Pyrometallurgical Process Simulations using CALPHAD Thermodynamic Databases

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ABSTRACT

In order to utilize the powerful thermodynamic databases for process simulations, a concept called Effective Equilibrium Reaction Zone (EERZ) was introduced to couple thermodynamic database calculations and reaction kinetics. Using the EERZ concept, many process simulation models for steelmaking processes have been developed within the FactSage steelmaking consortium. After validation of the simulation results by comparing with plant data, the simulation models have been applied to improve plant operations. Several success stories of the improvement of real steelmaking operations are shared. A new user-friendly FactProSim software developed for building process simulations is introduced.

INTRODUCTION

In pyrometallurgical processes, changes in phase amounts and their composition are mainly controlled by the thermodynamics of the system, and reaction kinetics. In order to produce liquid metal in industrial scale, for example, the complex chemical reaction thermodynamics and kinetics between liquid metal and other phases (solid and liquid slag, sulfide, salt flux and inclusion, refractories, and gas) should be considered. Most industrial processes involve multicomponent and multiphase systems, so even the thermodynamics of the system itself is difficult to understand.

Thermodynamic databases based on the CALPHAD (CALculation of PHAse Diagram) approach have been developed since 1960. Several commercial thermodynamic software packages containing extensive thermodynamic databases have been available since 1990 and widely used in both academic research and for industrial applications. One of the most well-known packages in particular for pyrometallurgical applications is FactSage software and database (www.factsage.com) (Bale et al., 2016). FactSage contains many critically evaluated and optimized thermodynamic databases for oxide, sulfide, salt, alloys, etc., and allows to calculate complex multicomponent thermodynamic equilibrium involving solids, liquids and gas up to 40 elements. Although the thermodynamic calculations give good insight into chemical reactions at reaction interface and tell the direction and the final equilibrium state of overall reactions in the system, the variations in amount, composition and temperature of stable phases cannot be directly calculated from thermodynamic calculations.

In metal production and metal refining processes, the precise control of impurities and alloying elements in liquid metal and alloy is important. In classical kinetic studies, a simple chemical reaction involving a target impurity or alloying element was usually considered to solve the flux equations. However, in order to simulate an industrial scale process, the chemical reactions of all components in liquid metal and other existing phases should be simultaneously considered. The reaction kinetics should also vary with process parameters and temperature. The temperature variations of all phases

should also be calculated considering the chemical reaction heats, heating by arcing, and heat loss during the process.

We (Van Ende et al., 2011) proposed the "Effective Equilibrium Reaction Zone (EERZ) Model" to couple the mass transfer kinetics with thermodynamic calculations based on CALPHAD-type databases to simulate high temperature materials processes. In the EERZ model, a complex process is divided into a finite number of reaction zones in which equilibrium conditions are calculated. The reaction kinetic mechanism involving chemical reaction at the interface can be considered with the EERZ model, and heat evolutions can be considered simultaneously to track the temperature variation of each phase in the process. This model is well accepted and used for many process simulations in the recent years. Some of highlight works include the simulations by Van Ende (2022), Moosavi-Khoonsari et al. (2022), Van Ende and Jung (2015), Van Ende et al. (2011), Paek and Jung (2015), Van Ende and Jung (2017), Van Ende et al.(2018), Van Ende and Jung (2020), Van Ende and Jung (2014), Van Ende and Jung (2019), Kumar et al.(2019), Shin and Park (2020), Coetsee et al.(2023), Mason et al.(2020).

In this study, the concept of the EERZ model and process simulation models for steelmaking developed based on the EERZ model are overviewed. A couple of success stories for the implementation of such process models to improve the real steelmaking process are shared. In addition, the new FactProSim software recently developed to assist in building process simulations is introduced.

CRITICAL WEAKNESS OF AI BASED MODEL FOR DIGITAL TWINS

Recently, artificial intelligence (AI) based predictions have been widely used for industrial process improvement. For the applications of the AI-based model, numerous sensors have been installed in pyrometallurgical processes to collect plant operation data. Although the sensors can collect a good amount of valuable data, the maintenance of sensors at high temperatures and reducing the noise in data constitute the main problems in high temperature processes. In addition, not only the total inputs but also the scheduling of input addition can significantly affect the quality (chemistry and temperature) of the final products. Therefore, it is rather difficult to implement an AI-based process model in pyrometallurgical processes.

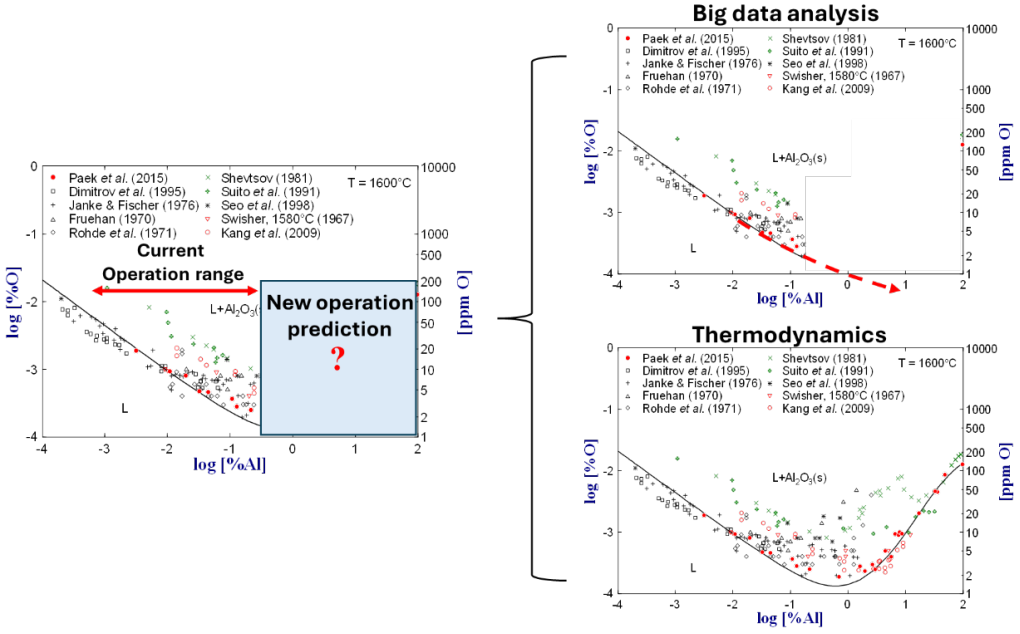


FIG 1 – Al deoxidation in liquid steel: Comparison of AI model based on big data analysis and thermodynamics-based model.

