State of the thermodynamic database for the BOFdePhos project

K. Hack, T. Jantzen, GTT-Technologies, Herzogenrath

Contents

- „Old“ LD converter model database
- Necessary components for BOFdePhos
- Contributions covering sulphur
- Contributions covering phosphorous

The „old“ thermodynamic data

- **Source**: THERDAS system and literature
- **Elementary components**:

  Ar, Al, C, Ca, Fe, H, O, S, Si, Mg, B, N, Mn, P
- **Solution phases**:

  GAS (*ideal*): 60 species in total

  SLAG (*IRSID cell model*):

  CaO, MgO, Al2O3, SiO2, FeO,

  Fe2O3, MnO,(PO)2O3

The „old“ thermodynamic data

- **Solution phases** (continued):

  LIQ_Fe (*Wagner dilute sol.*)

  Fe and Al,C,Ca,O,S,Si,Mg,B,N,H,Mn,P

  BCC_Fe (*Wagner dilute sol.*)

  Fe and Al,B,C,N,O,S,Si,Mn,P,H

  FCC_Fe (*Wagner dilute sol.*)

  Fe and Al,B,C,N,O,S,Si,Mn,P,H

The „old“ thermodynamic data

- **Solution phases** (continued):

  MeS (*ideal*)

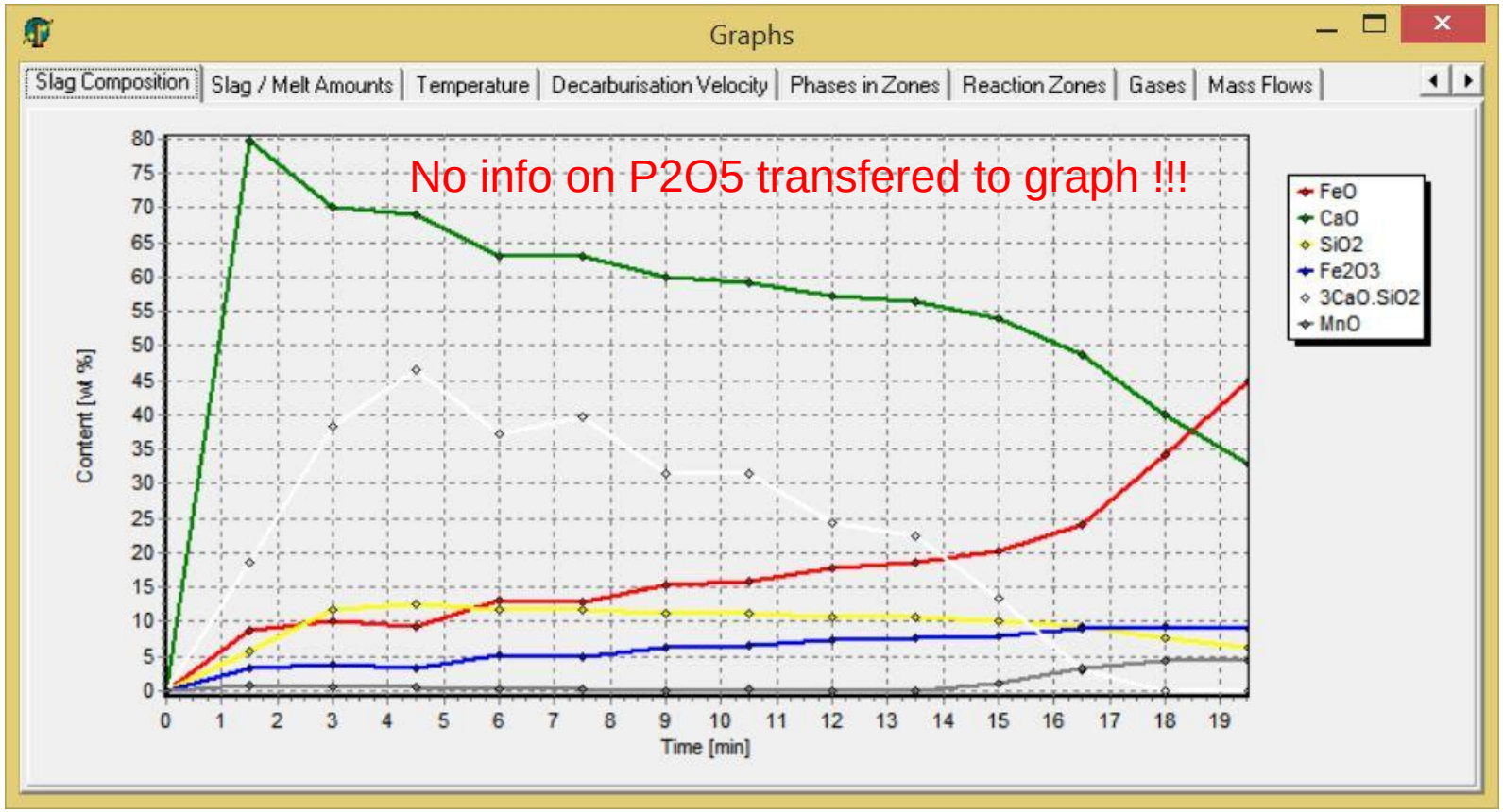
  CaS,FeS,MnS

- **Stoichiometric phases**:

