

Dynamic Simulation of Batch Copper Converting Using SysCAD with ChemApp

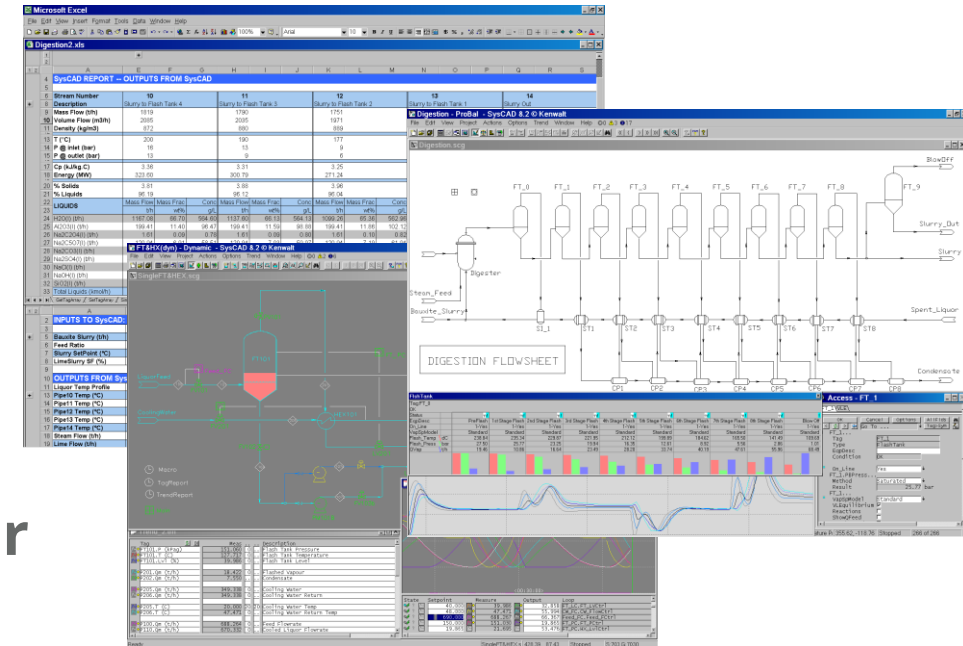
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GTT Users Meeting 2022

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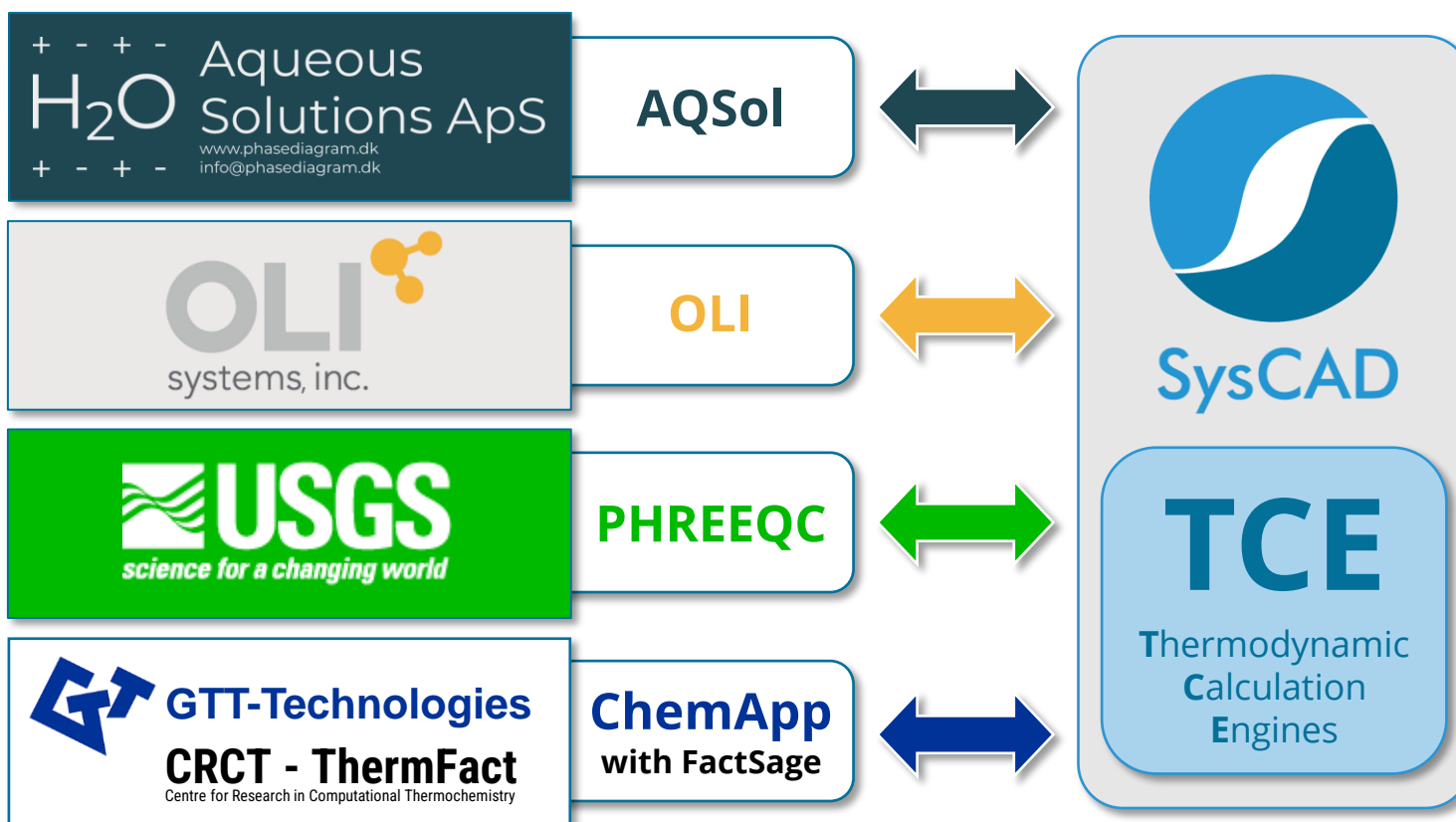
- **Batch Cu Converting, Process Description**
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What is SysCAD?