The AI-based process model delivers the benefit of an accurate interpolation based on the available data. However, one of the critical weaknesses of AI-based model is the extrapolation capability. For example, the deoxidation of liquid steel is very important in the steelmaking process to reduce the amount of oxide inclusions in the final products. As shown in Fig. 1, an AI-based model trained using

the current operation data would predict a decreasing oxygen content with increasing Al content even above 1 wt.% Al. But thermodynamics predict that the oxygen content increases again above 1 wt.% Al in liquid steel. That is, a big data-based Al model can significantly mislead the oxygen prediction, but a thermodynamic-based model can improve the prediction accuracy at process conditions which have not been operated before. In particular, the process models based on thermodynamics and reaction kinetics can even be used as Digital Twins for the current and future plant operations.

OVERVIEW OF THE EERZ MODEL

Recently, we (Van Ende et al., 2011) proposed the "Effective Equilibrium Reaction Zone (EERZ) Model" to couple mass transfer kinetics with thermodynamic databases to simulate high temperature materials processes. In the EERZ model, a complex process is divided into a finite number of reaction zones in which equilibrium is calculated. For example, let's consider a slag and liquid steel reaction, as shown in Fig. 2. The interfacial reaction zone size can be determined by the mass transfer coefficient which is influenced by the operation conditions. So, at each given time interval, the mass transfer coefficient is calculated using the operation conditions, and the effective volumes of steel (V2 in Fig. 2) and slag (V3) participating in the interfacial reaction can be determined using the mass transfer coefficient of steel and slag, respectively. FactSage thermodynamic database can be used to calculate the interfacial equilibrium between V2 and V3. The reaction products after the interface reaction can be homogenized with remaining volumes of steel (V1) and slag (V4). If we run the calculation iteratively reflecting the change in the operation conditions, the evolution of the steel and slag composition and mass can be calculated with time.

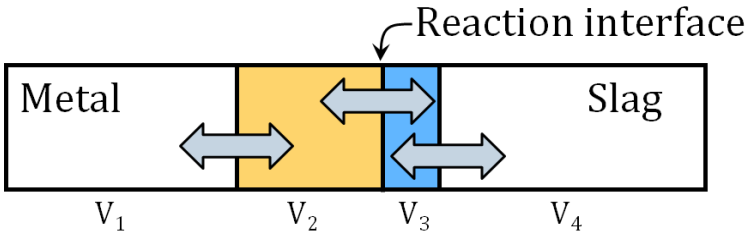


FIG 2 - Schematic diagram of the EERZ model: for the reaction between slag and liquid metal (Jung and Van Ende, 2020)

Using the thermodynamic database, the enthalpy change caused by the interface reaction can also be calculated, which can be used to predict the temperature profile of steel and slag. The heat loss and heat addition can also be included in the simulation. For example, we can add a certain amount of heat to liquid metal and slag due to arcing energy, which can increase the temperature of liquid metal and slag. As the heat capacities of liquid metal and slag are different, the temperatures of these phases can have very different values. Of course, heat transfer between liquid metal and slag can be considered too.

In steelmaking, complex reactions between slag / molten steel / inclusion / refractory / gas / input materials (fluxes, alloys, scraps, etc.) should be considered. In fact, to accurately analyze the thermodynamics between these reactions, kinetic concepts such as reaction efficiency, material mass, and time of the input material additions must be considered. In the EERZ model, the reaction mechanism should be first defined based on literature laboratory study or plant sampling results.

For example, the change in the chemical composition of liquid steel and molten slag can be mainly determined by process kinetics at the slag/metal interface. In steelmaking process, the chemical reactions at reaction interface are usually fast enough so that reaction rates are mainly controlled by mass transfer of species to and/or from the reaction interface. If the interfacial reaction is the first order reaction, the change in composition at the interface can be calculated by:

$$J_i = k_i \, (\%C_{i,\,bulk} - \%C_{i,\,interface}) \qquad (1)$$

where J_i and k_i are flux of i and mass transfer coefficient of i, respectively, and $\%C_i$, bulk and $\%C_i$, interface are concentration of i species at bulk and interface, respectively. That is, J_i is the flux of i species which can be consumed or gained by the interfacial reaction. $\%C_i$, interface can be determined by thermodynamic equilibrium at the interface. For nitrogen removal process involving

liquid steel and gas interface, the adsorption of surface active elements like sulfur and oxygen can influence to the equilibration at the interface, which can be taken into account in the description of $\%C_i$, interface. If k_i of all species in the given solution are the same values regardless of species, the amount of each solution participating in chemical reaction at the interface can be simply derived as follows:

$$RW_{solution} = (k\rho A)_{solution}\,\Delta t \qquad (2)$$

where RW, k and ρ are reacting amount, overall mass transfer coefficient, and density of given solution, respectively, A is the area of reaction interface, and Δt is time step of reaction.

That is, if we consider that the interfacial reaction between slag and liquid metal, we can put the amount of reacting mass of slag ($(k\rho A)_{slag}\,\Delta t$) and liquid metal ($(k\rho A)_{metal}\,\Delta t$) at given time into the chemical equilibrium reaction. These slag and metal amounts can be assigned as effective reaction zone volumes at the interfacial reaction in Fig. 2. This is the key concept of the EERZ model. k_{slag} and k_{metal} are the key parameters which can be varied with temperature, stirring energy, etc., and can be determined from the plant operation data.

The overall mass transfer coefficient k in Eq. (2) can vary with operation condition. For example, when the stirring energy of liquid metal becomes larger, k_{metal} becomes higher, which increases in general the reaction rate at the slag/metal interface. The k_{slag} can be also largely influenced by the viscosity of slag. The k value can be obtained from literature, or can be directly determined by the plant sampling data. Depending on the k values of slag and liquid metal, the rate determining step can be identified automatically in the calculations.

PROCESS SIMULATION MODELS: FATSAGE STEELMAKING CONSORTIUM

Using the EERZ concept, we have developed many process simulation models in collaboration with our industrial partners of the FactSage Steelmaking Consortium. These include steelmaking processes simulation models for Electrical Arc Furnace (EAF) (Van Ende, 2022), hot metal treatment (powder injection) (Moosavi-Khoonsari et al, 2022), Basic Oxygen Furnace (BOF) (Van Ende and Jung, 2015), RH Degasser (Van Ende et al, 2011), Vacuum Tank Degasser (VTD) (Paek and Jung, 2015), Ladle Furnace (LF) (Van Ende and Jung, 2017, Van Ende et al., 2018), Tundish (Van Ende and Jung, 2020), Continuous Casting (Van Ende and Jung, 2014), and Argon Oxygen Decarburization (VOD) (Van Ende and Jung, 2019).