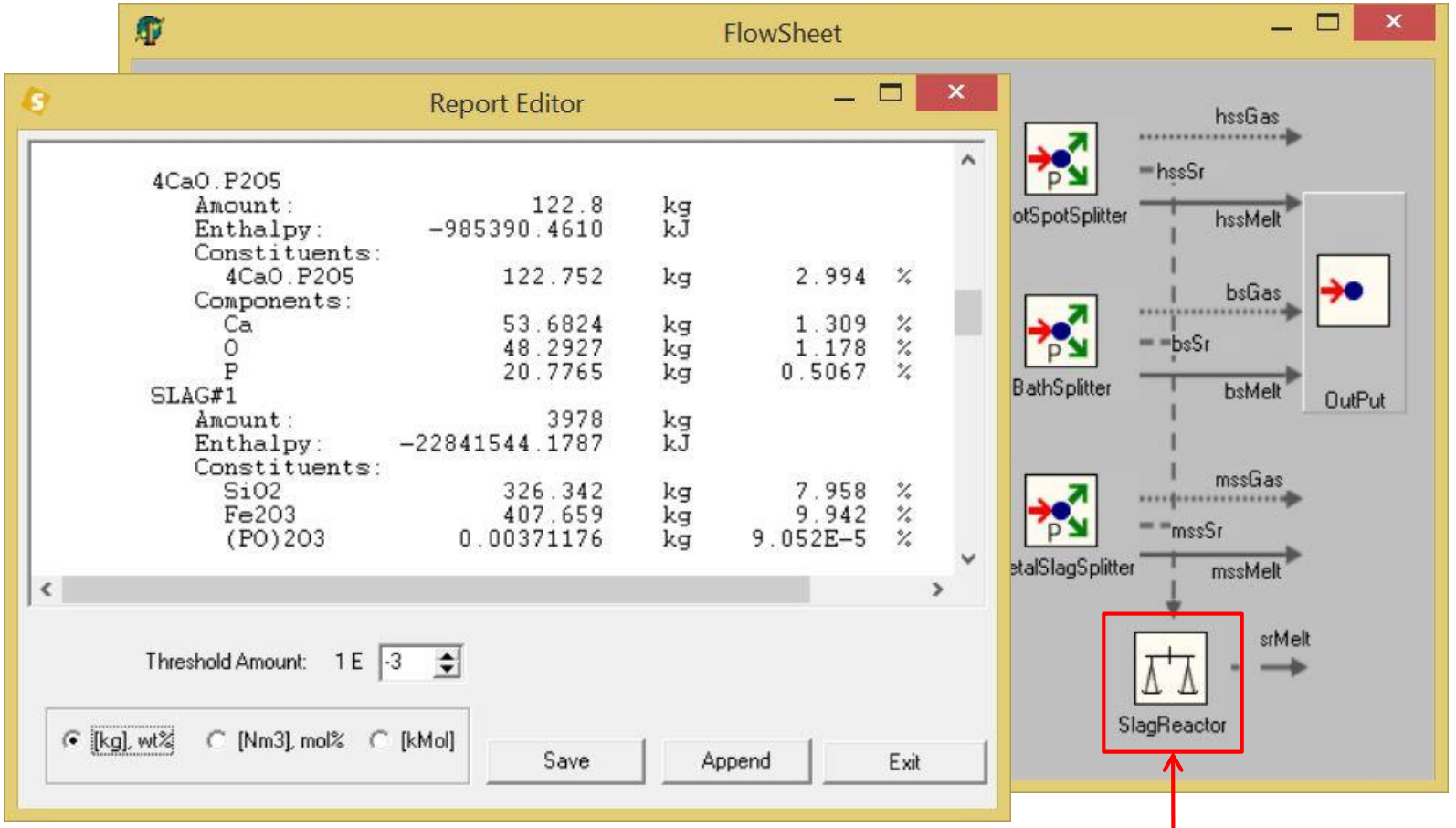
  100 compounds, among these P2O5 and three calcium phosphates

  CaCO3, MgCO3, dolomite as input substances

Output from LD-Sage
„old“ database, Jalkanen reference data



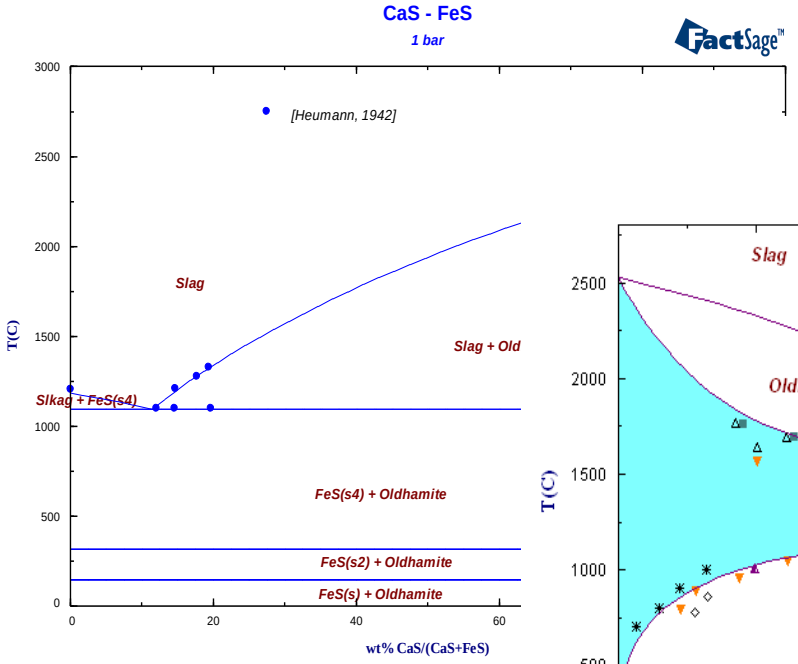
Output from LD-Sage
„old“ database, Jalkanen reference data

