI	264 Na2CO3(m) M1	351 Bi2S3(g) G	C
20 Mo 42	80 Cu3AsO4(s SI	228 NaCI(a) LI	265 Na2SO4(m) M1	352 BiS(g) G	C
21 Ag 47	81 Cu3AsS4(s SI	229 NiO(a) LI	266 NaCl(m) M1	353 C(g) G	C
22 Sb 51	82 CuSFeS4(s SI	230 NiSO4(a) LI	267 N1(m) M1	354 CH4(g) G	C
23 Te 52	83 CuSFeS4(s SI	231 PbO(a) LI	268 N13S2(m) M1	[355 CO(g) G	C
24 Au 79	84 Cu6A12(OH SI	232 SO2(a) LI	269 N13S2(m) M1	356 CO2(g) G	C
25 Pb 82	85 Cu0#Fe203 SI	233 SiO2(a) LI	270 NiS(m) M1	357 Ca(OH)2(g GC	
26 Bi 83	86 CuO#Fe2O3 SI	234 ZnO(a) LI	271 Pb(m) M1	358 CaO(g) GC	1.64

Figure A-1: Elements and Compounds which are shown in METSIM program

	108						
Collahuasi (nev	w)	la ala ini almanatha il in anangkial		ngang pang tang tang tang tang tang tang tang t	en elle constitution a fois		
108		SI U	M1	М3		0	Cancel
Collahuasi		LO		GC		Un	Cancer
	MT/DY		Wt.Frac.	Mol.Frac.	-	Wt.Frac.	Mol.Prace*
SOLID	694.63794	Cu20(s)	0	0	H 1	0	0
SLD-ORG	0	Cu25(C) (s	0.0547	0.0450816	c 6	0	0
AQUEOUS	1.39206	Cu25(s)	0	0	F 7	0	0
ORGANIC	0	Cu25(s)	0	0	0 8	0.0408984	0.1045002
MOLTEN	0	Cu25(s)	0	0	Na 11	0	0
MATTE	0	Cu2Se(s)	0	• _	Mg 12	0.0007237	0.0012169
SLAG	0	Cu2Se(s)	0	0	AL 13	0.0058746	0.0089008
GAS	0	Cu3 (As04)	0	0	Si 14	0.0288692	0.0420203
TOTAL	696.03	Cu3As(s)	0	0	s 16	0.358006	0.4564434
& SOLID	0.998	Cu3As04 (s	0	0	Cl 17	0	0
Contrl C	0	Cu3AsS4 (s	0.0018996	0.0006326	к 19	0	0
Temp C	20	Cu5PeS4 (s	0.0234	0.0061162	Ca 20	0.0009291	0.0009476
Temp F	68	Cu5FeS4 (s	0	0	T1 22	0	0
Pres kPa	101.325	Cu6A12 (OH	0	0	Pe 26	0.2648169	0.1938475
Pres psis	14.695949	CuO*Fe203	0	0	Ni 28	0	0
Pres psig	• •	CuO*Fe203	0	•	Cu 29	0.2747857	0.1767914 🖕

Figure A-2: Flow rate and composition which are required for input stream

(3) Draw all the units and insert input and output streams. In this study, a FRL furnace is used as a primary smelting reactor (PSR) (Figure A-3).