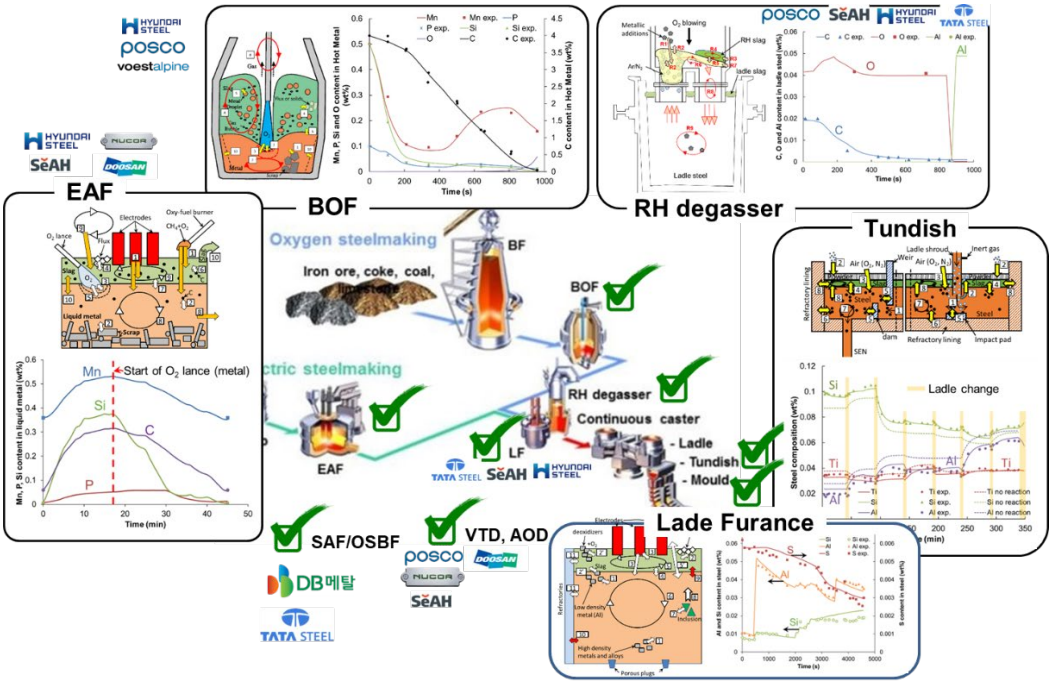


Fig. 3 – Overview of the process simulation models (simulators) developed within the FactSage Steelmaking Consortium.

Originally, the process simulation models were developed using the FactSage macro processing code to connect thermodynamic calculations, but all of them were converted to ChemApp (GTT Tech., 2024) based standalone programs to significantly improve the simulation speed. Most of the process simulations can be completed within 1/4 to 1/10 of real process operation time.

As shown in Fig. 3, each process model has been tested using real plant data from several industrial members. When the model is applied to plant simulation, small tunings in the model parameters like mass transfer coefficient *k* and heat loss are usually necessary to more accurately reproduce the plant sampling data. The *k* and heat loss (heat transfer coefficient) parameters are mainly dependent on stirring condition, slag viscosity, reactor dimension, etc. The influences of steel composition and additive schedule to the chemistries and temperatures of liquid steel, slag, inclusion and gas can be well predicted by EERZ model based on accurate thermodynamic database.

To validate and improve the model predictions, many sampling data of steel, slag and inclusions are necessary and the data and simulation results are analysed together with industrial partners. After the validation of model simulations, the process models can be applied to improve the plant operations. For example, the scheduling of flux addition, alloy addition and gas injection can be varied in the simulations to investigate their influences to the chemistry and temperature of liquid steel and slag. By employing the simulations, the current plant operation can be further optimized to improve the productivity and quality of the products and the future production scenarios can be designed virtually.

Some of the success stories by our industrial partners are presented below.

BOF process model

Fig. 4 shows the schematic diagram of BOF process simulation model. In the BOF model, ten reaction zones are considered. For example, the semi-empirical drop generation model is incorporated in the present simulation to calculate the droplet generation rate depending on the process conditions. The decarburization and oxidation of liquid steel, and reduction of Fe oxide in slag at hot spot and emulsion zone are calculated. A numerical simulation equation for scrap melting is taken into account. The dissolution rate of fluxes such as lime, dolomite, hematite, and other slag making flux is calculated considering thermodynamic driving force, temperature and slag viscosity. Other empirical parameters for interfacial reactions are fixed based on plant sampling data. In every time step, all these ten interfacial thermodynamic calculations are performed with the FactSage thermodynamic database, and heat loss/post combustion of the BOF is also considered for the accurate temperature calculations of slag and liquid metal.

- R1 : Scrap melting in metal bath and heat gain/loss
- R2: Burning of hot metal surface (O_2/metal reaction for FeO formation)
- R3: Hot spot (O_2/metal reaction for direct de-C)
- R4: Flux dissolution in slag
- R5: Metal droplet/slag reaction
- R6: Bulk metal/slag reaction
- R7: Bulk metal homogenization
- R8: Slag homogenization + post-combustion of the exhaust gas
- R9: Heat exchange between slag and metal
- R10: Mixing between active and dead zones in hot metal