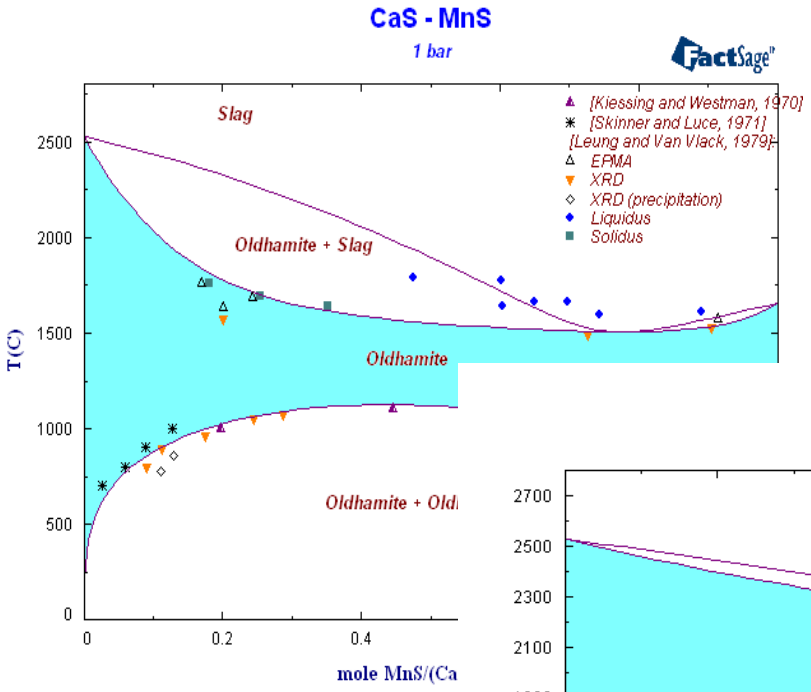


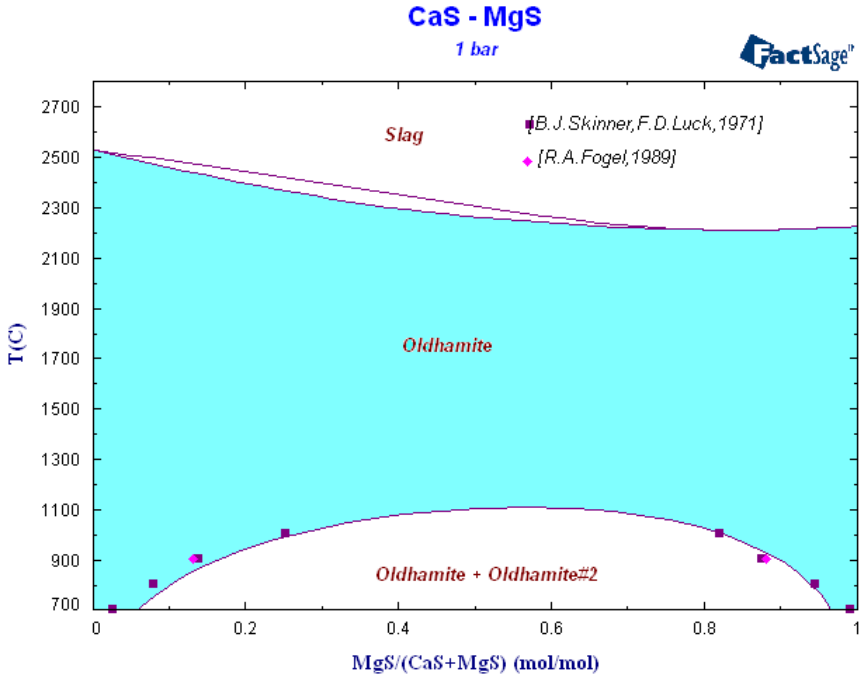
Click here to obtain report !