- Powerful & versatile Process Plant simulator
- Steady State or Dynamic mode
- Simulate simple to complex full plant operation
- An invaluable process tool that will help users gain tremendous insights into their process operation
 - Good process knowledge aids better decision making
 - Improved plant operation performance
 - Cost saving
 - More efficient and knowledgeable operators



Thermodynamic Calculation Engines (TCE)



- Detailed thermodynamics applied *as needed*
- One SysCAD model, multiple TCEs and chemistry models
- Parallel processing
- User-friendly features

Batch Cu Converting

Process Description

Process Description

- Cu converting is traditionally carried out in Peirce-Smith converters.
- It is a batch process receiving furnace matte. Mainly consisting of two distinctive steps
 - Slag blows → removal of Fe to slag to produce white metal (“Cu₂S”)
 - Depending on initial matte grade
 - Could consist of 2 or 3 slag blows, each receiving fresh furnace matte and skimming slag at the end of the blow
 - Fe end-point might be higher for initial blows
 - Cu blow → removal of S from Cu to produce Blister Cu
 - Longer blow, needs cold charge (high grade reverts) for temperature control
 - Transition through Cu-S miscibility gap
 - In a converter aisle, several 2-4 converters typically operate in staggered sequence, with one in Cu blow (high and continuous SO₂ stream) whereas other converters are in slag blow, or down for rebrick.

