Using Computational Thermochemistry in Metallurgical Plants

Contents

- General issues concerning the use of FACTSAGE
- Several practical examples

General

- General FACTSAGE approach:
  - Fit full (multi-component) system
  - Present results in phase diagrams etc.

- Industry wants:
  - Focus on limited compositional ranges
  - Results in terms of grade/degree of conversion

    More process minded vs. reaction minded
  - Mass and heat balance

General

- Metallurgical systems
  - Multi-component systems
  - Multi-phase “but not that many”

General

- Possible and risky use of FACTSAGE:

- Enter your chemical elements:
- Fe, Si, Al, Mg, Ca, Ti, P, Mn, C, O, H (multi-component)
- Only the default databases etc.
- Pure condensed phases ('many' multi-phase)

General

- At least investigate a sample of the material:

1) XRD phase identification
2) Optical microscopy
3) Microprobe analysis / EDS

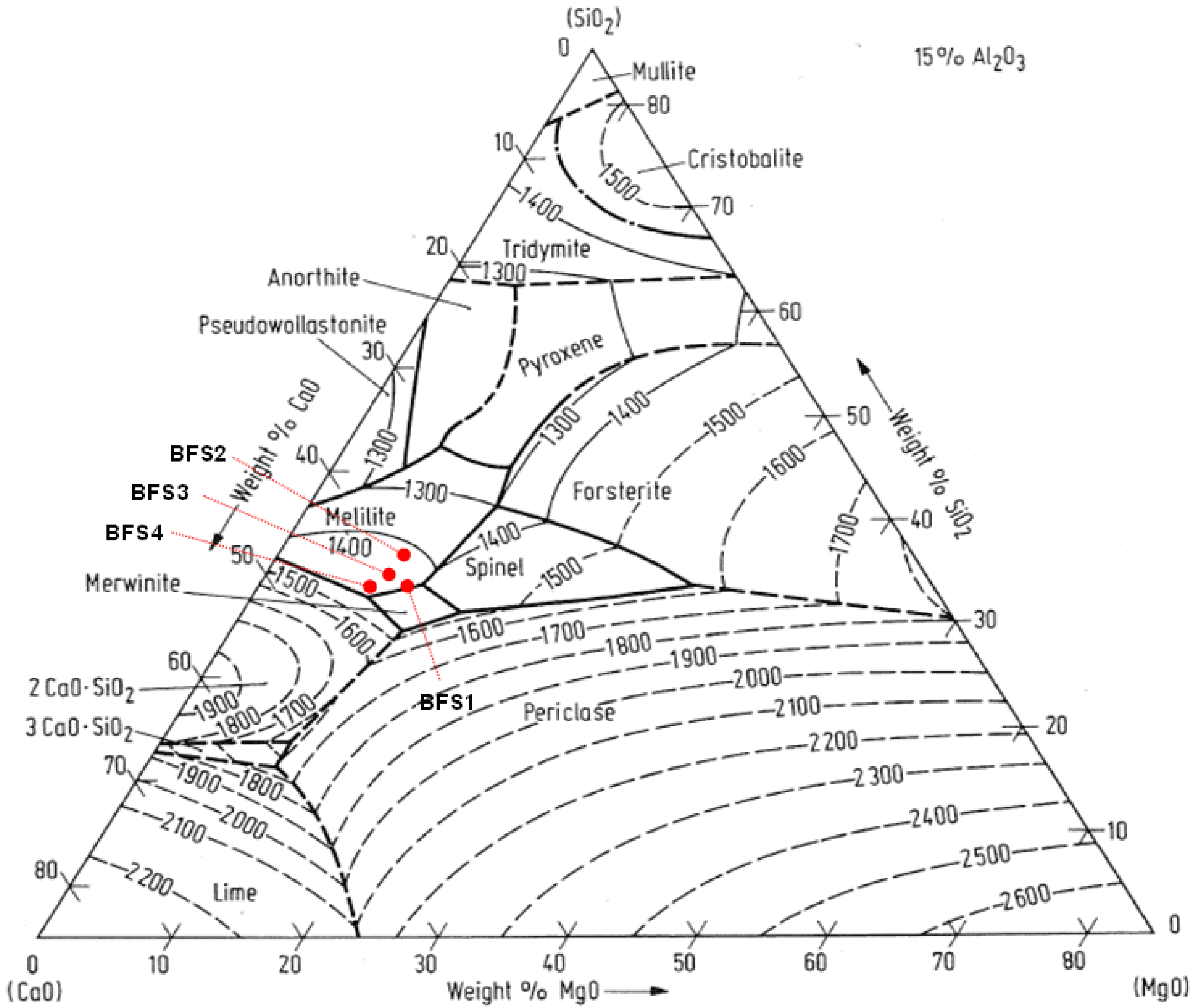
Examples

- Blast furnace slag (liquidus temperature)
- Converter slag (3 times): Lining attack (chemical)
Liquidus temperature
Free CaO
- Slag washing (lining protection; physical)
- Sinter process (prediction of phase composition)