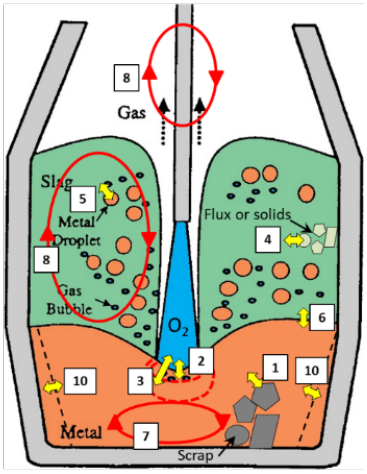


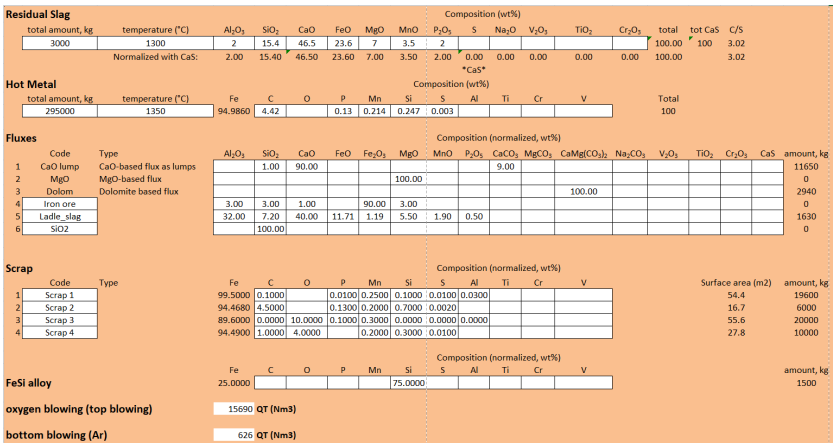
FIG 4 – Overview of the reaction zones for BOF process simulation model (Van Ende and Jung, 2015).

BOF process model was applied to optimize the process and test the possible operation scenario of low quality hot metal. The main purpose of BOF is the decarburization and dephosphorization of hot metal to produce liquid steel. Due to the ever-decreasing availability of high quality BF (blast furnace) grade iron ores, many steel producers are looking alternative iron ores. For example, high P_2O_5 containing iron ore is one possibility. In order to evaluate whether it is possible to economically

produce low P content liquid steel in BOF process or not, virtual operation patterns were studied with the BOF process model and operation cost could be calculated.

Fig. 5 shows the BOF simulation results of hot metals containing different initial P content. The standard BOF operation condition is as follows (see the details in Fig. 5 (a)):

- Scraps: 4 kinds of scraps with 45.6 ton in total
- Hot metal: 295 ton of hot metal (Fe-4.42C-0.214Mn-0.247Si-0.13P-0.003S in wt.%) at 1350 °C
- Residual slag: 3 ton of the end of BOF slag at 1300 °C
- FeSi: 1.5 ton of Fe-Si (75%Si)
- Flux: 11.65 ton of lump CaO, 2.94 ton of dolomite, and 1.63 ton of ladle slag
- Gas blowing: 15,690 Nm^3 of oxygen top blowing, and 626 Nm^3 Ar bottom bubbling
- Double slag operation: 20 min of total blowing time, and 40% of slag discharged after 6 min



Residual Slag

total amount, kg	temperature (°C)	Al_2O_3	SiO_2	CaO	FeO	MgO	MnO	P_2O_5	S	Na_2O	V_2O_3	TiO_2	Cr_2O_3	total	tot CaS	C/S
3000	1300	2	15.4	46.5	23.6	7	3.5	2						100.00	100	3.02
	Normalized with CaS:	2.00	15.40	46.50	23.60	7.00	3.50	2.00	0.00	0.00	0.00	0.00	0.00	100.00		3.02
									CaS							

Hot Metal

total amount, kg	temperature (°C)	Fe	C	O	P	Mn	Si	S	Al	Ti	Cr	V	Total
295000	1350	94.9860	4.42		0.13	0.214	0.247	0.003					100

Fluxes

	Code	Type	Al_2O_3	SiO_2	CaO	FeO	Fe_2O_3	MgO	MnO	P_2O_5	$CaCO_3$	$MgCO_3$	$CaMg(CO_3)_2$	Na_2CO_3	V_2O_3	TiO_2	Cr_2O_3	CaS	amount, kg
1	CaO lump	CaO-based flux as lumps		1.00	90.00						9.00								11650
2	MgO	MgO-based flux						100.00											0
3	Dolom	Dolomite based flux											100.00						2940
4	Iron ore		3.00	3.00	1.00		90.00	3.00											0
5	Ladle_slag		32.00	7.20	40.00	11.71	1.19	5.50	1.90	0.50									1630
6	SiO2			100.00															0

Scrap

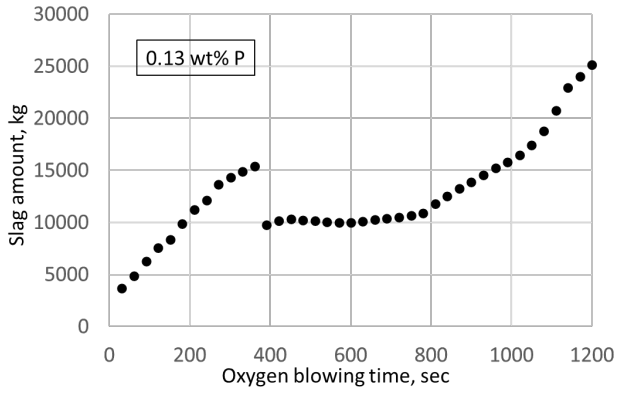
	Code	Type	Fe	C	O	P	Mn	Si	S	Al	Ti	Cr	V	Surface area (m2)	amount, kg
1	Scrap 1		99.5000	0.1000		0.0100	0.2500	0.1000	0.0100	0.0300				54.4	19600
2	Scrap 2		94.4680	4.5000		0.1300	0.2000	0.7000	0.0020					16.7	6000
3	Scrap 3		89.6000	0.0000	10.0000	0.1000	0.3000	0.0000	0.0000	0.0000				55.6	20000
4	Scrap 4		94.4900	1.0000	4.0000		0.2000	0.3000	0.0100					27.8	10000

	Fe	C	O	P	Mn	Si	S	Al	Ti	Cr	V	amount, kg
FeSi alloy	25.0000					75.0000						1500

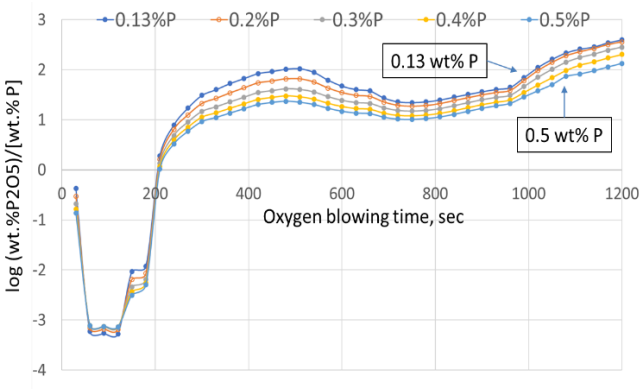
oxygen blowing (top blowing) 15690 QT (Nm3)

bottom blowing (Ar) 626 QT (Nm3)

(a)



(b)



(c)

FIG 5 – BOF process simulation input and simulated results: (a) Input and overall operation condition, (b) slag amount in BOF, and (c) phosphorus distribution depending on the initial P content in hot metal.