Thermodynamic database

Sulphide subsystems

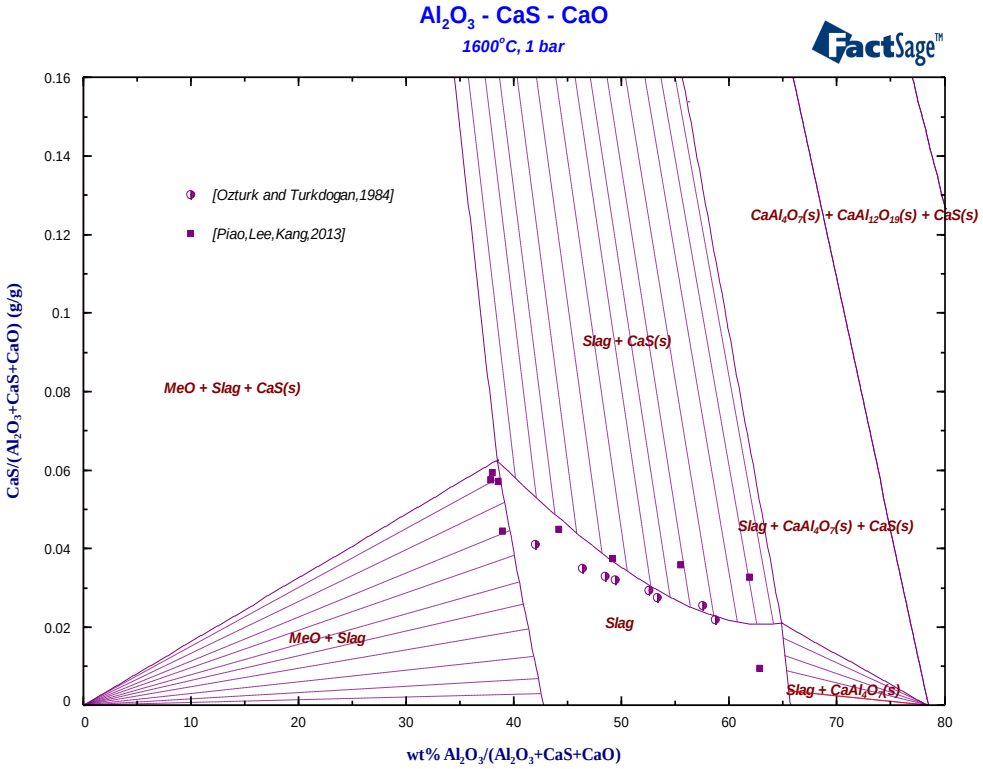


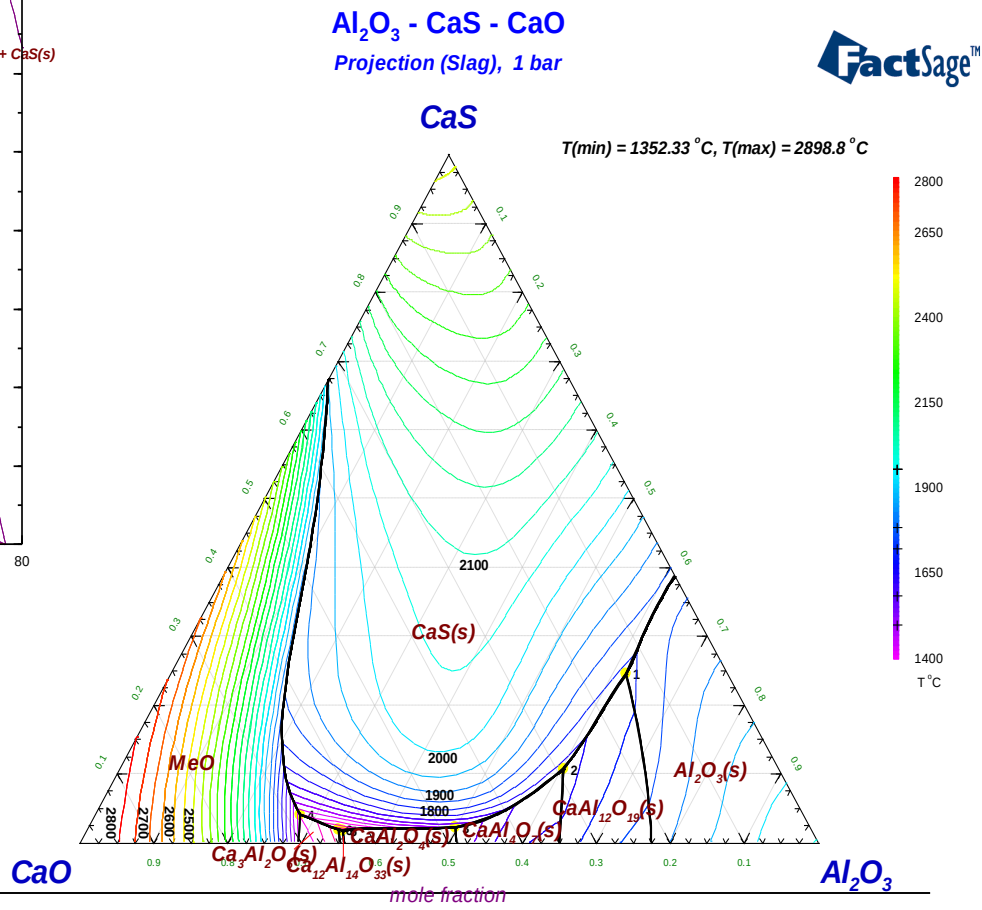




Thermodynamic database

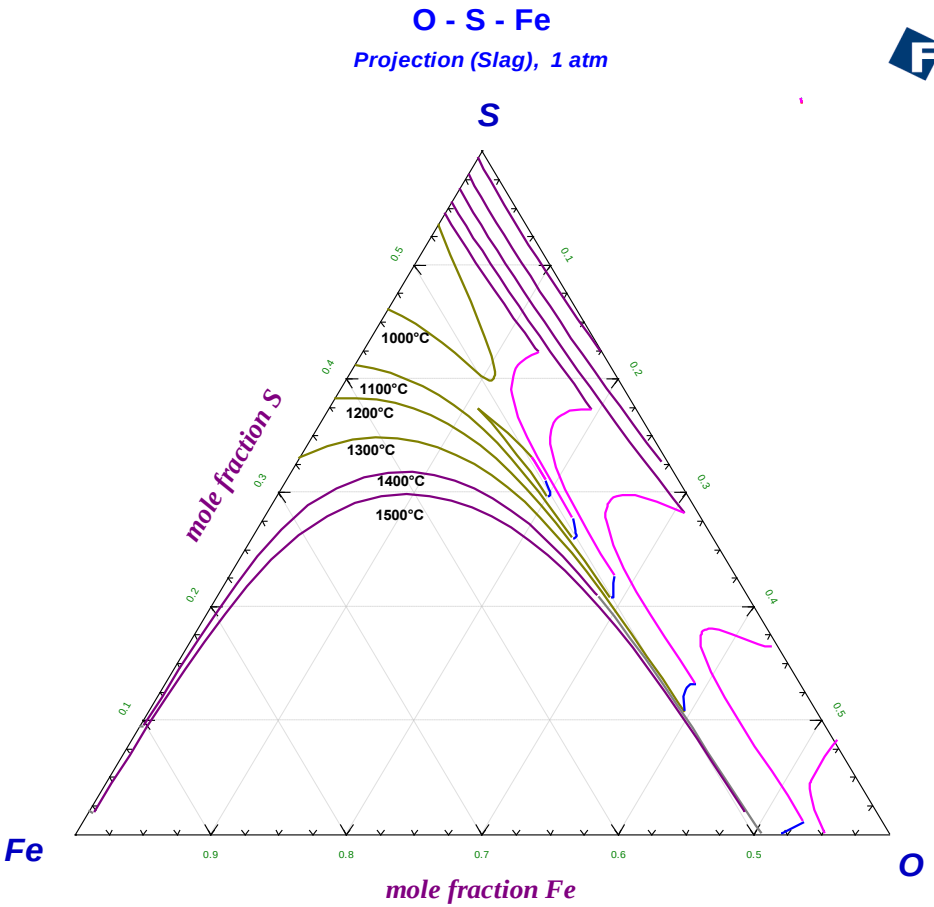
Ternary systems with sulphide component



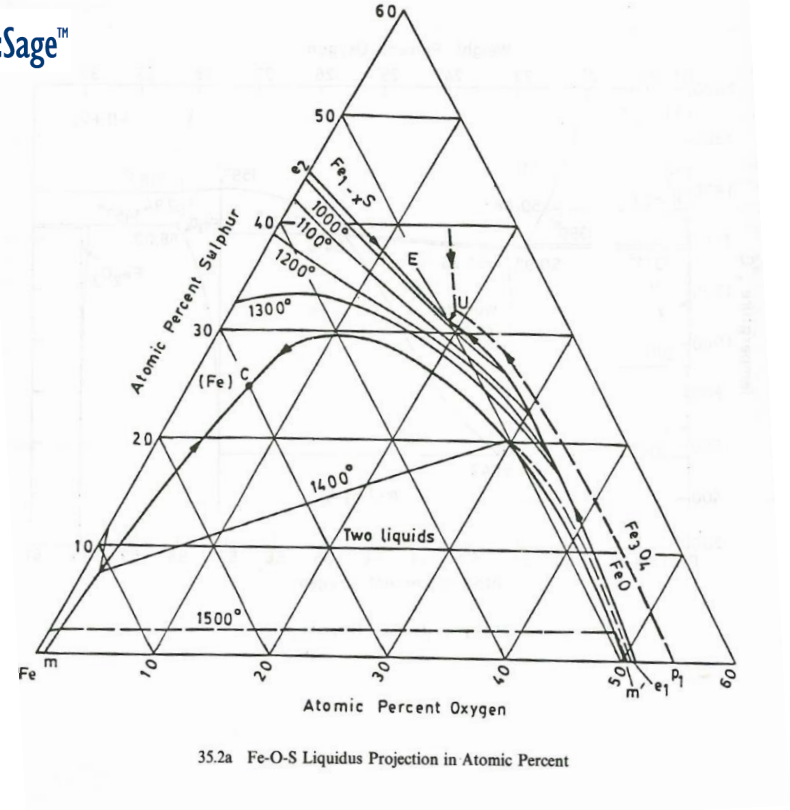