Thermodynamic System

Cu-Fe-S-O-Si+ System, Definition of thermodynamic ChemSage input file

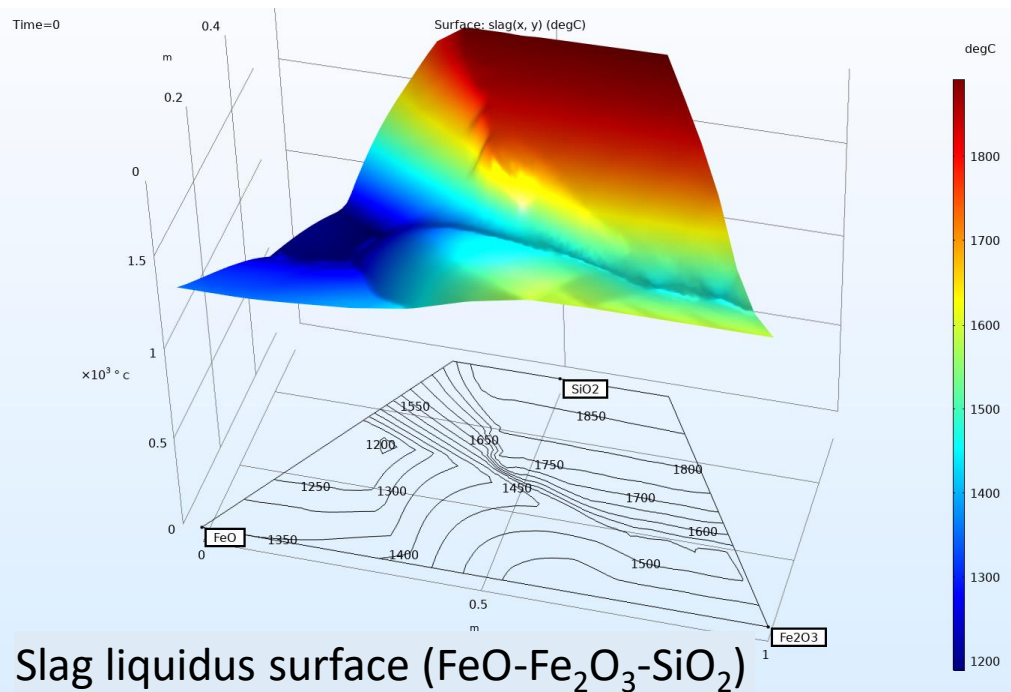
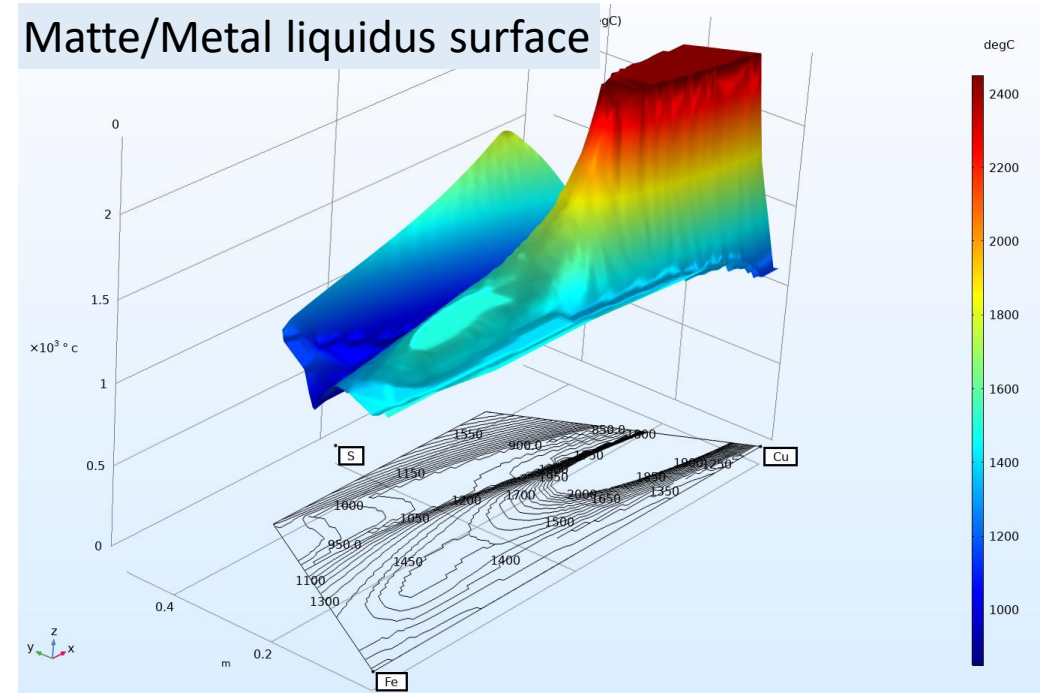
ChemSage Input File

A thermodynamic input file consisting of:

- **7 System components (plus electron):**
 - Cu-Fe-S-O-N-H-Si-e
- **9 Solutions:**
 - gas_ideal, Spinel, Monoxide, Liq(Matte_Metal)#1#2, fcc#1#2, Slag#1#2, etc.
- **39 Pure Components:**
 - Fe_2O_3 , CuO, Cu_2O , CuFeO_2 , S, FeS, FeS_2 , CuS, Cu_2S , CuFeS_2 , $\text{H}_2\text{O}_{(l)}$, SiO_2 , Fe_2SiO_4 , etc.
- **Built from published thermodynamic parameters^[1-9]**