In the simulations, only the initial P content in hot metal was varied from 0.13 to 0.5 wt.% without changing any other operation conditions. Certainly the increasing P content in hot metal results in much lower phosphorus distribution ($Lp = (\%P_2O_5)_{slag}/[wt\%P]_{metal}$) in the end of BOF process: Lp = 396 for 0.13 wt.% P to 135 for 0.5 wt.% P hot metal. According to the simulations, the final P content in steel can be changed from 72 wt.ppm for 0.13 wt.% P to 817 wt.ppm for 0.5 wt.% P hot metal. Of course, the operation condition in Fig. 5 is not optimized for each specific hot metal condition. This kind of simulation results can provide a plant operation team with the information whether a certain quality of liquid steel with low P can be still produced in BOF plant or not even when low quality hot metal is used, and if yes, how much operation cost can increase.

BOF simulation model was also used to analyse the slopping in BOF process. When excessive foam growth happens, it cannot be contained within the converter and flow down the outside of the converter. This phenomenon is the slopping. The model can calculate the CO generation rate,

undissolved solid flux, formation of Ca_2SiO_4, and chemistry and temperature of slag. Using the information, viscosity of slag and slag foaming index can be calculated, which can be used to evaluate the slopping in BOF operation. A dynamic BOF model was also developed to predict the final carbon and oxygen content and temperature of liquid steel for online motoring of the BOF process. Recently, many virtual BOF operation simulations for processing low carbon hot metals (2.5 ~ 3.5 wt.%) and operating low HMR (hot metal ratio: 70 to 80) have been carried out using the BOF model to more towards the carbon neutrality in steelmaking.

LF process model

The schematic diagram of the LF simulation model is presented in Fig. 6. In total,11 reaction zones are considered to describe LF process. The addition of ferro-alloy, shred Al and lump Al, and slag flux are considered. The overall mass transfer coefficient of liquid steel and slag are allowed to be changed by the stirring energy determined by Ar bubbling. Arcing can provide heat to liquid steel and slag, and also induce more chemical reaction between slag and liquid steel. Steel reoxidation due to open eye formation and formation of non-metallic inclusion are also taken into account in the model. At each time step, all equilibrium reactions at each reaction zone are performed using the FactSage thermodynamic database.

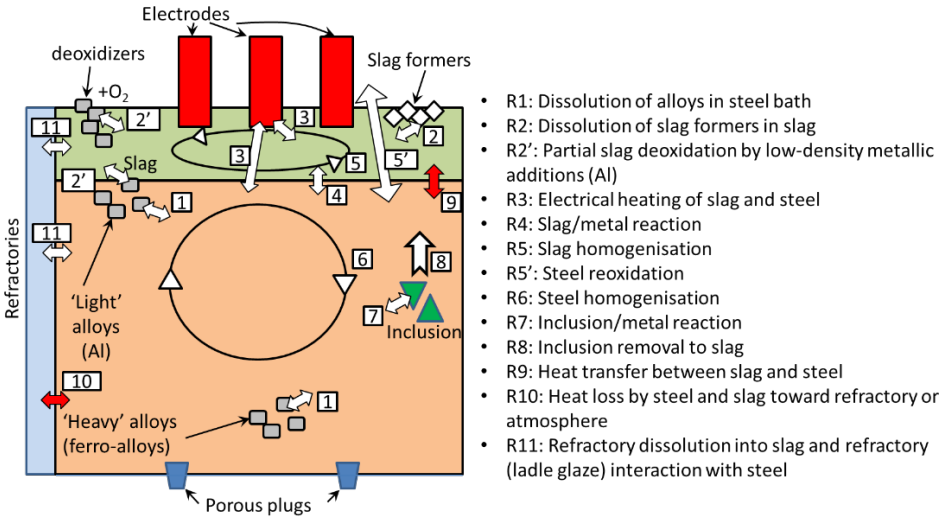
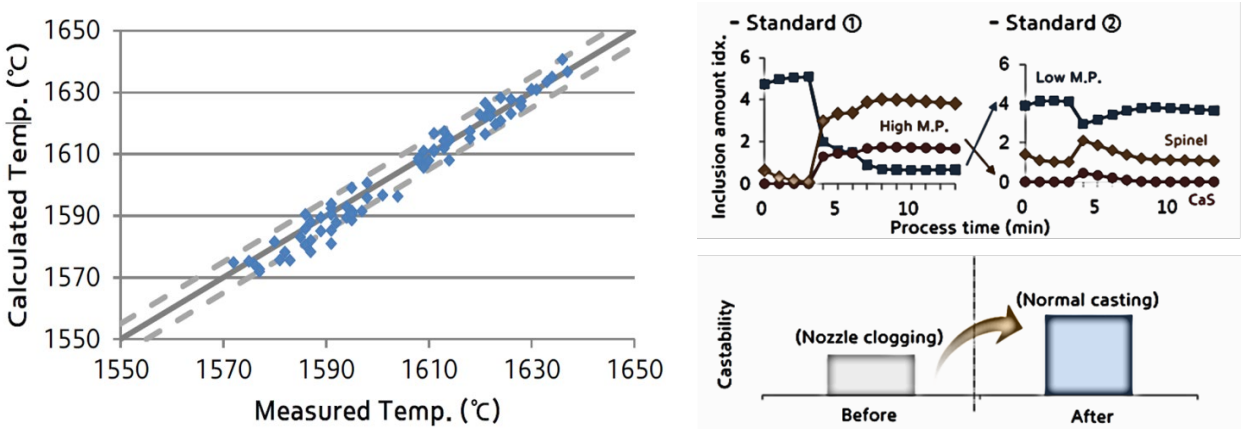


FIG 6 – Overview of the reaction zones for LF process simulation model (Van Ende and Jung, 2017).