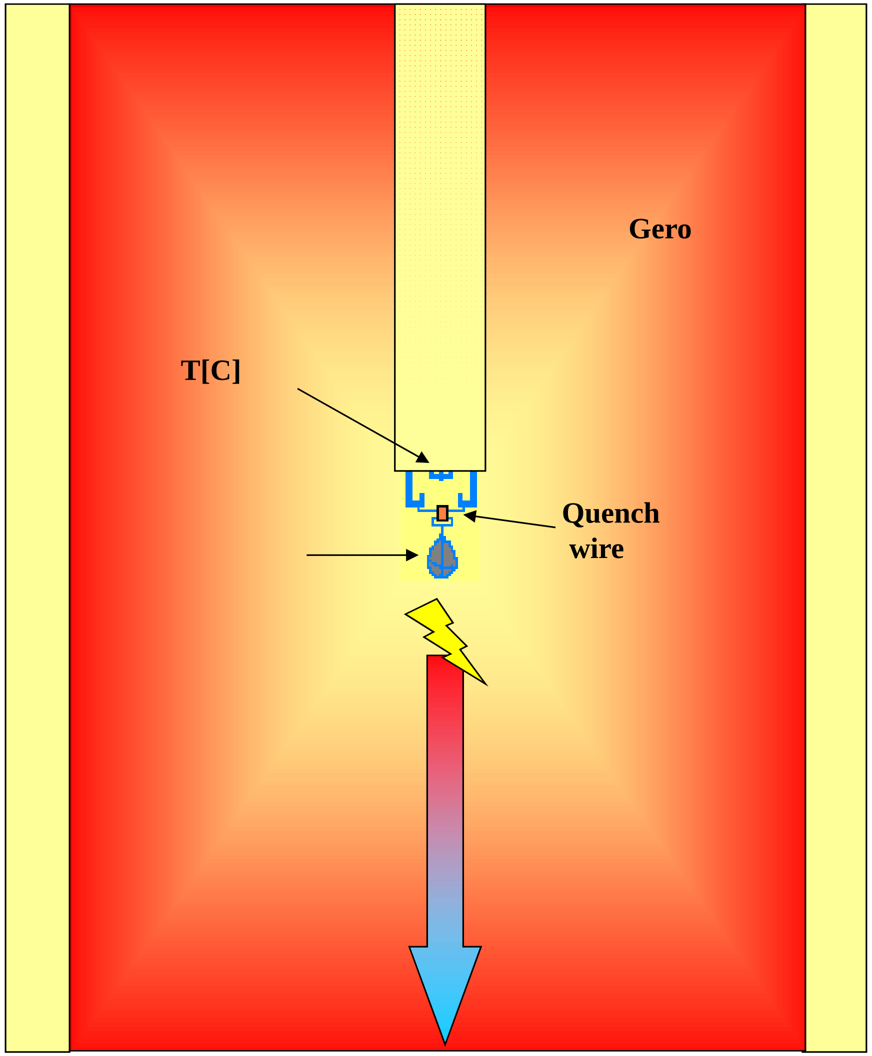
Blast furnace slag

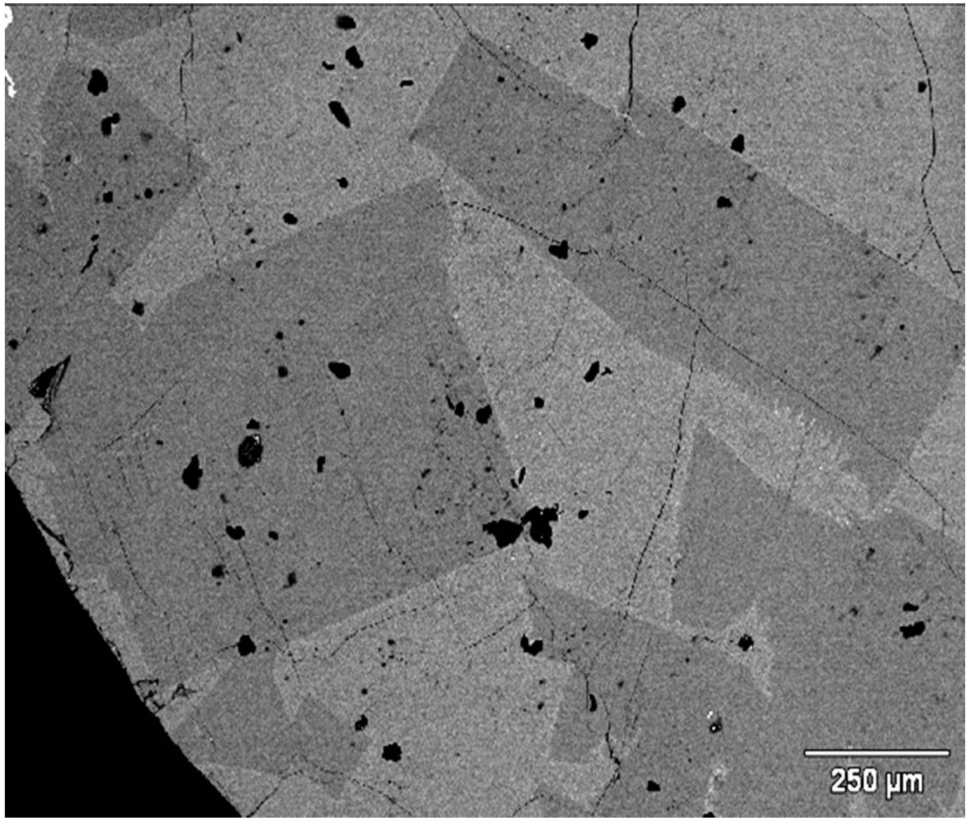
- Ex iron ore
- FeO nothing left
- SiO_2
- CaO added to neutralise the silica
- Al_2O_3
- MgO added for refractory protection

