Usage of thermochemical calculations in SMS Siemag AG

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VES2 Fundamentals and Models Steelmaking/Reduction

Thermochemical calc. in SMS Siemag AG

Introduction

FactSage

SimuSage

Conclusion

SMS Siemag AG

Part of SMS Holding GmbH: internationally active in plant construction and mechanical engineering relating tp the processing of steel and non ferrous metals.

Research and development departement

VES: Fundamentals and models steelmaking and reduction processes.

Main Tasks:

- Static and dynamic models: EAF, BOF, AOD, SAF → Endpoint prediction and optimized process control
- Optimisation of metallurgical processes
- CFD Models

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Application of Factsage: Equilibrium Calculations

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➢ Verification of existing static models:

- for charge requirement calculations
- based on desired end point chemistry and temperature

- Comparison with the Equilib Results:

1. Model calculations for a typical charge composition were made
2. The charge requirement (input on elements: C, Fe, FeO, CaO ….) was determined
3. Elements (and their corresponding amount) were input as reactants in Equilib-FactSage
4. FactSage : determines the expected products at the end of the process and their corresponding amounts
5. Comparison with those expected by the model

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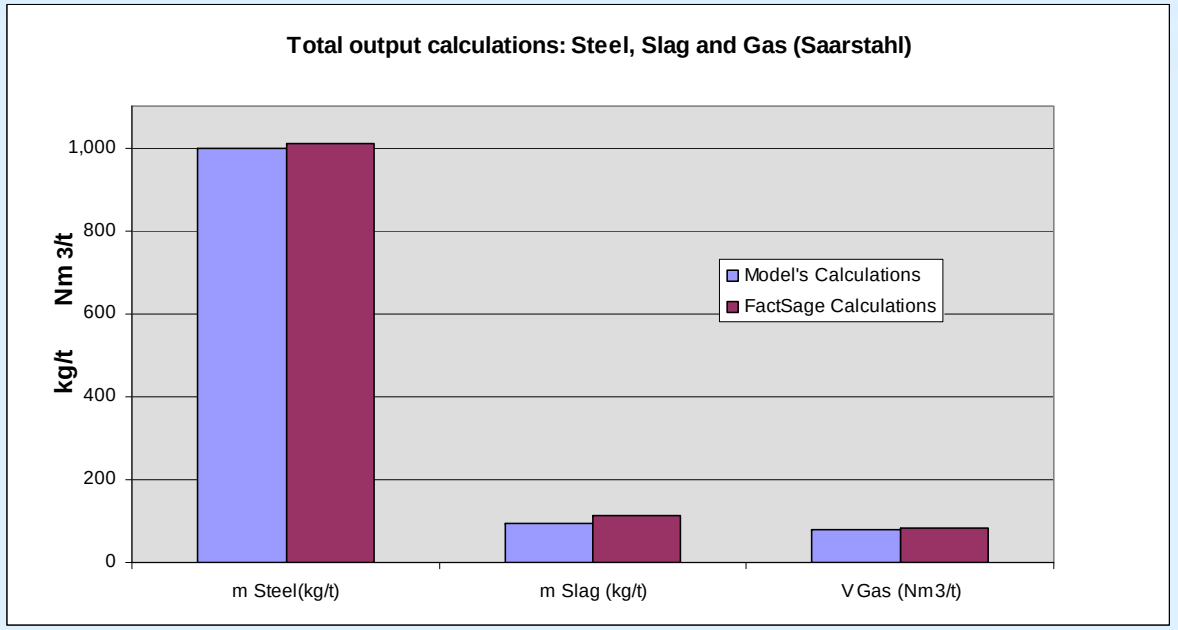
Application of Factsage: Equilibrium Calculations



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- ➢ Mass of steel: deviation of 0.9%
- ➢ Mass of slag: deviation of 18%

⇒ Dust/skulls formation not considered in FactSage

- ➢ Volume of off gas: deviation of 3%

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Application of Factsage: Equilibrium Calculations

Steel composition (Model/FactSage)			
	Model	**Factsage**	Difference%
Steel			
[%Fe]	99.72	99.73	0.01
[%C]	0.04	0.03	-29.67
[%Mn]	0.06	0.15	150.68
[%O]	635ppm	627ppm	-4.50
[%P]	0.011	-	-
m Steel(kg/t)	1000	1,009	0.93

- Fe content: deviation of 0.01%
- C content:
  - Factsage: 0.03%
  - Model: 0.04%