Main Solutions

Liquid Metal/Matte
SUBG model
Cu, Cu²⁺, Fe, Fe²⁺, S and O



Slag
SUBG model
SiO₂-FeO-Fe₂O₃-Cu₂O

SysCAD Implementation

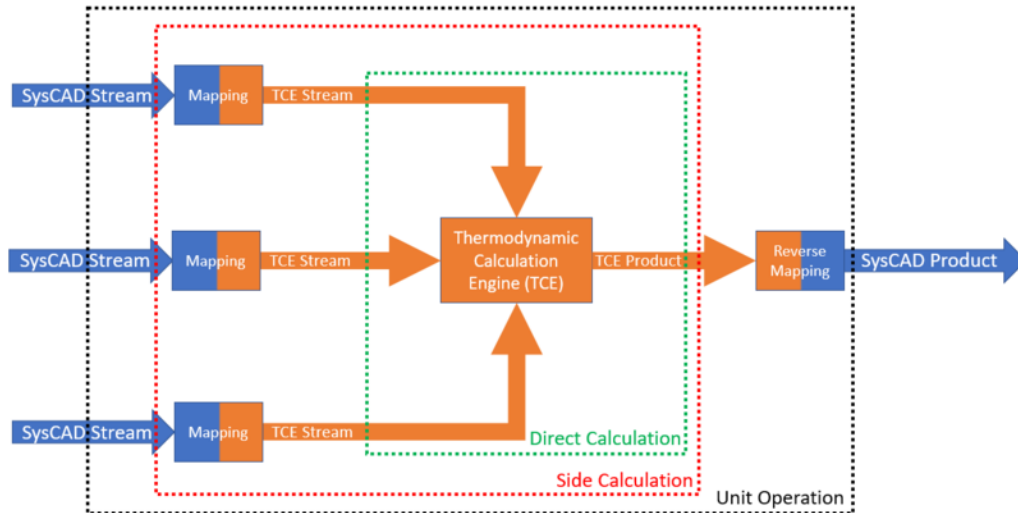
Dynamic Converter Model

Species Mapping

ChemApp species are mapped to SysCAD species

Mapping process is automated but also allows user customization

Species/Phase suppression is supported



gas_ideal	Sup	Molewt	MappedSpecies
H2O	<input type="checkbox"/>	18.02	H2O(g)
N2	<input type="checkbox"/>	28.01	N2(gas_ideal)
O2	<input type="checkbox"/>	32.00	O2(gas_ideal)
SO2	<input type="checkbox"/>	64.06	SO2(gas_ideal)
SO3	<input type="checkbox"/>	80.06	SO3(gas_ideal)

gas_ideal ...
Suppress Suppress A11 : Suppress 5 for gas_ideal
Unsuppress Unsuppress 0

Spinel	Sup	Molewt	MappedSpecies
Cu1Cu2O4[2-]	<input type="checkbox"/>	254.64	Cu1Cu2O4[2m](Spinel)
Cu1Fe2O4	<input type="checkbox"/>	239.23	CuO.Fe2O3(Spinel)
Cu1Fe2O4[2-]	<input type="checkbox"/>	239.23	Cu1Fe2O4[2m](Spinel)
Cu1Va2O4[6-]	<input type="checkbox"/>	127.54	Cu1Va2O4[6m](Spinel)
Fe1Cu2O4[1-]	<input type="checkbox"/>	246.93	Fe1Cu2O4[1m](Spinel)
Fe1Cu2O4[2-]	<input type="checkbox"/>	246.93	Fe1Cu2O4[2m](Spinel)
Fe1O4[5-]	<input type="checkbox"/>	119.84	Fe1O4[5m](Spinel)
Fe1O4[6-]	<input type="checkbox"/>	119.84	Fe1O4[6m](Spinel)
Fe3O4	<input type="checkbox"/>	231.53	Fe3O4(Spinel)
Fe3O4[1+]	<input type="checkbox"/>	231.53	Fe3O4[1p](Spinel)
Fe3O4[1-]	<input type="checkbox"/>	231.53	Fe3O4[1m](Spinel)
Fe3O4[2-]	<input type="checkbox"/>	231.53	Fe3O4[2m](Spinel)

Spinel ...
Suppress Suppress A11 : Suppress 12 for Spinel
Unsuppress Unsuppress 0

Monoxide	Sup	Molewt	MappedSpecies
CUO	<input type="checkbox"/>	79.55	CUO(Monoxide)
(Fe2O3):2	<input type="checkbox"/>	79.84	[Fe2O3]2(Monoxide)
FeO	<input type="checkbox"/>	71.84	FeO(Monoxide)

Monoxide ...
Suppress Suppress A11 : Suppress 3 for Monoxide
Unsuppress Unsuppress 0

Liq(Matte_Metal)#1	Sup	Molewt	MappedSpecies
Cu	<input type="checkbox"/>	63.55	Cu(Liq_Matetal_#1)
Cu2+	<input type="checkbox"/>	63.55	Cu(Liq_Matetal_#1)
Fe	<input type="checkbox"/>	55.84	Fe(Liq_Matetal_#1)
Fe3+	<input type="checkbox"/>	55.84	Fe(Liq_Matetal_#1)
O	<input type="checkbox"/>	16.00	O(Liq_Matetal_#1)
S	<input type="checkbox"/>	32.06	S(Liq_Matetal_#1)

Liq(Matte_Metal)#1 ...
Suppress Suppress A11 : Suppress 6 for Liq(Matte_Metal)#1
Unsuppress Unsuppress 0

Liq(Matte_Metal)#2	Sup	Molewt	MappedSpecies
Cu	<input type="checkbox"/>	63.55	Cu(Liq_Matetal_#2)
Cu2+	<input type="checkbox"/>	63.55	Cu(Liq_Matetal_#2)
Fe	<input type="checkbox"/>	55.84	Fe(Liq_Matetal_#2)
Fe3+	<input type="checkbox"/>	55.84	Fe(Liq_Matetal_#2)
O	<input type="checkbox"/>	16.00	O(Liq_Matetal_#2)
S	<input type="checkbox"/>	32.06	S(Liq_Matetal_#2)