Blast furnace slag



Blast furnace slag

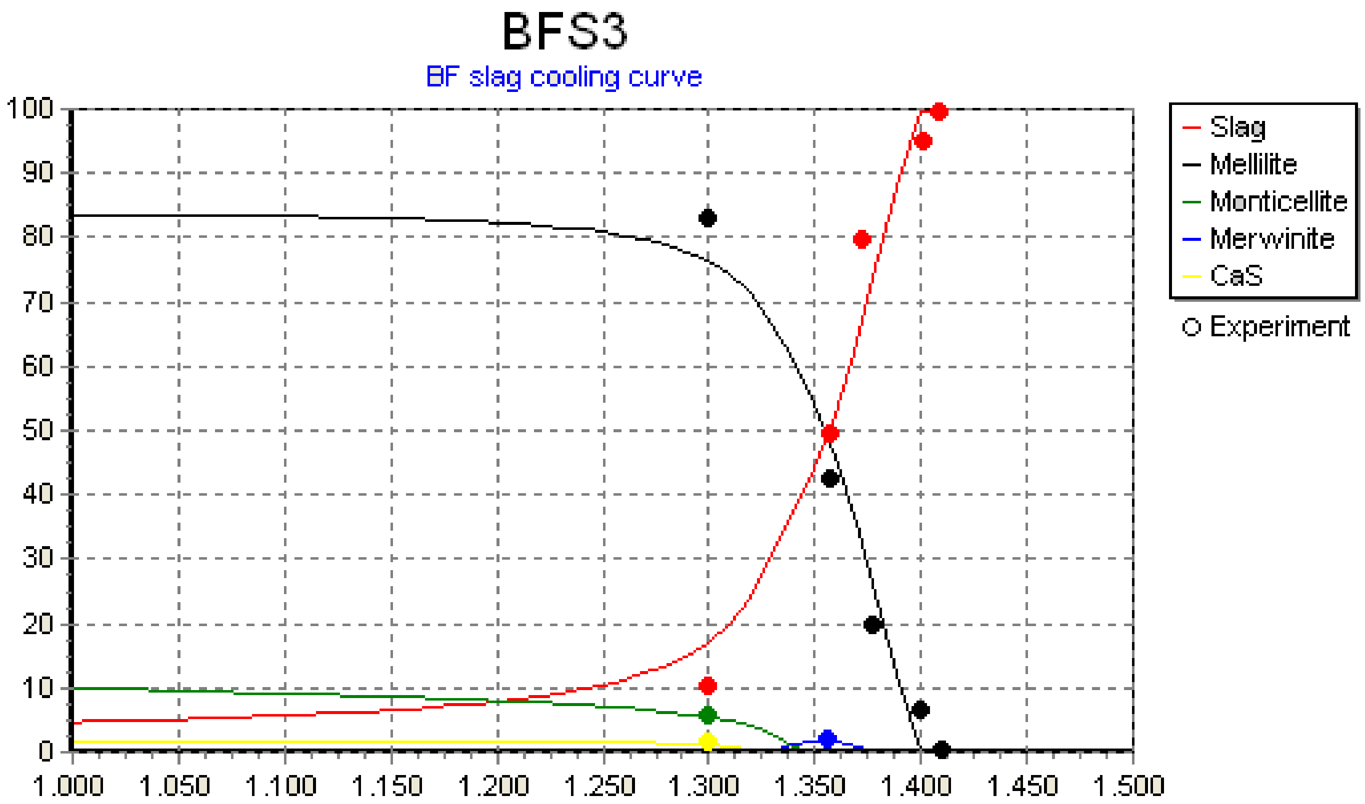




Blast furnace slag

Mass fraction of crystals observed?