Thermodynamic database

The Fe-O-S system



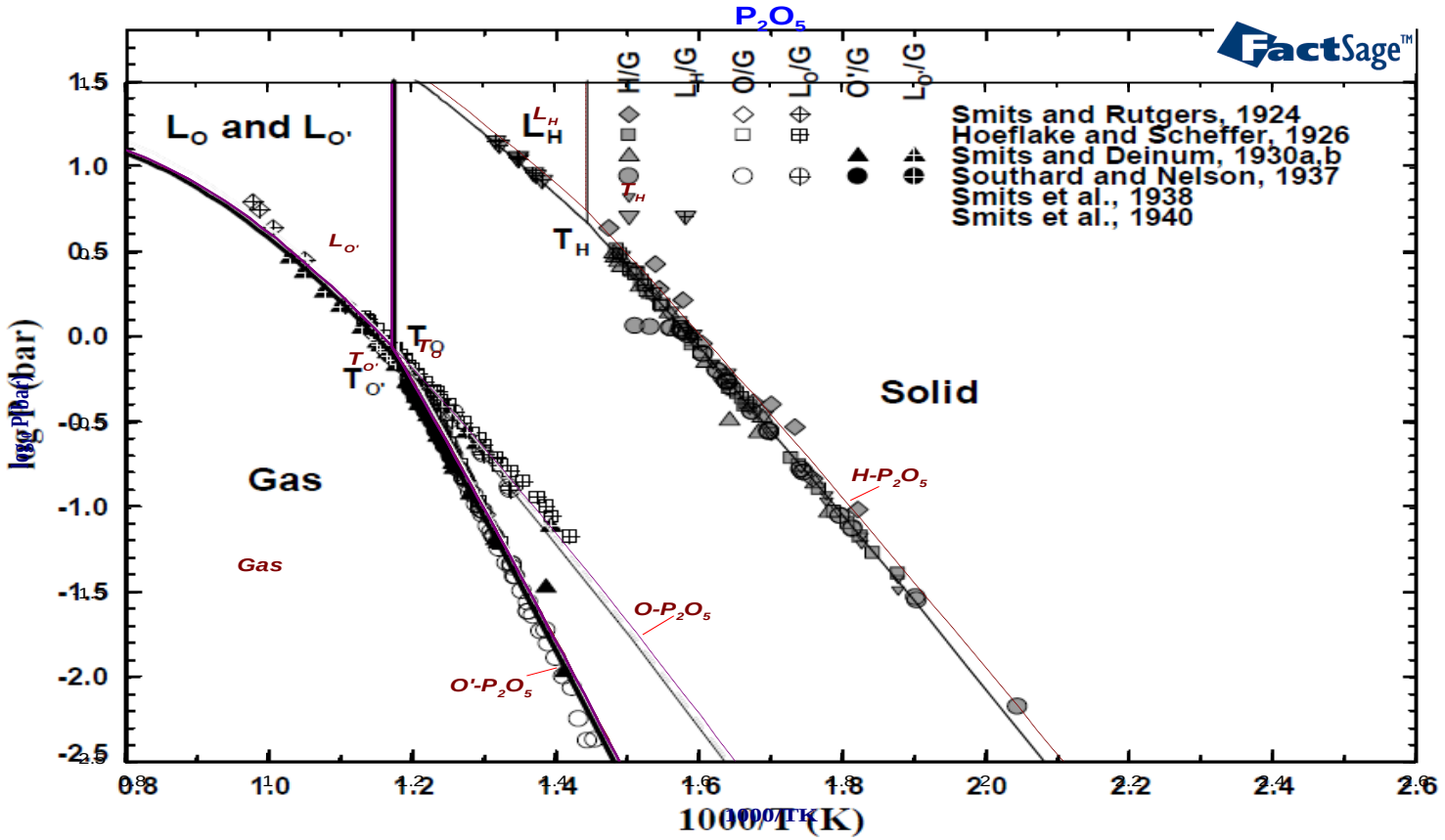
FactSage™



V. Raghavan, Phase diagrams of Ternary Iron Alloys, Part 2, Ternary systems containing Iron and Sulphur, The Indian Institute of Metals, Calcutta,1988.