Figure A-3: PSR Model in METSIM

Tenie	nte Dimer	sions	PI	hases React	ons	E	quil.	H	cat Ba	4 1	.09	ic C	ontrols	Labo	# Mate	alais	Reagents	Notes
Rea	tion							同情										Inser
1	H20(a)		1	H20(g)														5.0
1	ENAP6	(0)	+91	87 02(g)		=	4	NO	2(g))	1	5	502(0	;)	+550	H20	(g)	COR
1	Ganga(s	s) =	: 1	Ganga(de)												1.8	Cu/D
2	Cu6A12	(OH=	2	CO2(g)		24	H20	0 (g)	٠	5	A120	3(s)	+ 6	Cu20	(s)	• 3	
1	Zn6A12	(OH=	1	CO5(d)		12	H50	0(g)	٠	6	Zn0 (s)	+ 1	A120	3(s)		Copy
5	Ag 20 (s) =	: 1	05(d)	•	4	Ag	(s)										Contraction of the second
4	KFe3(S	54)=	8	502(g)		7	02	(g)		+1	2	H20 ((g)	• 2	K20(s)	+1	Paste
4	NaFe3(504:	: 2	Na 20(e)	•	8	50	2(g)	•	7	02(g)	+12	H20(g)	+1	Clea
1	Fe3(As	04):	: 1	As205(s)	+	3	Fe	0(H)(s))							6	
2	CaSOBH	4(s:	: 2	CaO(s)	•	2	50	2(g)	•	1	02(9	1)	• •	H50(g)		+ Up
2	Ca504(s):	: 2	CaO(s)	•	1	02	(g)		*	2	5020	(g)				3	* Dow
1	Ca 3As 2	06(:	: 3	CaO(s)	.*	1	As	203	(s)								- 2	
1	MgCO3(s) :	- 1	MgO(P)(s	:)+	1	co	2(g)								16	Sort
2	ZnS04(s):	: 2	502(g)	•	1	02	(g)		*	2	Znot	(s)				1	
2	CuFe02	(s):	- 1	Cu20(s)		1	Fe	203	(s)									Uno
4	CuS(s)		= 2	Cu25(s)	1	1	52	(g)									3	Save
4	CuFeS2	(C):	= 2	Cu25(s)		4	Fe	SIT)(s	•	1	52(0	12				8	A CHARTER
4	CuFe52	(s):	= 2	Cu2S(s)		4	re	5(1)(\$	•	1	5210					6	OK
4	cusses	4(5)	=10	Cu25(s)		1	10	5(1	JUS	۰.	1	5219						
4	Cu13(A	SSD	- 4	As253(s.		1	50	253	(s)	• 4		cuzs	sisi	•	5219	,		Canc
2	Cu3Ass	4(5	= 3	Cu2S(s)	1	1	AS	253	(5)	•	1	52(0	1)					
1	Cu504x	5H2	= 1	cusoats.	1	5	HZ	org									-	

Figure A-4: Input reaction and extent of reaction in PSR reactor

(4) Define chemical reactions together with the reaction sequence and assign the degree of reactions (Figure A-4).

(5) Assign the distribution coefficients of each phase for all process streams (Figure A-5). For example, 20% of matte contaminates in slag stream. The total number of phases that can be specified is 8 as shown in Table A-1. The chemical species such as pure chemicals, minerals or elements, can exist in one or more of eight phases.

	DUST LO	331		
DL	10	* Unveace	d solids bypass,	, <1 fraction, §1 tonnage
	DISTRIB	UTION OF	PHASES TO	OUTLET STREAMS:
	Motal	Slag	Olfgas	
PD	0.005	0.005	0.99	* GC Gas
	0	0	11	* LC Liquid
	0	0	1	# SC Solids
	0	1	0	* M3 Slag
	0	1	0	* M2 Maze
	0.87	0.13	0	* M1 Meral

Figure A-5: Input distribution coefficient in PSR reactor

Component	Phase	Phase No.	Types of components
Solid Components	SC		Includes SI & SO
Solid Inorganic	SI	1	Minerals, Salts
Solid Organic	SO	2	Coal, Resin, Carbon
Fluid Components	FC		Includes LC & GC
			Includes LI, LO, M1, M2 &
Liquid Components	LC		M3
Liquids Inorganic	LI	3	Water, Acids, Dissolved Salts
Liquid Organic	LO	4	Fuel, Kerosene, Organics
Molten 1	MI	5	Molten Metals, Speiss
Molten 2	M2	6	Molten Sulfides, Halides
Molten 3	M3	7	Molten Oxides, Slags
Gaseous components	GC	8	Air, Gaseous, Metal Vapors

Table A-1: All phases in a PRS model

METSIM carries out mass balance calculations by tracking material flows. The phases are identified by their phase number. Prior to using any of the component input routines, a comprehensive list of the components is first prepared. Components are assigned to the phases in which they are present.

(6). Add all information required in each tab. It should be noted that the data of reactions and the extent of reactions are required as the input in METSIM. A modeler should know the correct reactions in the PSR and their extent of reactions (either in an exact value or in an expression) in order to obtain a appropriate reactor model.