  ⇒ Carbon content in steel at the end of BOF process > equilibrium
- O content:
  - current example: deviation of 3% ($[O]_{Model} > [O]_{FactSage}$)
  - Example dependent

  ⇒ model does not take interaction coefficients into account

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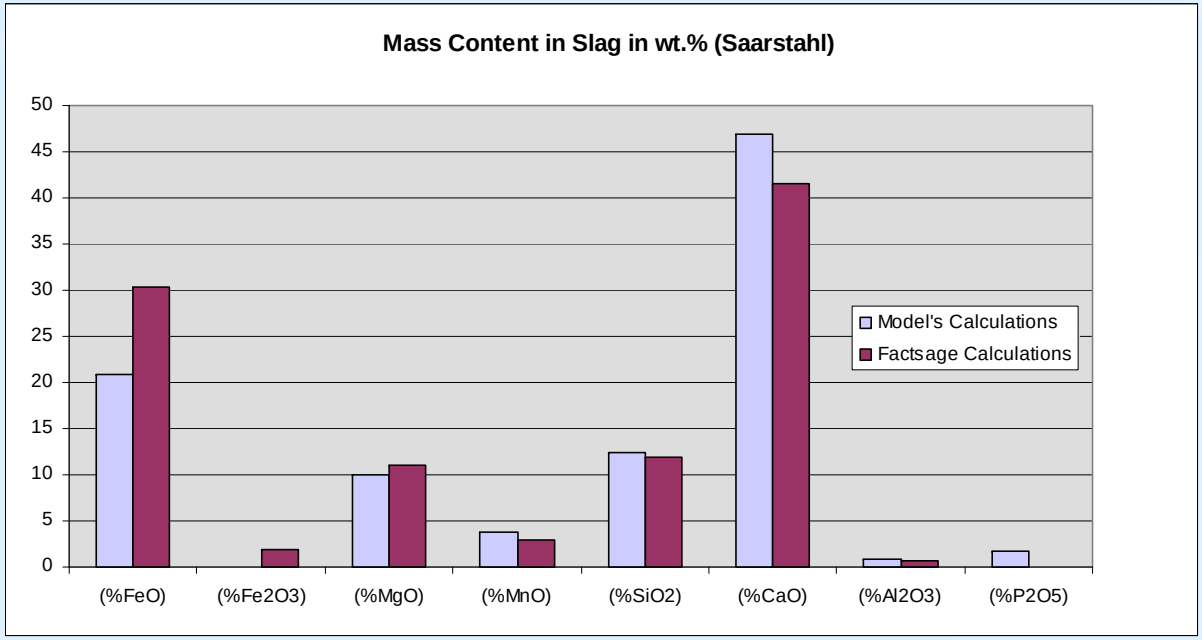
Application of FactSage: Equilibrium Calculations



- $(\%Fe_2O_3)_{FactSage}$ = 1.8% ⇒ Hematite formation is not considered in the model
- $(\%FeO)_{Model}$ << $(\%FeO)_{FactSage}$
  - Practice: more Fe is slagged to FeO in BOF than at equilibrium

- $(\%P_2O_5)$: FactSage estimation of P_2O_5 is not straight forward (especially when S is also considered as a reactant)