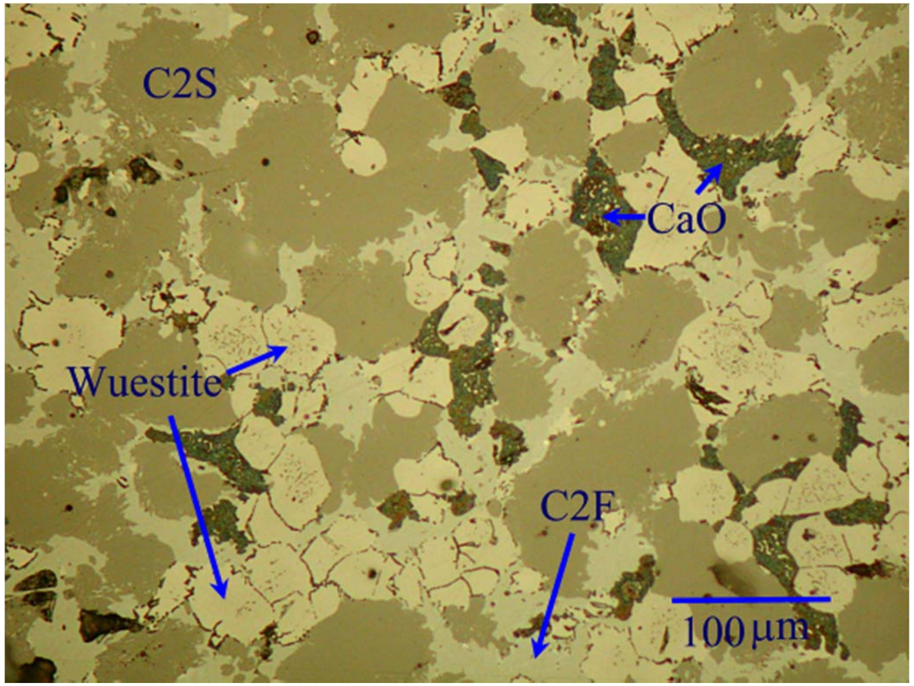
100% *Al_2O_3% in slag = x*Al_2O_3 in crystal + (100-x) * Al_2O_3 in liquid
For all components optimise

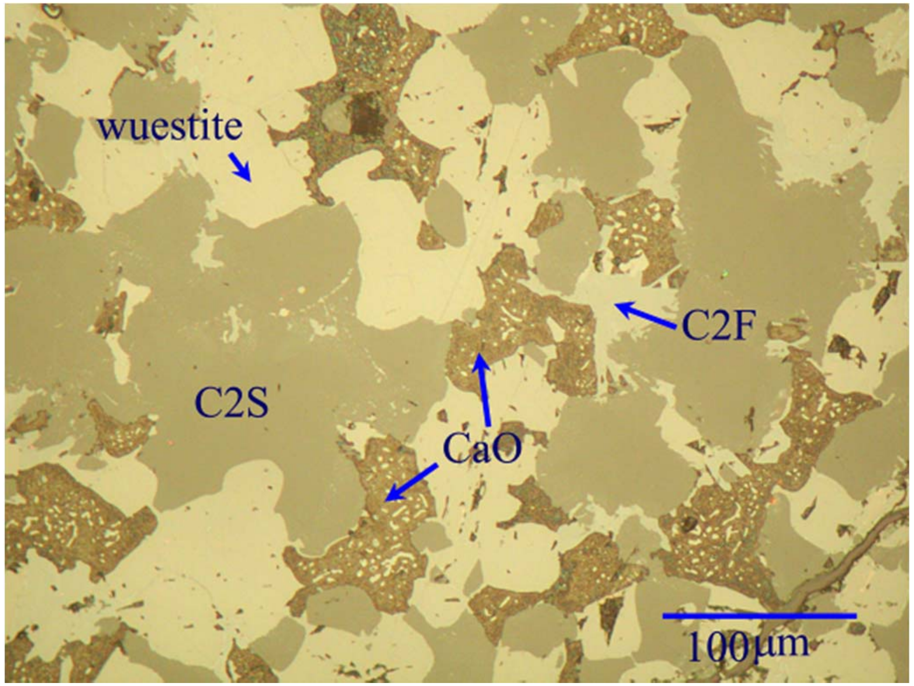


Blast furnace slag

- Need some minor adaptations of G(phase) or allow some systematic error which is NOT accepted
- Use full chemical analysis
- Prepare cst file within FACTSAGE
- Write dedicated software (e.g. in Delphi)
- Use ChemApp.dll (with saved cst file)

Converter slag

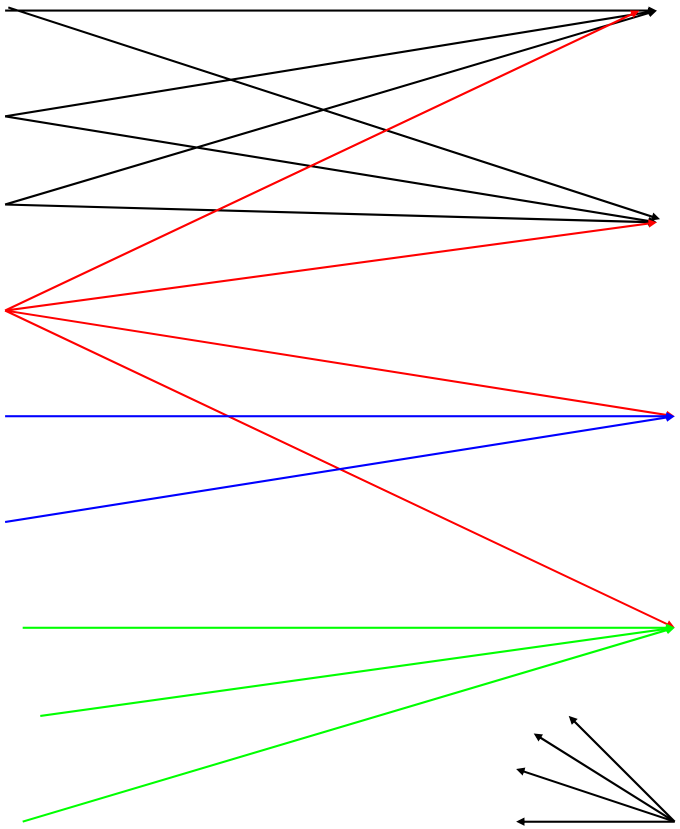




Components (9): FeO, MnO, MgO, CaO, SiO_2, P_2O_5, Al_2O_3, Fe_2O_3,TiO_2

Converter slag

- Components:
  - FeO
  - MnO
  - MgO
  - CaO
  - SiO_2
  - P_2O_5
  - Al_2O_3
  - Fe_2O_3
  - TiO_2