APPENDIX B

REACTIONS IN A PRIMARY SMELTING REACTOR

The reactions in a primary smelting reactor and their extent of the reactions are shown as follows;

No.	Reaction			Extent
1	H ₂ O(aq)	\Rightarrow	H ₂ O(g)	1
2	l Gangue(s)	\Rightarrow	lGangue(sl)	1
3	2Cu ₆ Al ₂ (OH)(s)	\Rightarrow	$1CO_2(g) + 12H_2O(g) + 6ZnO(s)$	
			$+ Al_2O_3(s)$	1
4	$Zn_6Al_{12}(OH)(s)$	\Rightarrow	$1CO_2(g) + 12H_2O(g) + 6ZnO(s)$	
			$+ Al_2O_3(s)$	1
5	$2Ag_2O(s)$	\Rightarrow	$1O_2(g) + 4 Ag(s)$	0.5
6	4KFe ₃ (SO ₄)	\Rightarrow	$8SO_2(g) + 7O_2(g) + 12H_2O(g) +$	
			$2K_2O(s) + 12FeO(s)$	1
7	4NaFe ₃ (SO ₄)	\Rightarrow	$2Na_20(e) + 8SO_2(g) + 7O_2(g) +$	
			$12H_2O(g) + 12FeO(sl)$	1
8	$1 \operatorname{Fe}_3(\operatorname{AsO}_4)$	\Rightarrow	$1As_2O_5(s) + 3FeO(s)$	1
9	$2CaSO_6H_4(s)$	\Rightarrow	$2CaO(s) + 2SO_2(g) + O_2(g) + 4H_2O(g)$	1
10	2CaSO ₄ (s)	\Rightarrow	$2CaO(s) + 1O_2(g) + 2SO_2(g)$	1
11	Ca ₃ As ₂ O	\Rightarrow	$3CaO(s) + 1As_2O_3(s)$	1
12	MgCO ₃ (s)	\Rightarrow	$1MgO(s) + 1CO_2(g)$	1
13	2ZnSO ₄ (s)	\Rightarrow	$2SO_2(g) + 1O_2(g) + 2ZnO(s)$	1
14	2CuFeO ₂ (s)	\Rightarrow	$1Cu_2O(s) + 1Fe_2O_3(s)$	1
15	4CuS(s)	\Rightarrow	$2Cu_2S(s) + 1S_2(g)$	1
16	$4CuFeS_2(s)$	\Rightarrow	$2Cu_2S(s) + 4FeS(s) + 1S_2(g)$	1
17	4Cu ₅ FeS ₄ (s)	\Rightarrow	$10Cu_2S(s) + 4FeS(s) + 1S_2(g)$	1

No.	Reaction			Extent
18	$2Cu_3AsS_4(s)$	\Rightarrow	$3Cu_2S(s) + 1As_2S_3(s) + 1S_2(g)$	1
19	1CuSO ₄ .5H ₂ O(s)	\Rightarrow	$ICuSO_4(s) + 5H_2O(g)$	1
20	4CuSO ₄ (s)	\Rightarrow	$4SO_2(g) + 3O_2(g) + 2Cu_2O(s)$	1
21	$2\text{FeS}_2(s)$	\Rightarrow	$2\text{FeS}(s) + 1\text{S}_2(g)$	1
22	$1Fe_2As_4O_{12}(s)$	\Rightarrow	$2As_2O_5(s) + 2FeO(w)(s)$	1
23	2FeAsO ₄ (s)	\Rightarrow	$As_2O_5(s) + 1Fe_2O_3(s)$	1
24	$1Fe_2(SO_4)_3$	\Rightarrow	$3SO_2(g) + 2O_2(g) + 2FeO(w)(s)$	1
25	2FeSO ₄ (s)	\Rightarrow	$1O_2(g) + 2SO_2(g) + 2FeO(w)(s)$	1
26	$4Cu(s) + 1O_2(g)$	\Rightarrow	2Cu ₂ O(s)	1
27	$1Cu_2O(s) + 1FeS(T)(s)$	\Rightarrow	$1Cu_2S(s) + 1FeO(sl)$	0.896
28	$1Cu_2O(e) + FeS(T)(s)$	\Rightarrow	$1Cu_2S(s) + 1FeO(sl)$	l
29	$2Na_3AsO_3$ (s)	\Rightarrow	$1 As_2O_3(s) + 3Na_2O(s)$	I
30	1Bi ₂ O ₃ (s)	\Rightarrow	$1Bi_2O_3(e)$	0.995
31	1Sb ₂ O ₃ (s)	\Rightarrow	1Sb ₂ O ₃ (e)	0.995
32	lAg (s)	\Rightarrow	lAg (m)	0.995
33	lAu (s)	\Rightarrow	lAu (m)	0.995
34	1Mo(s)	\Rightarrow	1Mo(m)	0.995
35	lPbS(G)(s)	\Rightarrow	1PbS(m)	0.995
36	1PbO(L)(s)	\Rightarrow	1PbO(e)	0.995
37	$PbSO_4(A)(s)$	\Rightarrow	1PbSO ₄ (m)	0.995
38	$1 Na_2 O(s)$	\Rightarrow	$1 \operatorname{Na}_2 \operatorname{O}_9(e)$	0.995
39	1CaSiO ₃ (s)	\Rightarrow	1CaSiO ₃ (e)	0.995
40	CaAl ₂ SiO ₂ O ₃ (s)	\Rightarrow	$CaAl_2Si_2O_3(e)$	0.995
41	$1 \text{Al}_2 \text{O}_3(s)$	\Rightarrow	$1 Al_2O_3(sl)$	0.995
42	$1Al_2SiO_5(s)$	\Rightarrow	$1Al_2SiO_5(e)$	0.995
43	$1Ca_2Fe_2O_5(s)$	\Rightarrow	$1Ca_2Fe_2O_5(e)$	0.995
44	1MgSiO ₂ (s)	\Rightarrow	1MgSiO ₃ (sl)	0.995
45	$1Na_2O(s)$	\Rightarrow	$1 Na_2 O(e)$	0.995
46	1Na ₂ SiO ₃ (s)	\Rightarrow	$1Na_2SiO_3(e)$	0.995
47	$1Cu_2O(s)$	\Rightarrow	$1Cu_2O(e)$	0.995
48	lFeO(s)	\Rightarrow	1FeO (de)	0.995