LF is a secondary refining unit widely used in most of the steel plants for deoxidation, desulfurization, and alloying of liquid steel. In addition, the modification and removal of non-metallic inclusion can be carried out in LF. Accuracy in temperature prediction of liquid steel in LF process is presented in Fig. 7(a). In general, it is well predicted within ± 5 °C compared to the plant data. This is possible because the chemical reaction heat is well reflected from thermodynamic calculations. The precise control of temperature is important for the subsequent casting process. Therefore, when new high alloyed steel grades are developed, the process condition can be already well designed with LF simulation model. The modification of non-metallic inclusion can be also possible by changing the operation condition and flux. Fig 7 (b) shows a plant example of inclusion modification from high melting temperature inclusions to low melting temperature inclusions, which resulted in the improvement of steel castability. High melting temperature Al_2O_3 and $MgAl_2O_4$ spinel type inclusions can be modified by Ca injection to liquid inclusion. Instead of Ca injection, low quality ferro-alloy can be even employed to modify the inclusion as well, which can be well simulated by the LF simulation model.

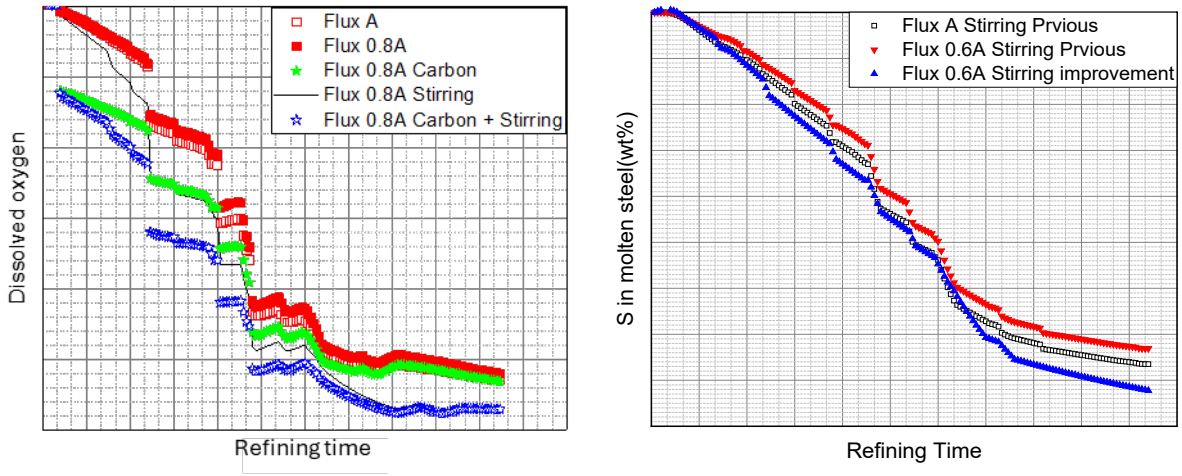
The complex process optimization to obtain ultra low sulfur and low oxygen content in liquid steel can be also performed using the LF process model. In particular, when a company produces a wide range of steel grades from low carbon steel to special steel in a single steelmaking line, the LF operation is even more tricky because the delay in LF refining operation can affect the operation schedule of the entire plant. Therefore, operators prefer to adopt a conservative operation schedule to reduce the risk of operation delay instead of producing the best quality steel. In order to change the standard operation procedure (SPO), many trials in the plant are required but usually not possible

in such a plant with a single steelmaking line. One of examples for the process optimization is presented in Fig. 8. Using the LF simulation model, flux addition and stirring condition for each specific steel grade were optimized to obtain higher desulfurization and higher deoxidation level beyond the existing level, while the refining time, electrical energy, and lime input amount were even reduced. These optimum operation conditions were applied to SPO in LF plant and contributed to improving the quality of steel as well as productivity. When new steel grades are ordered from clients, the plant engineers can use the LF process simulation to design the SPO to meet the specification of new steel too.



(a) (b)

FIG 7 – LF simulation results: (a) Accuracy of temperature prediction, and (b) non-metallic inclusion modification by process optimization and influence to castability.



(a) (b)

FIG 8 – LF simulation results: Variations of (a) oxygen content and (b) sulfur content in liquid steel depending on the operation conditions.

Online monitoring system

As the simulation speed is faster than the real operation, online process simulation is possible by receiving the inputs of simulation from HMI (Human Machine Interface) in plants. One of consortium members already tested online LF simulation and VTD simulation to monitor the plant operations and also compare the simulation results with the plant sampling data for a long period. Eventually, the reliability of simulation prediction is confirmed, significant reduction in operating cost will be achieved by replacing intermediate samplings with model predictions.

Generation of virtual data to assist big data analysis for AI based model

One of the critical weaknesses of AI model based on big data is the extrapolation capability. Using the simulation model, it is possible to generate virtual plant data for the operation conditions which are outside of the current operation range. By combining these virtual plant data to the real plant

data set, the coverage of the available data set can be broadened and the prediction of AI model can be improved significantly.

FACTPROSIM: FLOWSHEET PROCESS SIMULATION SOFTWARE

The process simulation models we have developed so far were based on the FactSage macro processing code and ChemApp DLL (GTT-Tech., 2024). Although FactSage macro processing is rather easy to do the programming, the model can be only run under the FactSage environment and calculation speed is rather slow. On the other hand, process models based on ChemApp needs more programming skill for C++, Visual Basics, Python, etc.

In order to make process calculations without any coding, we have developed a new flowsheet program “FactProSim” for process simulation applications based on our experience on the variety of process simulation models in steelmaking and other metallurgical processes. FactProSim software employs accurate and reliable FactSage thermodynamic databases and Gibbs Energy Minimizer (ChemSage) through ChemApp (internally available in FactSage program) to perform complex multiphase, multicomponent equilibrium calculations. FactProSim uses an intuitive flowsheet diagram approach to model the process with modules, which interact with each other through the flow of materials. It is designed with a drag-and-drop approach, providing a user-friendly interface with no coding required. This software will be available in FactSage 8.4 version in 2025.

FactProSim Features

As shown in Fig. 9, the FactProSim software is designed with a complete graphical interface, allowing the user to interact with modules and the resulting flowsheet with relative ease. Modules can be added to the flowsheet by drag-and-drop operation, and modified through their respective windows, which also auto-populates relevant phases as and when needed. FactProSim is not process specific; it is a general-purpose process simulation tool. Flowsheeting is a systematic description of materials and energy flow in a process. A flowsheet is comprised of multiple streams interconnected to describe the process behaviour. A complex metallurgical process can be broken down into several local chemical equilibrium zones, where materials are assumed to be at equilibrium. Hence, a chemical equilibrium calculation is required to ascertain the local composition and enthalpy (heat) change using thermodynamic databases. This modelling approach based on local equilibrium is the basis of the EERZ model approach as shown in Fig. 1.