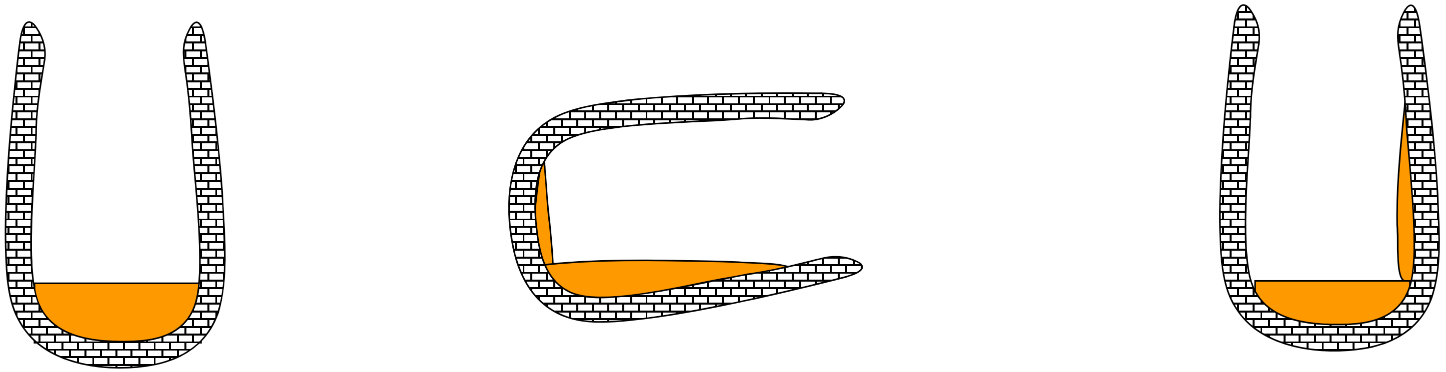


Phases:

- MgO wustite (MgO,FeO,MnO,CaO)
- free CaO (CaO,MnO,FeO,MgO)
- silicate ($Ca_2(Si,P)O_4$)
- ferrite ($Ca_2(Fe,Al,Ti)_2O_5$)
- slag (liquid)