No.	Reaction			Extent
49	1Fe ₃ O ₄ (s)	\Rightarrow	$1 \operatorname{Fe}_3 \operatorname{O}_4 (\operatorname{de})$	0.995
50	$1Fe_2SiO_4(s)$	\Rightarrow	$1 \operatorname{Fe}_2 \operatorname{SiO}_4(e)$	0.995
51	$1As_2O_3(s)$	\Rightarrow	$1As_2O_3(e)$	0.995
52	$1As_2O_3(s)$	\Rightarrow	$1 \text{As}_2 \text{O}_3(e)$	0.995
53	$1As_2O_5(s)$	\Rightarrow	$1 \text{As}_2 \text{O}_5(e)$	0.995
54	$l K_2 O(s)$	\Rightarrow	$1 K_2 O(e)$	1
55	1ZnS(s)	\Rightarrow	lZnS(s)(m)	1
56	lZnO(s)	\Rightarrow	1ZnO(sl)	0.995
57	$1 \text{TiO}_2(s)$	\Rightarrow	lTiO ₂ (m)	0.995
58	1CaO (s) + 1 SiO ₂ (s)	\Rightarrow	1CaSi ₂ O ₃ (e)	0.995
59	$1Al_2O_3(s) + 1CaSiO_3(e)$	\Rightarrow	1SiO ₂ (s) + 1CaAl ₂ O ₄ (s)	0.995
60	$1MgO(P)(s) + 1SiO_2(s)$	\Rightarrow	1MgSiO ₃ (sl)	0.995
61	1Na ₂ O(e) + 1 SiO ₂ (s)	\Rightarrow	1Na ₂ SiO ₃ (e)	0.995
62	1CuO(s)	\Rightarrow	1CuO (e)	0.995
63	3CuO(s) + 1FeS(T)(s)	\Rightarrow	3Cu(m) + 1FeO(sl)	
			+ 1SO ₂ (g)	1
64	$1PbSO_4(m) + 1PbS(m)$	\Rightarrow	$2Pb(m) + 2SO_2(g)$	1
65	$2PbS(m) + 3O_2(g)$	\Rightarrow	$2SO_2(g) + 2PbO(e)$	0.995
66	$1MoS_2(s) + 3O_2(g)$	\Rightarrow	$1 \text{MoO}_2(s) + 2 \text{SO}_2(g)$	0.995
67	$2MoO_2(s) + 1O_2(g)$	\Rightarrow	2MoO ₃ (g)	1
68	$2Sb_2S_3(s) + 9O_2(g)$	\Rightarrow	$6\mathrm{SO}_2(g) + 2\mathrm{Sb}_2\mathrm{O}_3(e)$	0.995
69	4Sb(s) + 3 O ₂ (g)	\Rightarrow	$2Sb_2O_3(m)$	0.995
70	$1Ag_2S(s) + 1O_2(g)$	\Rightarrow	$2Ag(m) + 1SO_2(g)$	0.995
71	$2Pb(s) + 1O_2(g)$	\Rightarrow	2PbO(e)	0.995
72	$2Bi_2S_3(s) + 9O_2(g)$	\Rightarrow	$6\mathrm{SO}_2(g) + 2\mathrm{Bi}_2\mathrm{O}_3(e)$	0.995
73	$2Zn(s) + 1O_2(g)$	\Rightarrow	2ZnO (de)	0.995
74	$4Cu(s) + 1O_2(g)$	\Rightarrow	$2Cu_2O(e)$	0.995
75	$4As(s) + 3O_2(g)$	\Rightarrow	$2\operatorname{Bi}(g) + 3\operatorname{SO}_2(g)$	0.995
76	$1Bi_2S_3(s) + 3O2(g)$	\Rightarrow	$2\mathrm{Bi}(\mathrm{g}) + 3\mathrm{SO}_2(\mathrm{g})$	1
77	$1C(s) + 1O_2(g)$	\Rightarrow	1CO ₂ (g)	1
78	$1S_2(g) + 2O_2(g)$	\Rightarrow	2SO ₂ (g)	1