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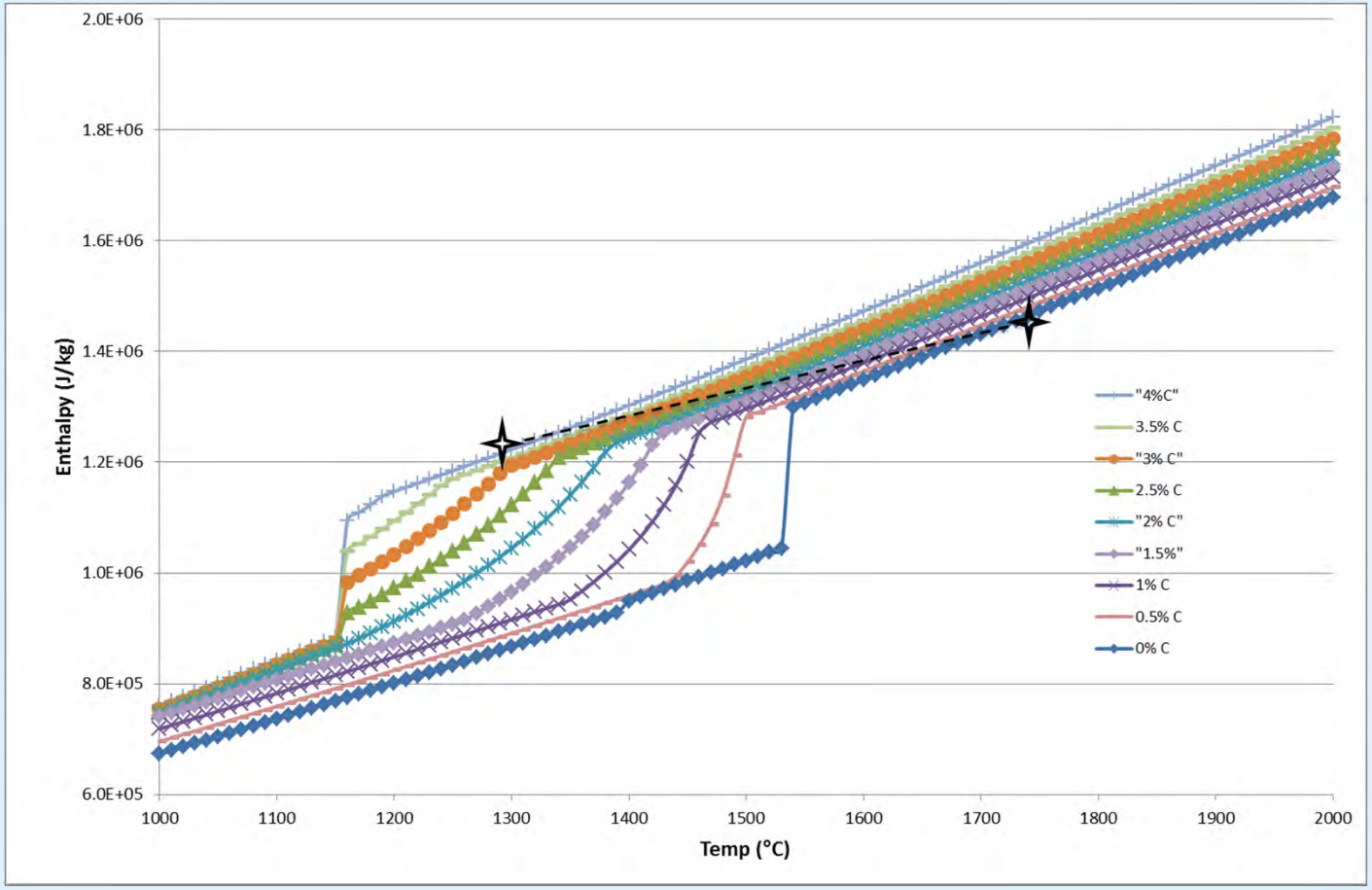
Application of FactSage: Equilibrium Calculations

Energy balance for dynamic calculations: Enthalpy of the melt during the progress of a BOF-heat