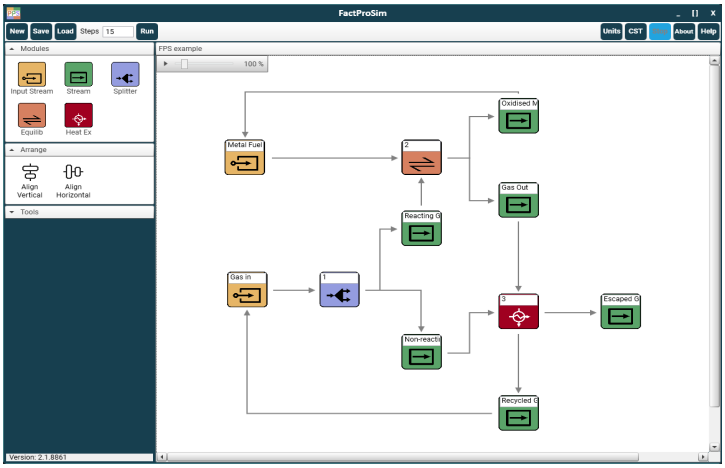


FIG 9 – Visualisation of the 5 main modules of FactProSim and the connections between them.

Any chemical reaction requires an equilibrium chemical reaction (Gibbs Energy minimization), input materials (reactants) and output materials (reaction products). In some cases, material flow needs to be divided into several flow branches to bypass or to take part in other reactions, which is done by a splitter. These four flowsheet components are sufficient to describe the material flow and local chemical equilibria in a metallurgical process. As shown in Fig. 9, these components are provided in FactProSim as five modules, namely, the Equilib module (orange module) to perform equilibrium calculation, the Input Stream module (yellow module) to define incoming material in the flowsheet, the Splitter module (purple module) to divide a material stream into several streams, the Stream module (green module) to save streams created by the Equilib and Splitter modules, and the Heat

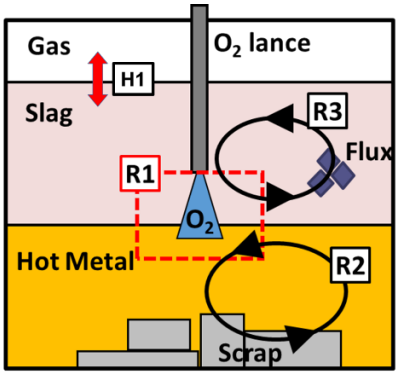
Ex module (red module) to allow the heat exchange between two streams without mass change or assign heat loss and heat gain. After chemical reactions at interfaces, the product streams can be allowed to mix with the remaining to begin the next cycle calculations. These modules can be easily added to the flowsheet diagram via drag-and-drop operation. Each module is connected by arrows to depict the flow of material in the flowsheet.

In addition, time-dependent process simulations can be performed with FactProSim by repeating a flowsheet for a certain number of time steps. The continuity in the simulation between the time step is carried out by designating the streams that will serve as input for the next time step.

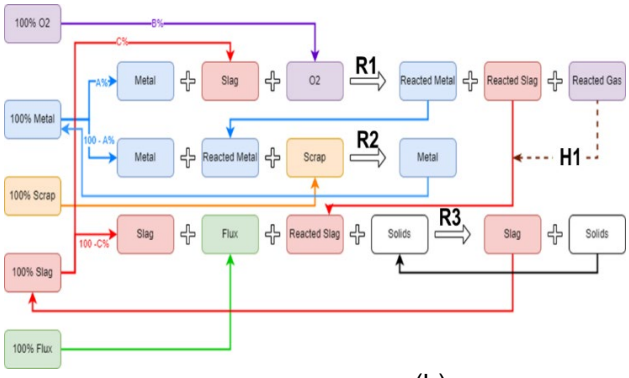
FactProSim offers the possibility to enter various inputs in the flowsheet modules (such as material composition, amount and temperature, equilibrium calculation conditions, etc.) through spreadsheets by linking one or several Microsoft Excel spreadsheets to a flowsheet. Furthermore, the output of the simulation is also saved in Microsoft Excel spreadsheets to provide a convenient way to analyse and represent the output data.

A simple model demonstration

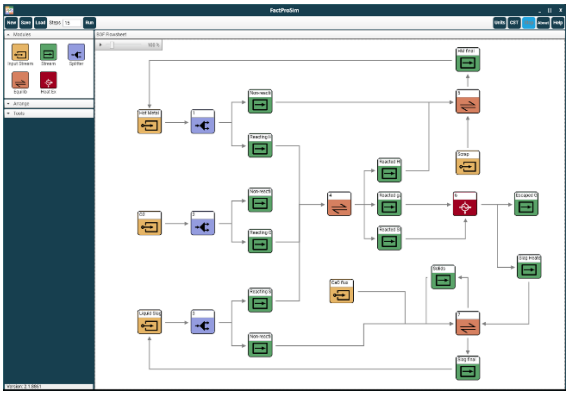
In order to demonstrate FactProSim, a simplified BOF process has been modelled. The schematic of the BOF process is presented in Fig. 10 (a). The simplified process flowsheet is prepared in Fig. 10 (b) to represent the BOF process. In this simple simulation, 3 reactions are included: (R1) hot metal oxidation reaction by O_2 involving fractions of hot metal and slag with incoming O_2 gas, (R2) scrap dissolution in hot metal and hot metal homogenization, and (R3) lime dissolution in slag and slag homogenization. In addition, the heat recovery (H1) from the exhaust gas to slag is also considered.