Thermodynamic database

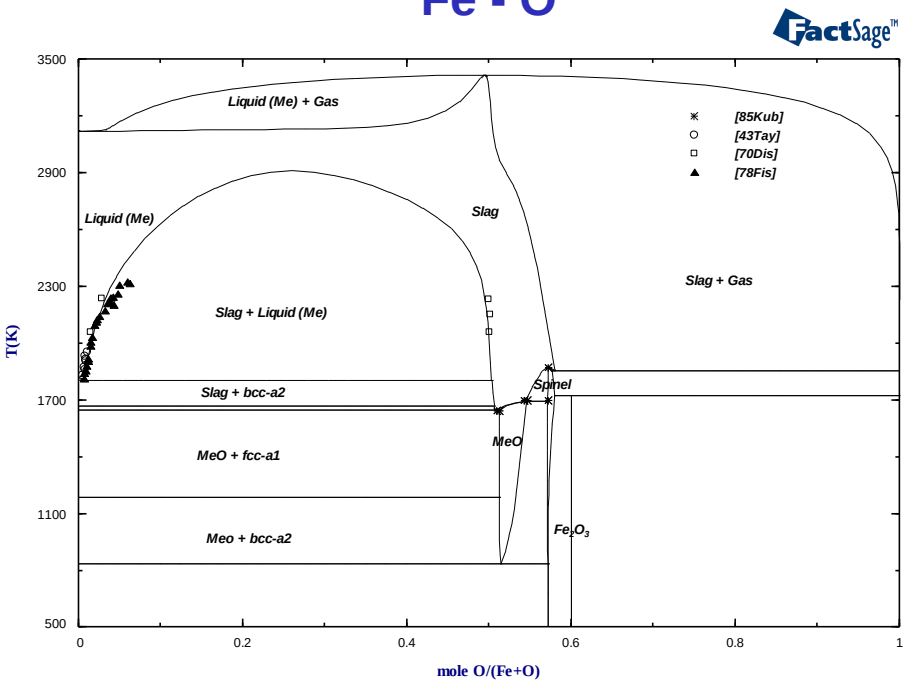
Data for pure P2O5



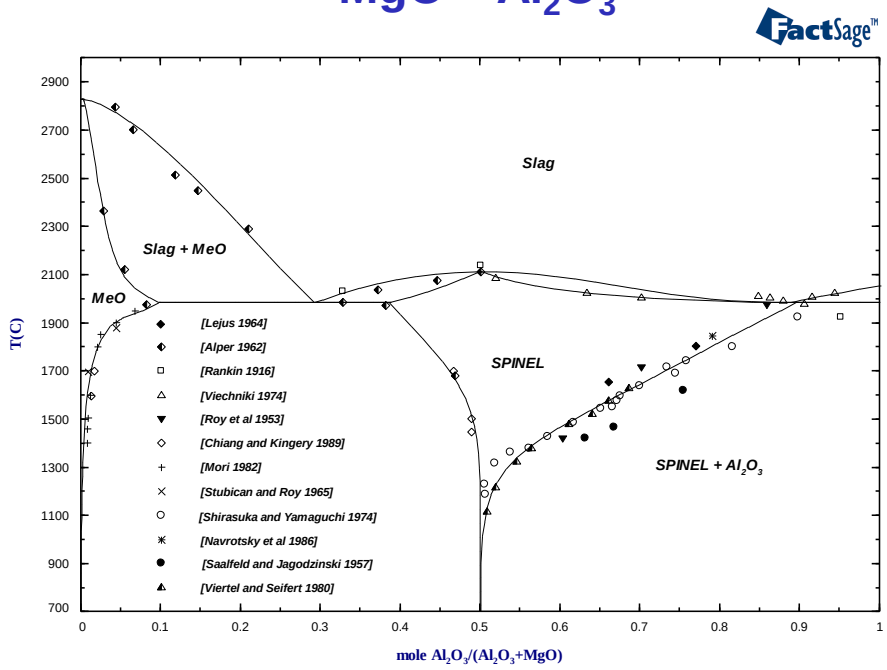
Thermodynamic database

Binary systems, including Fe-X

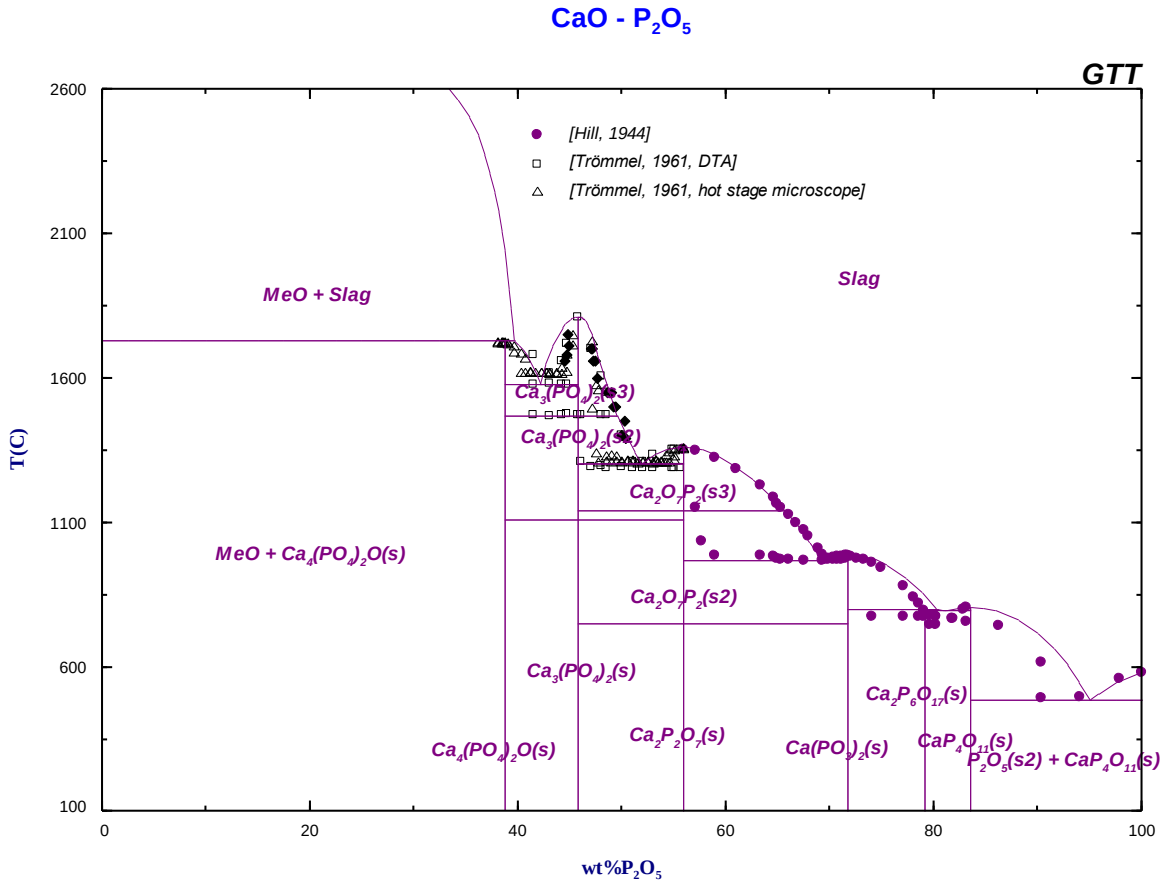
Fe - O

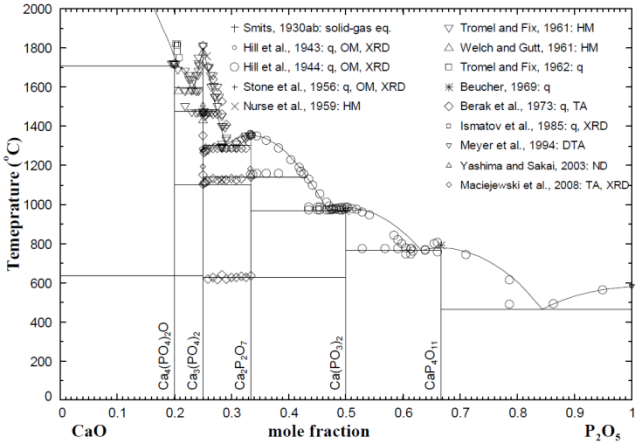