Slag washing

- Purpose: protective slag layer on top of refractory



- Enhance life-time converter

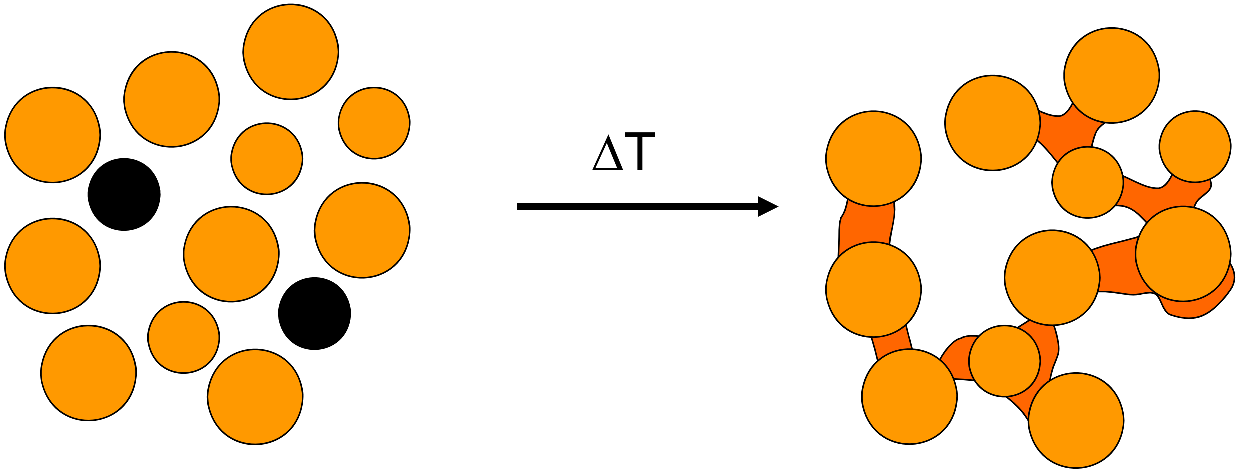
Key issue: viscosity □ S/L ratio

Slag washing

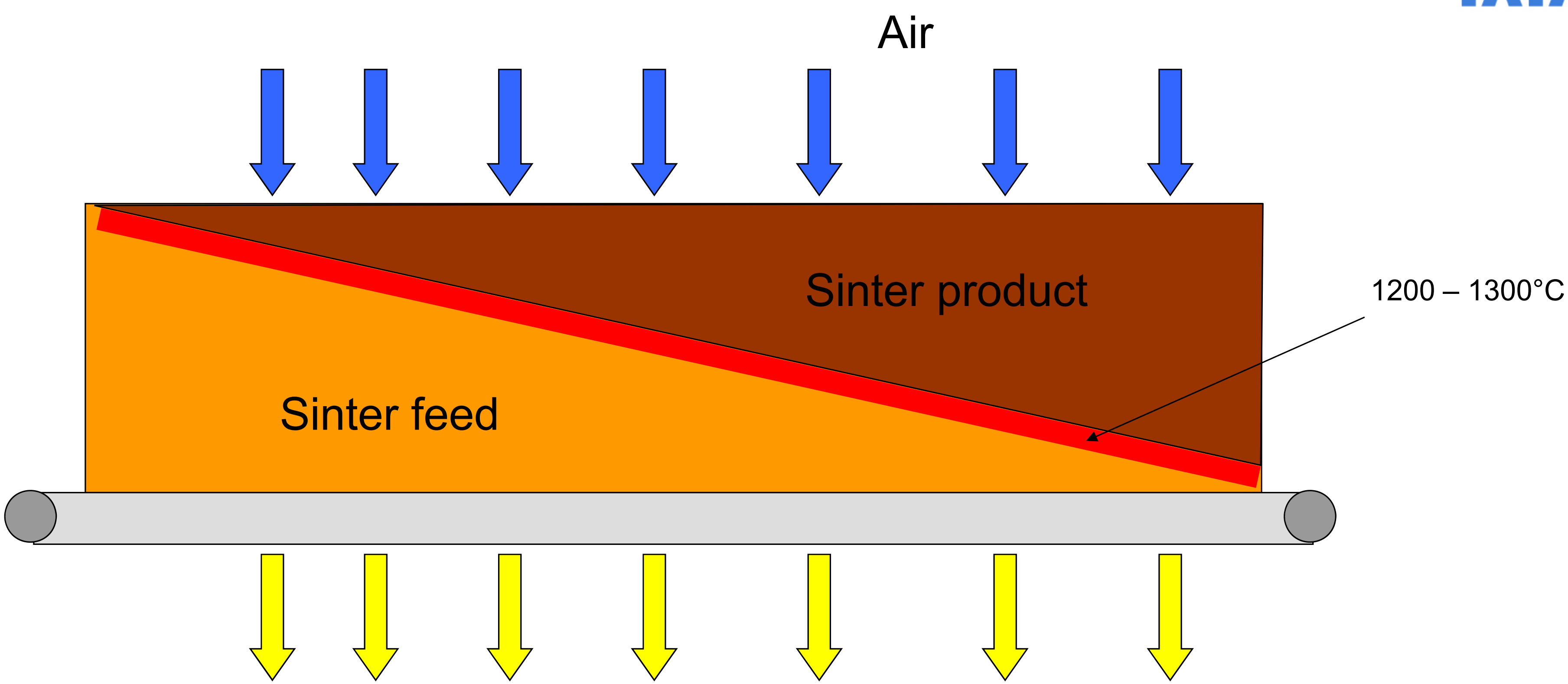
- Simple control: Temperature   desired S/L ratio
- Add cool slag to decrease T to the right level
- □Heat balance calculation (data ex FACTSAGE)