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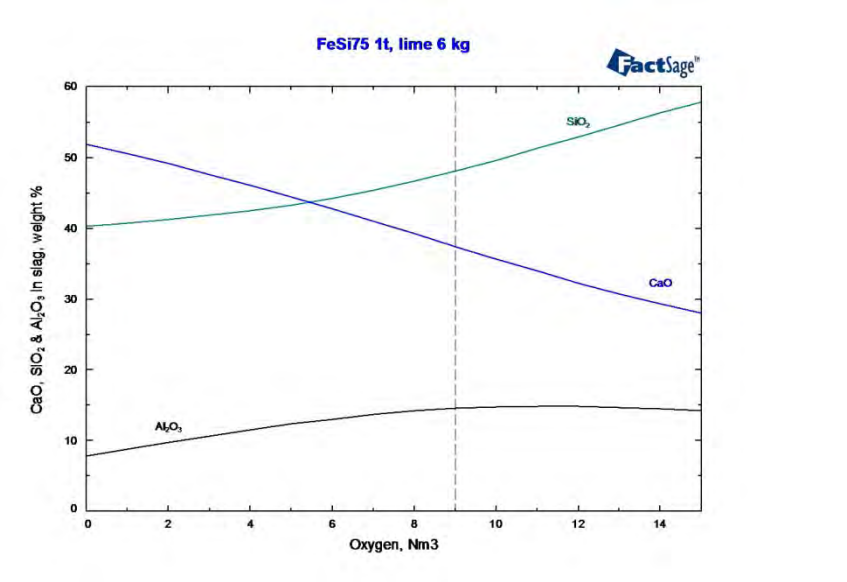
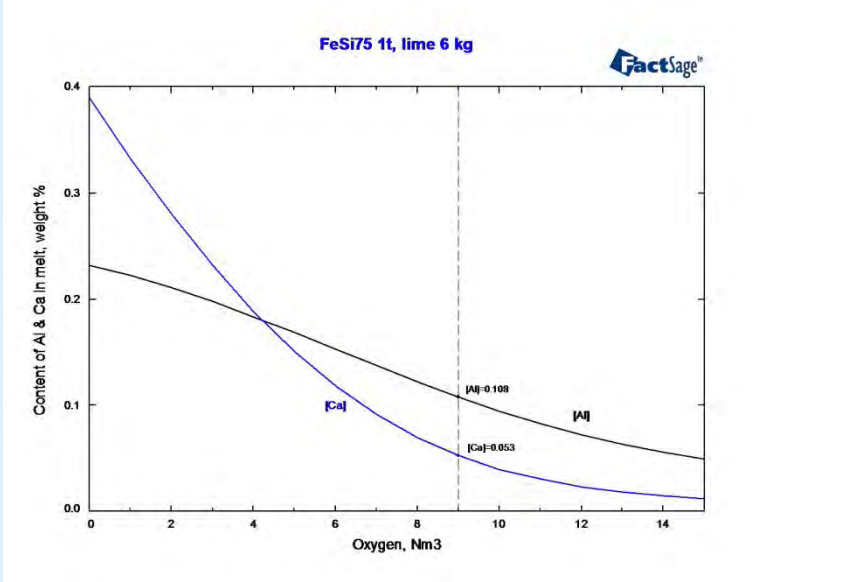
Application of FactSage: Equilibrium Calculations

- Si-Refining

Slag evolution during the blow



Equilib. [Al] and [Ca] during the blow



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Application of FactSage: Phase and Liquidus diagramms

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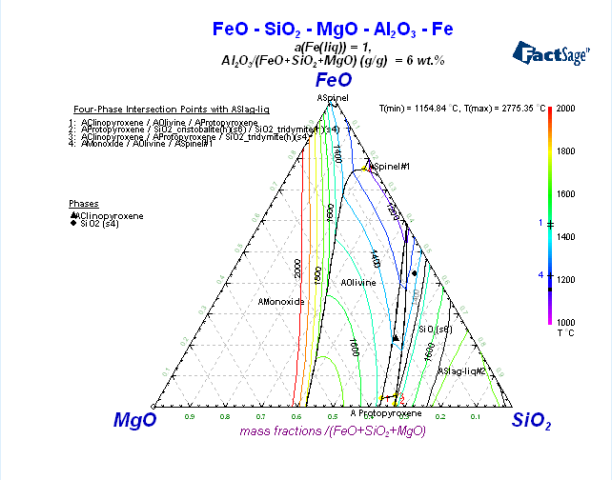
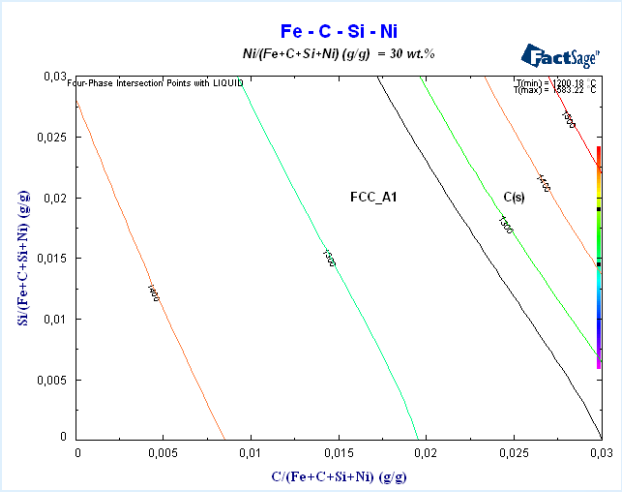
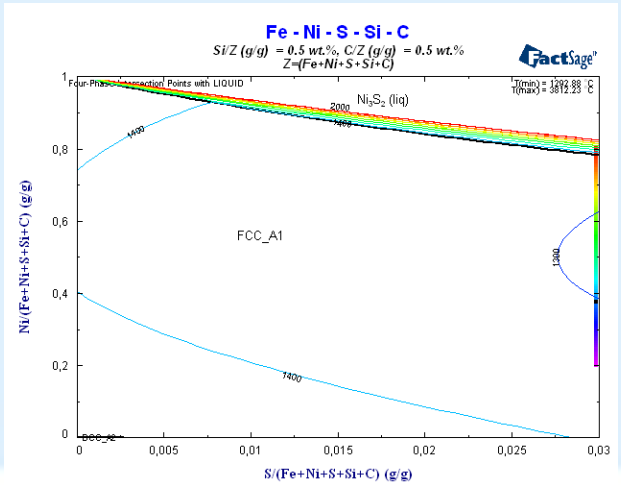
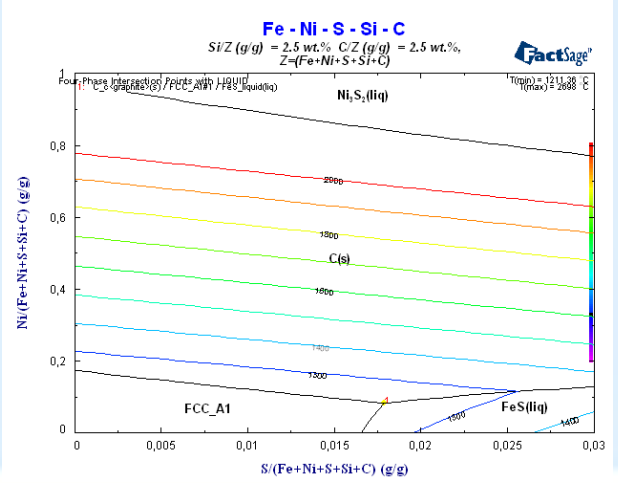
Reduction furnaces commisioning: (2 rectangular furnaces with 6 Elektrodes)