$MgO – Al_2O_3$



Thermodynamic database

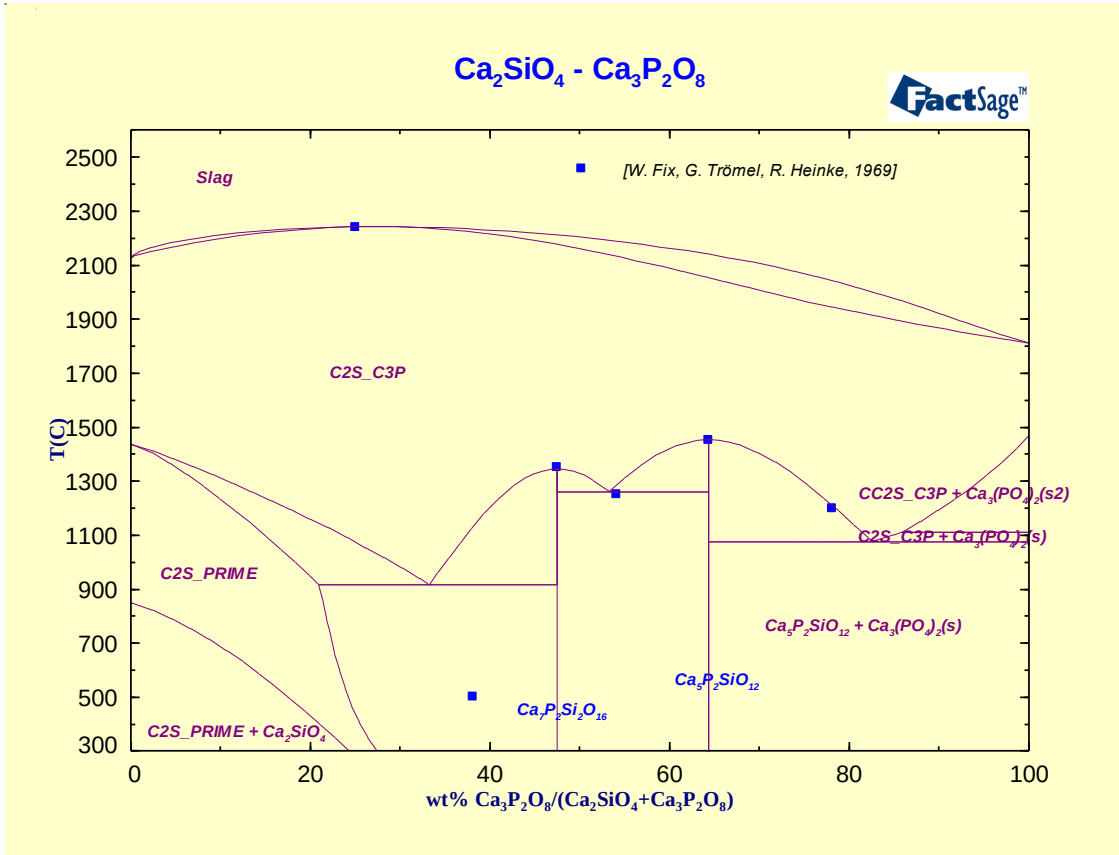


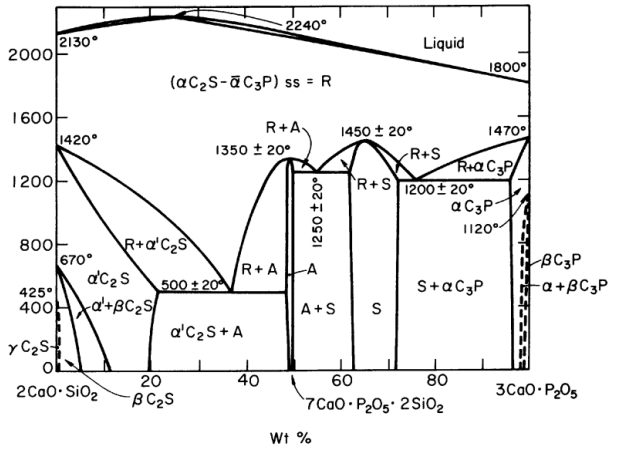


I.-H. Jung and P. Hudon, "Thermodynamic assessment of P_2O_5," *J. Am. Ceram. Soc.*, Vol. 95, No. 11, 2012.