Sinter process

- Input preparation for blast furnace
- Dust/ fine ore □ Lumps



Sinter process

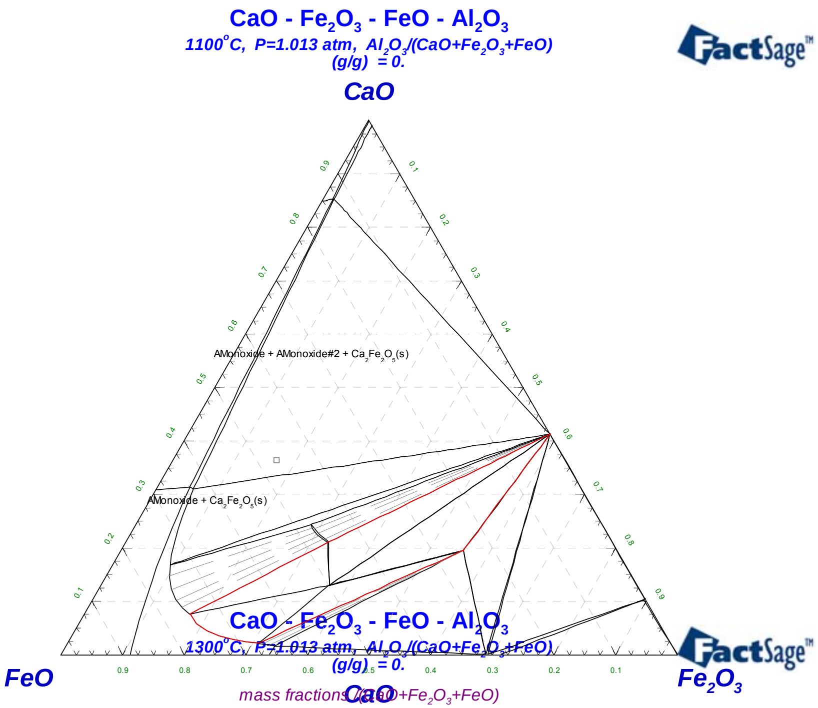


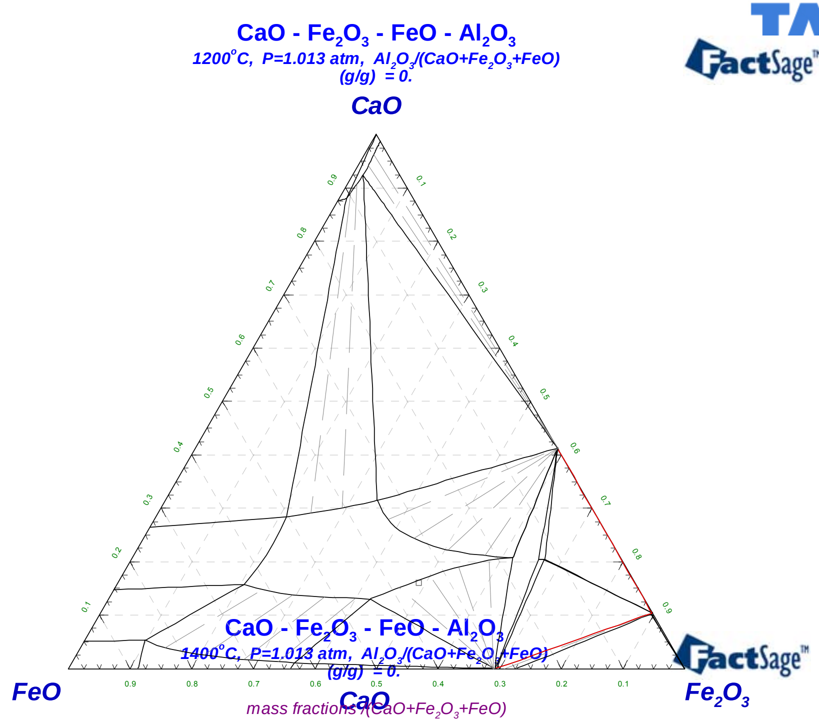
Iron ore: Fe_2O_3
SiO_2
Al_2O_3

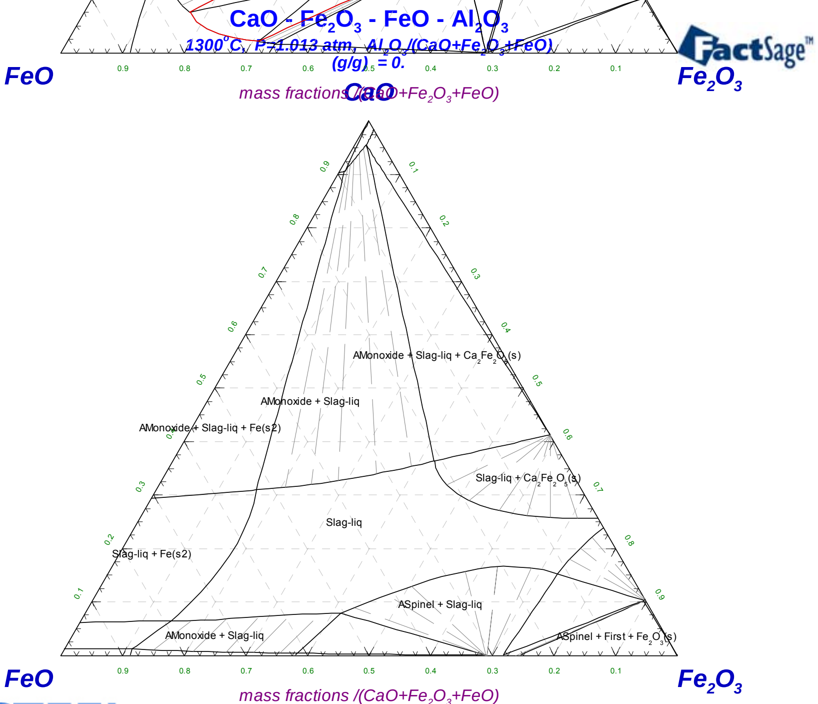
CaO
C
additives

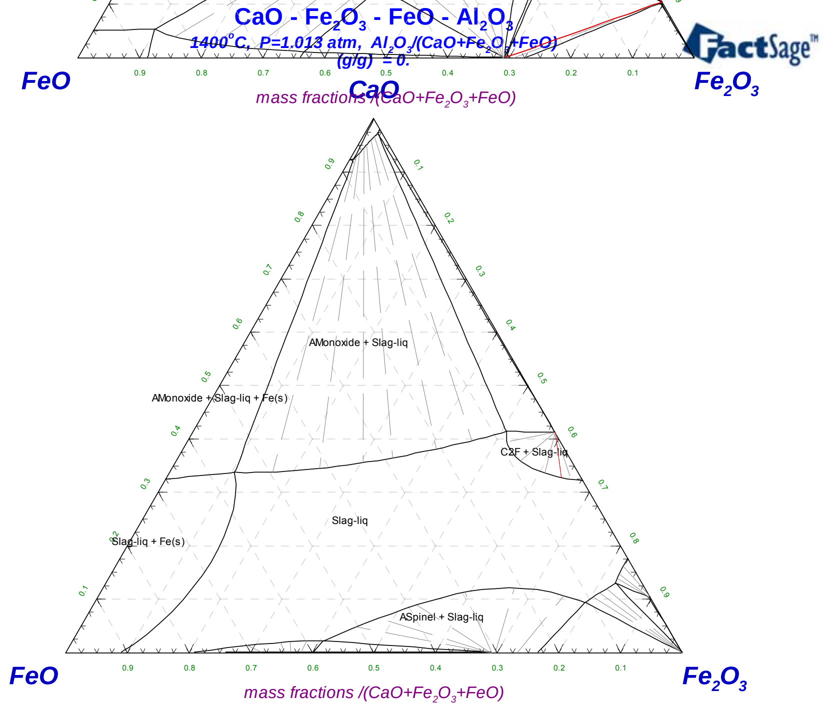
Fe_2O_3 + FeO + CaO