- MOP – Vale operacao Onca Puma
- Anglo American – Barro Alto









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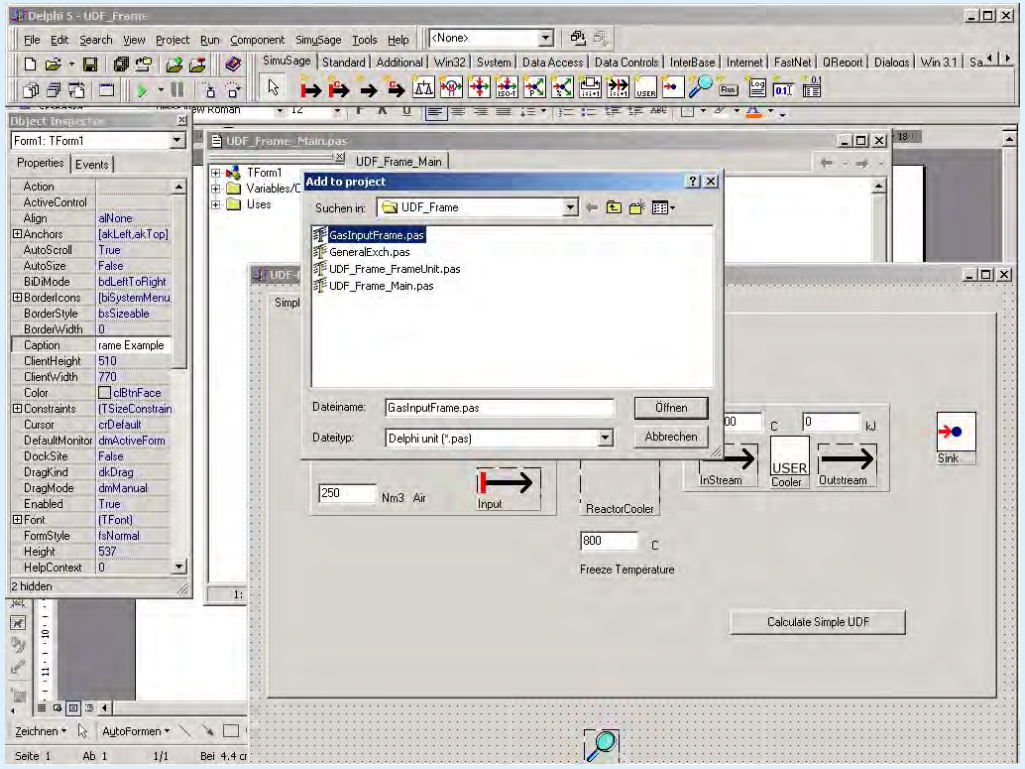
Application of Simusage: Energy balance for SAF- FeMn model