Liq(Matte_Metal)#2 ...
Suppress Suppress A11 : Suppress 6 for Liq(Matte_Metal)#2
Unsuppress Unsuppress 0

Dynamic Model Structure

The model centers around a generic “ChemApp Tank” unit model

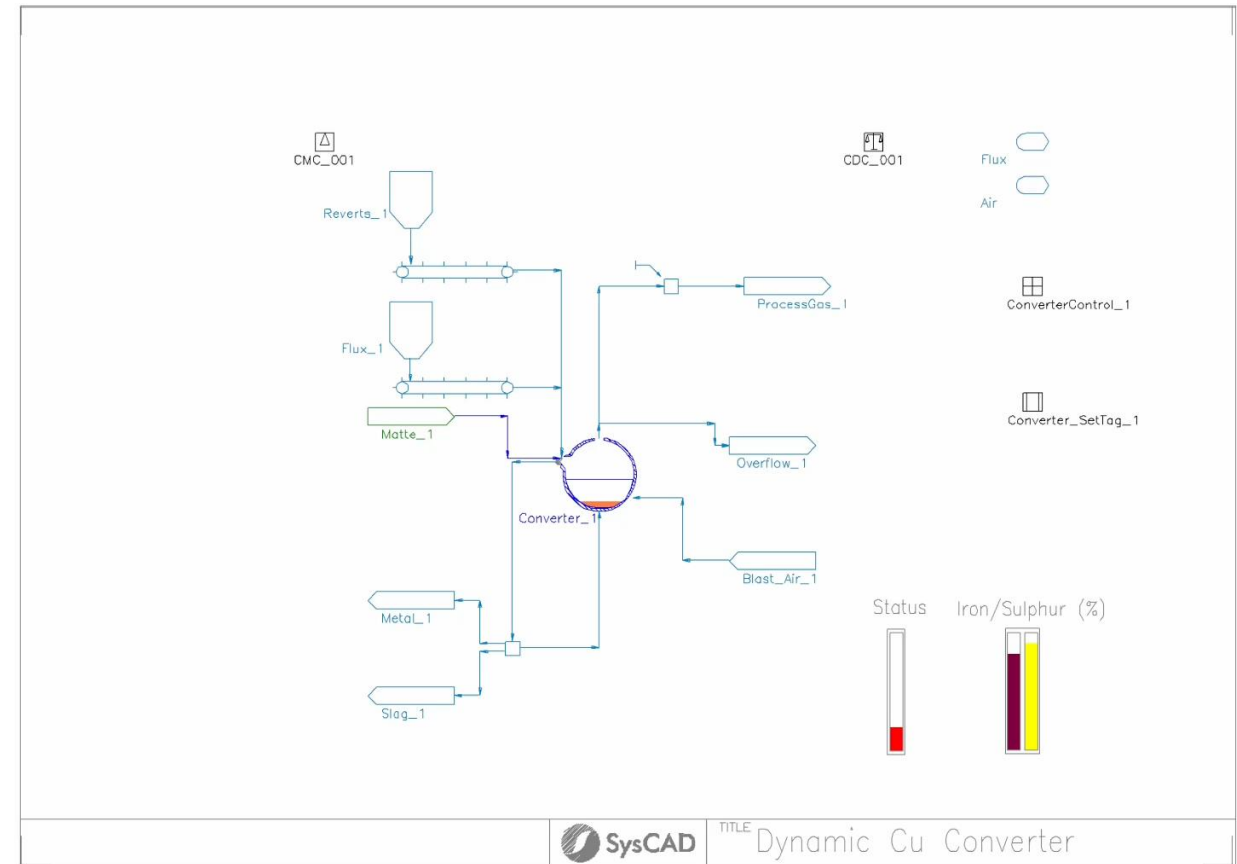
A converter class was built to simulate the batch process

Status: Idle, loading, Slag blow, Skimming, Cu Blow, Casting and Maintenance

Each status has a defined behaviour and set point

A “slag blow” subclass was defined to allow creating multiple slag blows, each with its own settings and configuration