Sinter process

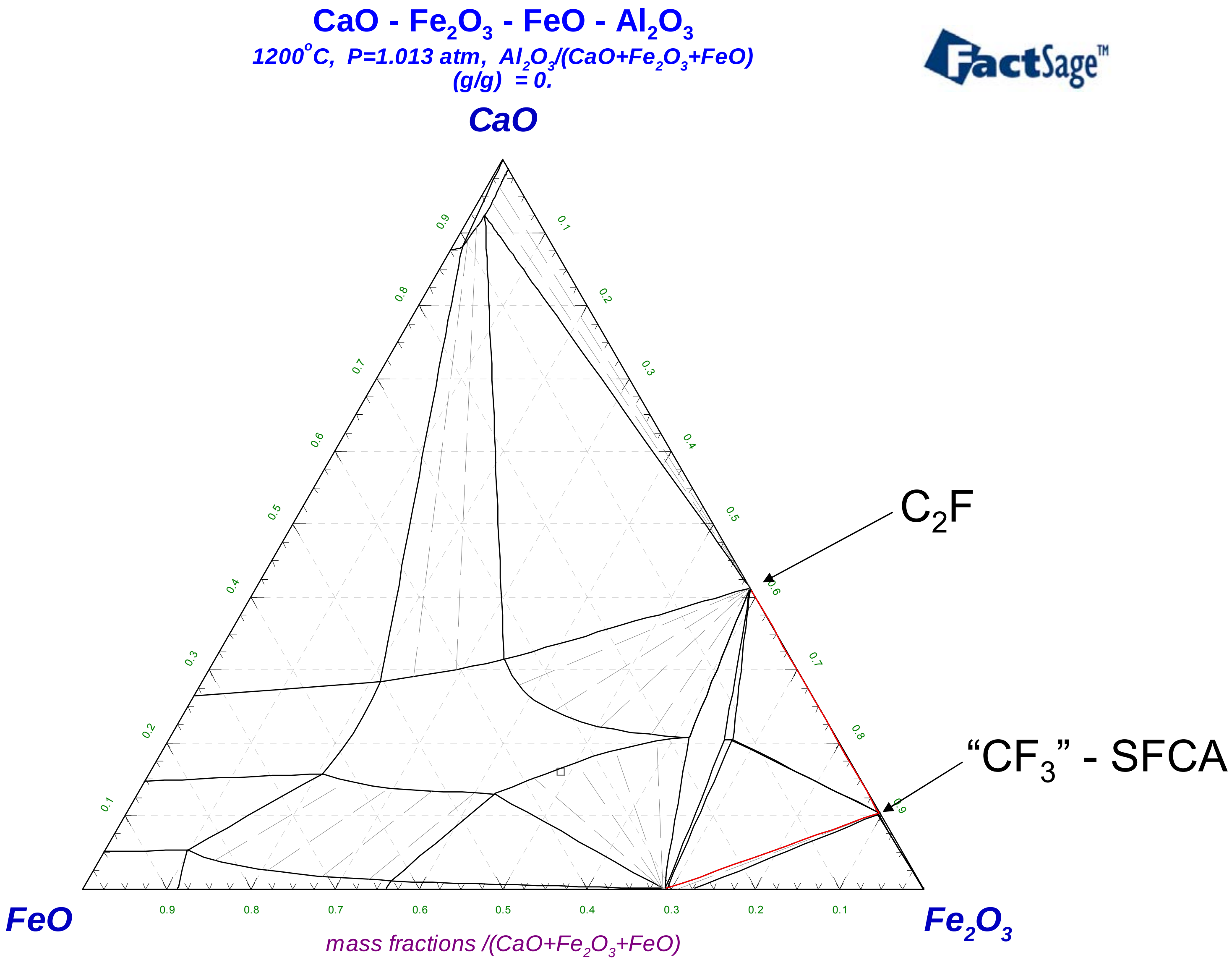








Sinter process



How to model

Thermodynamics == FACT

NOT by using the interactive FactSage interface

Step 1. Organise data needed in FactSage !

Step 2. Make sub-database in FactSage !

This case: slag, metal, gas phase

Step 3. Use ChemApp.dll instead