Enthalpy calculations with SimuSage: The enthalpy of input materials, of the melt , slag components (non ideal solutions) and offgas are determined and adapted in the models



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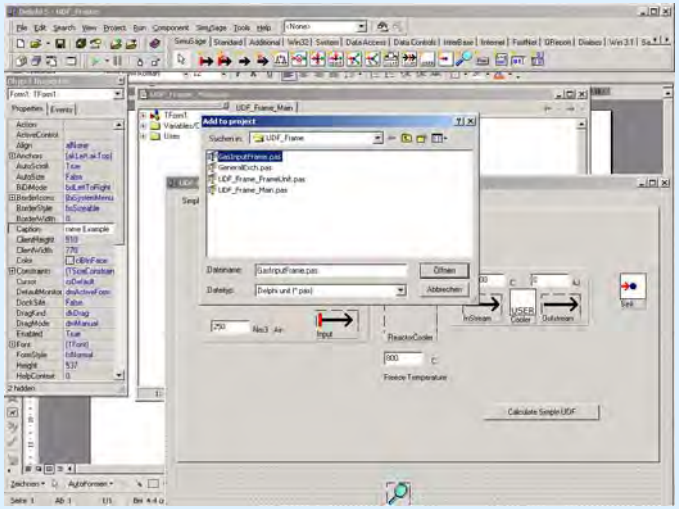
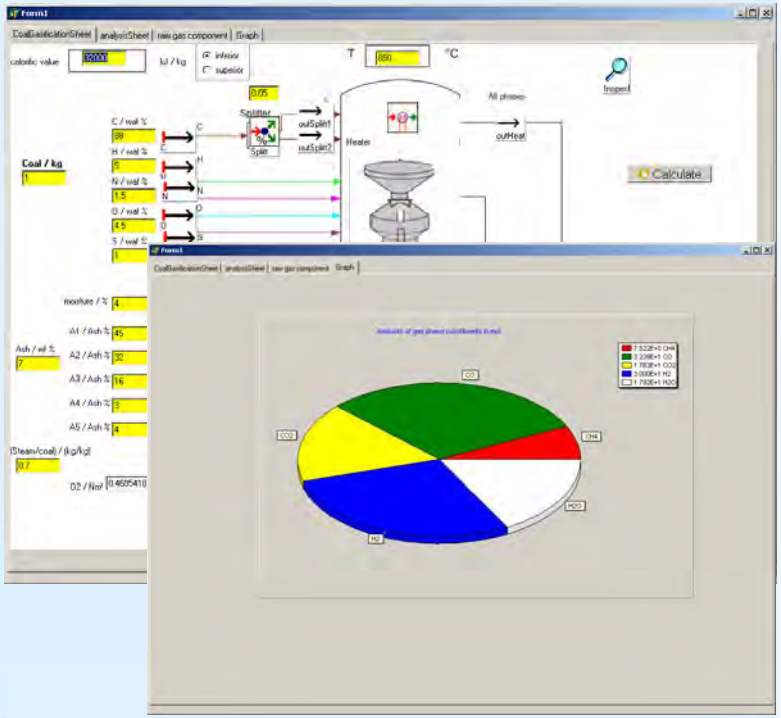
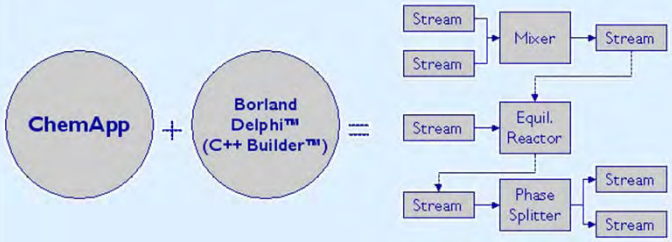
Application of Simusage: treatment of fossile fuels in thermodynamical calculations

Instruction example for Sasol: Determination of the enthalpy of coal gasification







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Summary

- FactSage / Simuage used in the SMS Siemag for:
  - Verification/comparison of practice models calculations with the equilibrium status.
  - Help generate accurate thermodynamic data especially for the energy balance calculations for different steelmaking processes.
  - With help of simusage it is possible to adapt the calculations automatically in the models
  - Generation of liquidus and phase diagramms

Future Work

- SimuSage-based:
- a dynamic dephosphorisation model
- a kinetic desoxidation model