No.	Reaction			Extent
79	$1S_2(g) + 2O_2(g)$	\Rightarrow	2SO ₂ (g)	1
80	$1Cu_2S(s)$	\Rightarrow	$1Cu_2S(m)$	0.995
81	1FeS(s)	\Rightarrow	1FeS(m)	0.995
82	$3\text{FeS}(m) + 5\text{O}_2(g)$	\Rightarrow	$1Fe_{3}O_{4}(m) + 3SO_{2}(g)$	0.010
83	$2As_2S_3(m) + 9O_2(g)$	\Rightarrow	$6SO_2(g) + 2As_2O_3(e)$	0.796
84	$2As_2O_3(e)$	\Rightarrow	$1As_4O_6(g)$	0.850
85	$2ZnS(s)(m) + 3O_2(g)$	\Rightarrow	$2SO_2(g) + 2ZnO(g)$	0.924
86	1ZnO(sl)	\Rightarrow	lZnO(g)	1
87	2ZnO(g)	\Rightarrow	2ZnO(sl)	0.322
88	$2\text{FeS}(m) + 3\text{O}_2(g)$	\Rightarrow	$2FeO(de) + 2SO_2(g)$	0.914
89	$1Fe_2O_3(s) + 1FeO(sl)$	\Rightarrow	$1Fe_3O_4(sl)$	1
90	1SiO ₂ (s)	⇒	1SiO ₂ (sl)	0.995
91	$2FeO(sl) + 1SiO_2(sl)$	\Rightarrow	$1Fe_2SiO_4(e)$	0.770
92	6 FeO(sl) + $1O_2(g)$	\Rightarrow	$2Fe_3O_4(sl)$	1
93	$2CuS(s) + 3O_2(g)$	\Rightarrow	$2Cu_2O(s) + 2SO_2(g)$	1
94	$3 \text{FeS}(s) + 5 \text{O}_2(g)$	\Rightarrow	$1Fe_3O_4(s) + 3SO_2(g)$	1
95	$2Ag_2S(s) + 3O_2(g)$	\Rightarrow	$2Ag_2O(s) + 2SO_2(g)$	1
96	$2As_2S_3(s) + 9O_2(g)$	\Rightarrow	$2As_2O_3(s) + 6SO_2(g)$	1
97	$2Sb_2S_3(s)+9O_2(g)$	\Rightarrow	$2Sb_2O_3(s) + 6SO_2(g)$	1
98	$2ZnS(s)(m) + 3O_2(g)$	\Rightarrow	$2ZnO(s) + 2SO_2(g)$	1
99	l Mo(m)	\Rightarrow	1Mo(e)	1

For the calculation, METSIM follows the order of reactions from number 1 to 99 and the rate of reactions is fixed by the extent of the reaction. It is noted that in this study, the extent of all reactions except the reaction no. 88 and 91 is specified following the technical data obtained form other smelters that uses the same Teniente converter technology. The extent of the reaction no. 88 and 91 are estimated from actual plant data.

VITA

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