Code is generic allowing use for multiple converters in a flowsheet



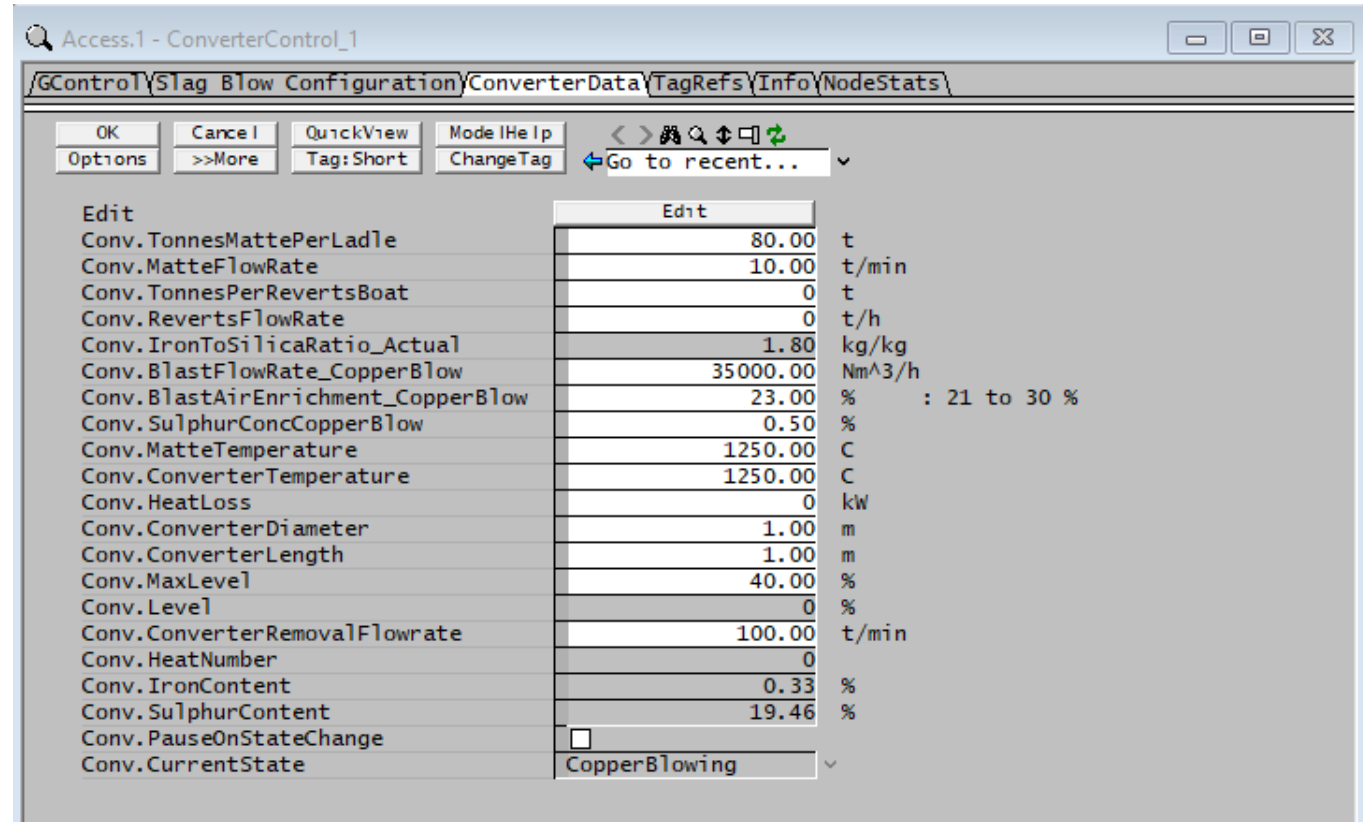
Main Class Settings

General settings for the overall converting process are defined by a custom interface

The user input interface is created with each “converter” instance

General Parameters:

- Ladle size (capacity)
- Loading flow rate
- Furnace and converter T (iso-thermal mode)
- Information variables: Fe/SiO₂, %Fe, %S, State, etc.



Slag Blow Class Settings

The Slag Blow subclass allows to define specific process conditions for each slag blow

- Number of ladles per blow
- Blast flow rate
- Enrichment
- Silica to O₂ ratio
- Fe end point

Access.1 - ConverterControl_1

/GControl/Slag Blow Configuration/ConverterData/TagRefs/Info/NodeStats

OK Cancel QuickView Mode Help
Options >>More Tag:Short ChangeTag < > 🔍 ↕ 🗨️ ↻
Go to recent...