(a)



(b)



(c)

Inputs	Comp. (wt%)				Amount (kg)	Temp. (C)
Metal	Fe	C	Mn	Si		
	95	4	0.5	0.5	100	1300
Slag	CaO	FeO	SiO2			
	55	25	20		2	1300
Gas	O2					
	100					25
Flux	CaO					
	100					25
Scrap	Fe					
	100					25

Kinetic factors						
Time (min)	O2 (kg)	CaO (kg)	Metal (A,%)	Gas (B,%)	Slag (C,%)	Scrap (kg)
1	0.57	0.25	10	50	50	2
2	0.57	0.25	10	50	50	2
3	0.57	0.25	10	50	50	2
4	0.57	0.25	10	50	50	2
5	0.57	0.25	10	50	50	2
6	0.57	0.25	30	80	80	2
7	0.57	0.25	30	80	80	2
8	0.57	0.25	30	80	80	2
9	0.57	0.25	30	80	80	2
10	0.57	0.25	30	80	80	0
11	0.57	0	30	80	80	0
12	0.57	0	30	80	80	0
13	0.57	0	30	80	80	0
14	0.57	0	30	80	80	0
15	0.57	0	30	80	80	0

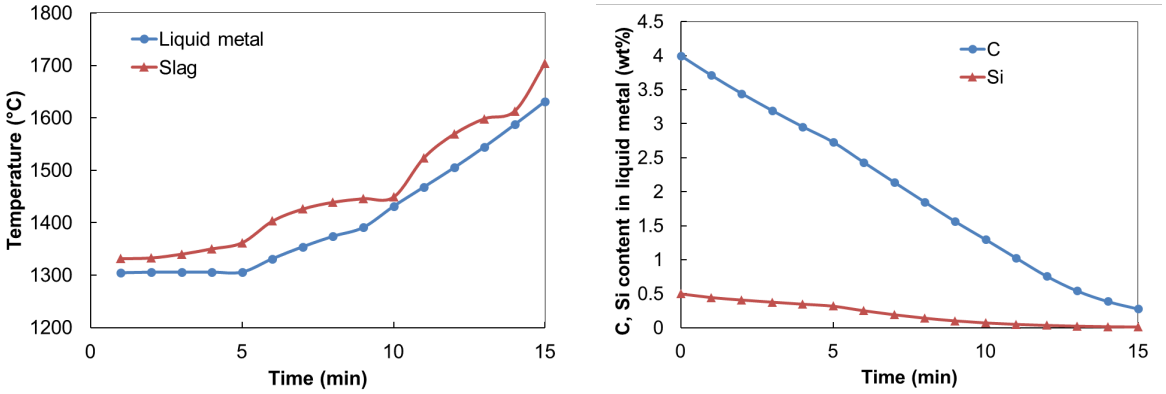
(d)

FIG 10 – (a) Schematics of BOF process, (b) flowsheet of the BOF process model, (c) corresponding simulation flowchart in FactProSim, and (d) Excel file for input condition of process simulation.

As seen in Fig. 10 (c), the process simulation in FactProSim can be constructed to be almost identical to the flowsheet in Fig. 10 (b). All reactions are set to be calculated under adiabatic equilibrium conditions for simplicity. Simple kinetic parameters A%, B% and C% in Fig. 10

(b) are set to adjust the material flow between each reaction, as listed in Excel file (see Fig. 10 (d)).

The simulation results of a 100 ton hot metal with 4.0 wt% C, 0.5 wt% Si and 0.5 wt% Mn at 1300 °C is shown in Fig. 11. The metal and slag temperature profile during the BOF process can be predicted from the heat balance of all chemical reactions. The evolution of the C and Si content in hot metal is presented. Of course, this is a simple model and not directly applicable to the BOF operation analysis. The real model should be much more complex as shown in Fig. 4. However, the present example can readily demonstrate the ease of simulating metallurgical processes with FactProSim.



(a) (b)

FIG 11 – Simulated evolution of (a) slag and metal temperature, and (b) C and Si content in liquid metal.

FactProSim is designed to handle very complex industrial scale simulations. One of examples for complex process simulation is shown in Fig. 12. This is a FactProSim flowsheet for the full scale LF model (Van Ende and Jung, 2017) shown in Fig. 6. In order to facilitate the setting of the EERZ amounts of reactants in the reaction zone depending on the stirring energy and other factors, a function builder which allows to use complex mathematical equation is also implemented in the FactProSim.

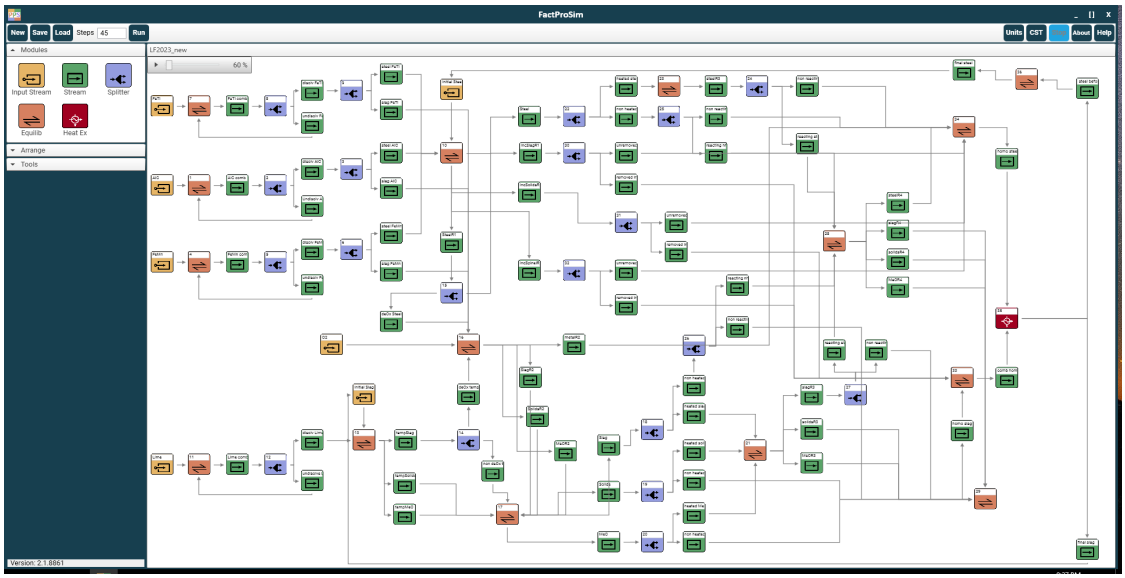


FIG 12 – FactProSim flowchart for LF process simulation.

We believe that FactProSim software can be a very useful tool for researchers and engineers in pyrometallurgy to build their own process simulation models to improve the current operation and design new process.

SUMMARY

The effective equilibrium reaction zone (EERZ) approach has been well applied to simulate the complex industrial processes that exhibit strong non-equilibrium and time-dependent characteristics. The steelmaking process simulation models for EAF, hot metal pre-treatment, BOF, LF, VTD, RH degasser, Tundish, continuous casting have been developed within the FactSage steelmaking consortium and applied to improving plant operations. New FactProSim software is also developed to assist in the development of process simulation models using the EERZ concept.

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