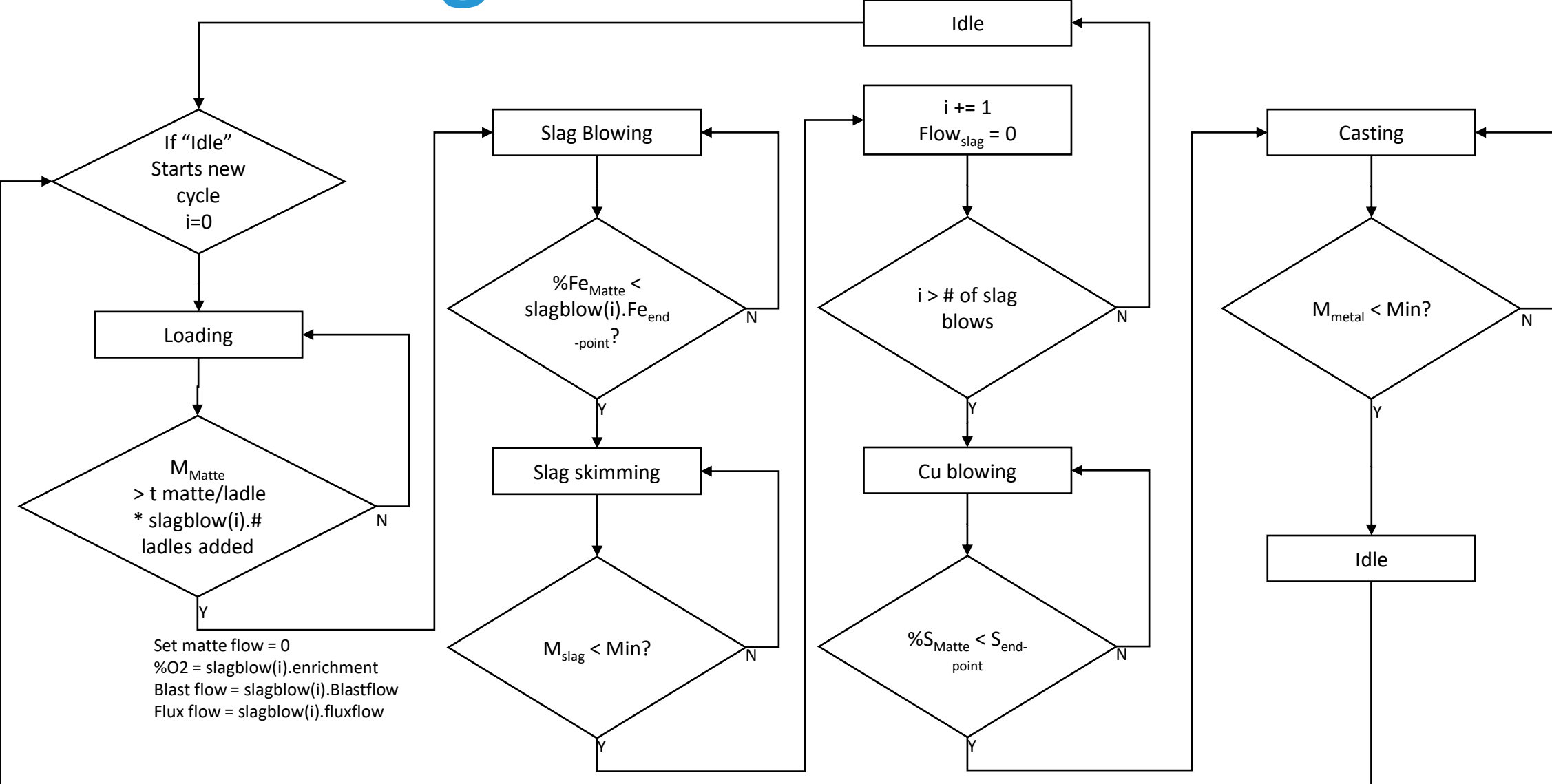
Edit Edit

Number of Slag Blows
NumberOfSlagBlows 3 : 1 to 3

Individual slag blow settings

SlagBlow[0].NumberOfLadlesAdded	3	
SlagBlow[0].BlastFlowRate	35000.00	Nm ³ /h
SlagBlow[0].BlastAirEnrichment	24.00	% : 21 to 30 %
SlagBlow[0].FluxToAirRatio	1.00	kg/kg
SlagBlow[0].IronEndPointConc	5.00	% : 1 to 5 %
SlagBlow[1].NumberOfLadlesAdded	2	
SlagBlow[1].BlastFlowRate	35000.00	Nm ³ /h
SlagBlow[1].BlastAirEnrichment	24.00	% : 21 to 30 %
SlagBlow[1].FluxToAirRatio	1.00	kg/kg
SlagBlow[1].IronEndPointConc	5.00	% : 1 to 5 %
SlagBlow[2].NumberOfLadlesAdded	1	
SlagBlow[2].BlastFlowRate	35000.00	Nm ³ /h
SlagBlow[2].BlastAirEnrichment	24.00	% : 21 to 30 %
SlagBlow[2].FluxToAirRatio	1.00	kg/kg
SlagBlow[2].IronEndPointConc	1.50	% : 1 to 5 %

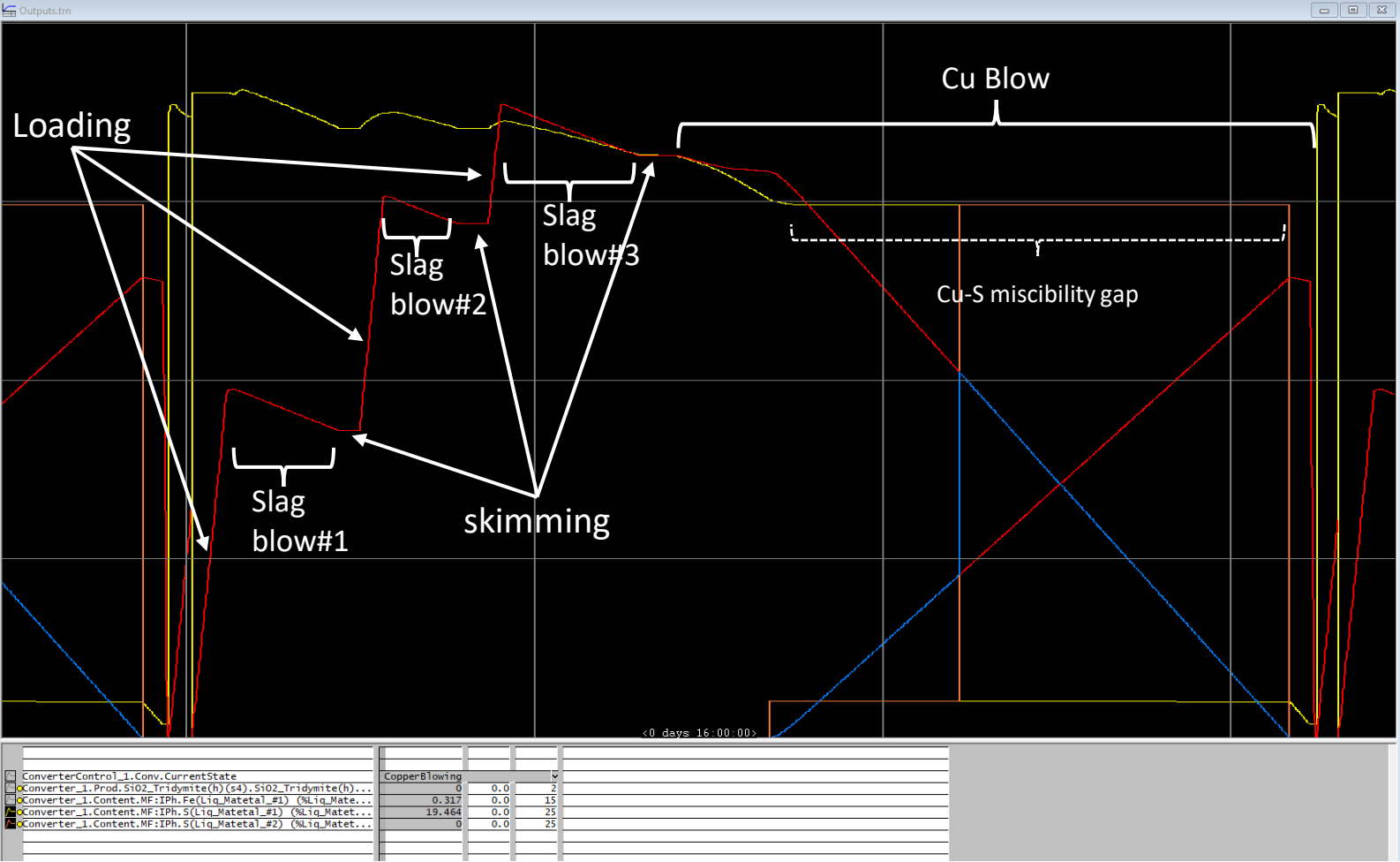
Process Logic



Results

Isothermal Case - Dynamic Model

Results



Selected Trends vs time:

- Liquid #1(matte): **red**
- Liquid #2 (blister): **blue**
- S wt% in liquid #1: **yellow**
- S wt% in liquid #2: **orange**

Summary

- A Batch Cu Converter model was implemented in SysCAD
- The model uses SysCAD dynamic solver
- ChemApp TCE was used to simulate the converter
 - The model centers on a generic ChemApp Tank unit model
 - A thermodynamic input file including matte, metal, slag, spinel and other phases was prepared in-house for this model
- A flexible and modular approach using a converter class definition was chosen to allow future expansion of the model
 - A sub-class for slag blows was also implemented

Next Steps

- **Enthalpy target run (Heat balance and cold charge)**
 - Automate addition of reverts and cold charge
 - Update tank discharge function (for individual phases)
- **Oxygen efficiency**
 - Use Constrained Free Energy to limit oxygen extent of equilibrium, particularly as a function of S concentration during late stages of Cu blow
- **Multiple converters in parallel**
 - Simulate converter aisle dynamics
- **Upstream/downstream units**
 - Add constraints originated from furnace, oxygen plant, off-gas handling system, acid plant, etc.
- **Expand/Enhance thermodynamic system**
 - Add additional impurities, expanding system of applicability

Thank you!



Questions?

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More Information:

- 🌐 syscad.net
- 🌐 help.syscad.net

Thermochemical Data References

References:

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