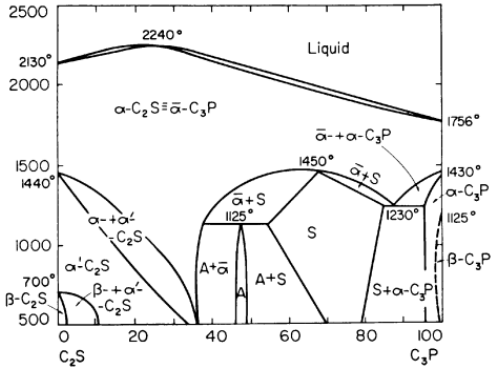
Thermodynamic database

Isopleth section Ca_2SiO_4-$Ca_3P_2O_8$



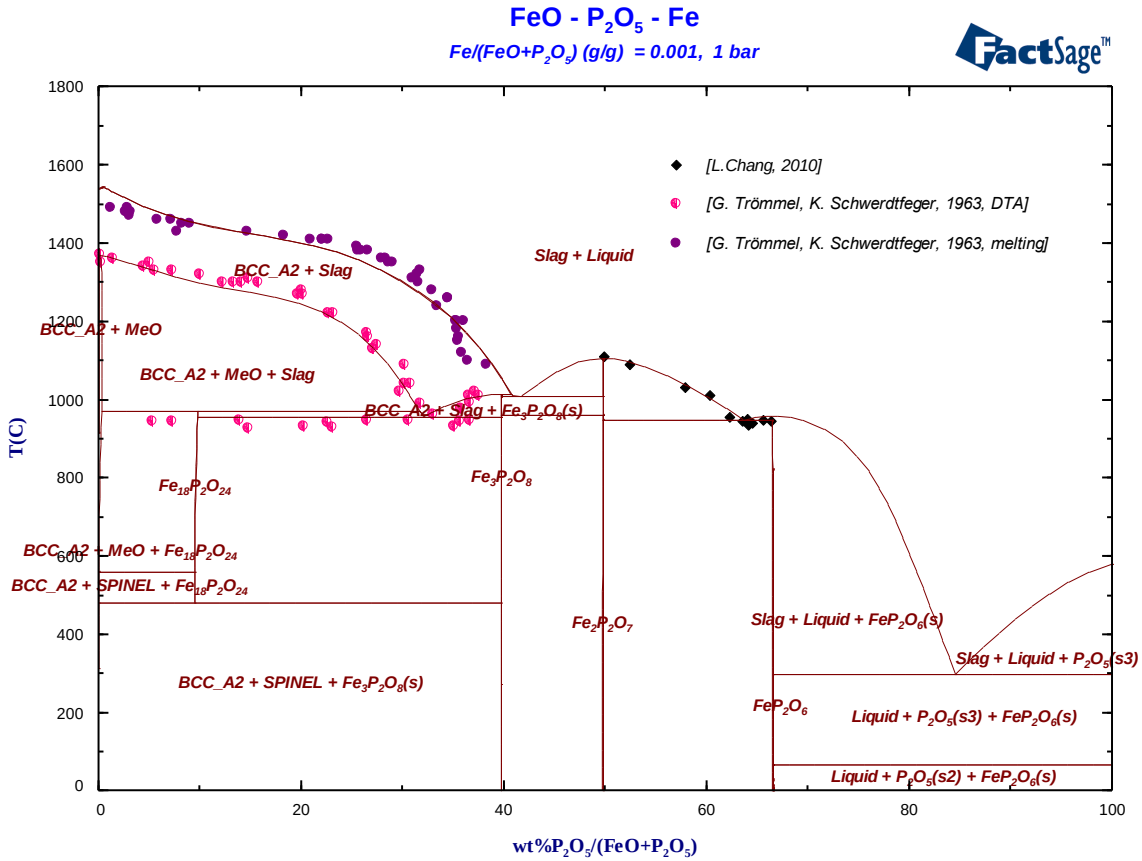


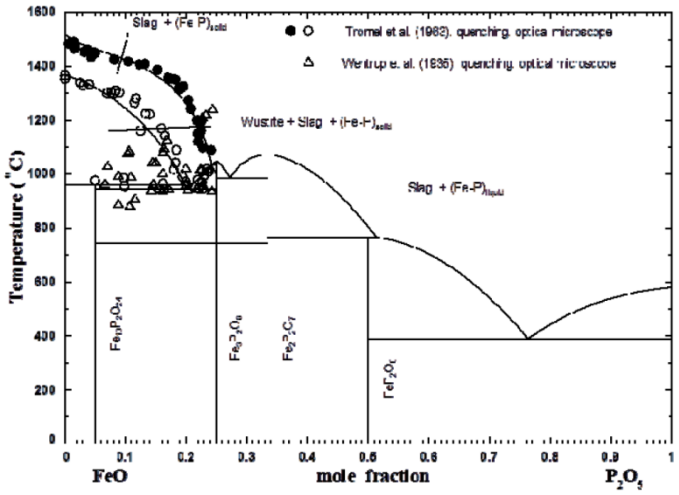
W. Fix, H. Heymann, and R. Heinke, J. Am. Ceram. Soc., 52 [6] 346-347 (1969).



R. W. Nurse, J. H. Welch, W. H. Gutt, J. Chem. Soc.,1077-1083 (1959).

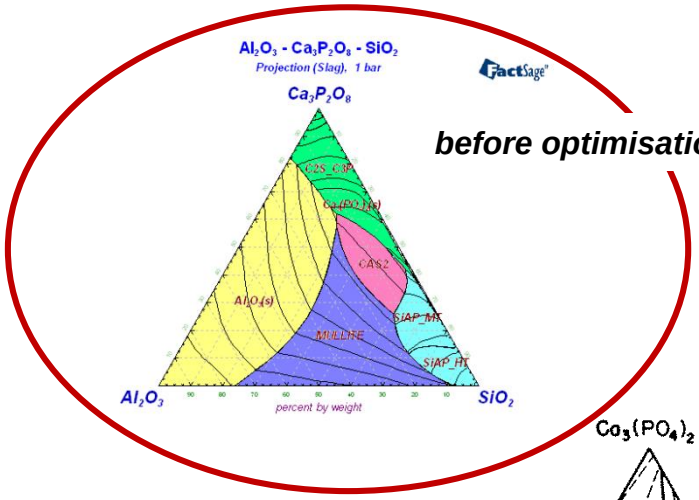
Thermodynamic database



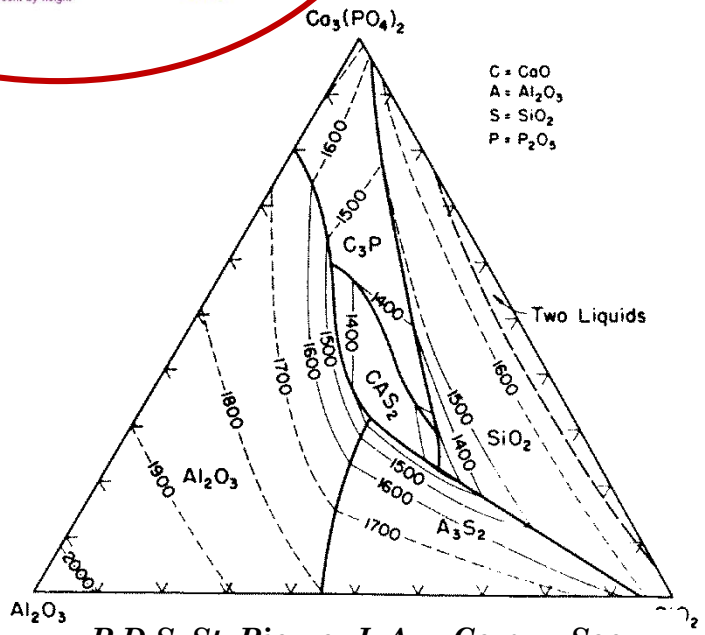


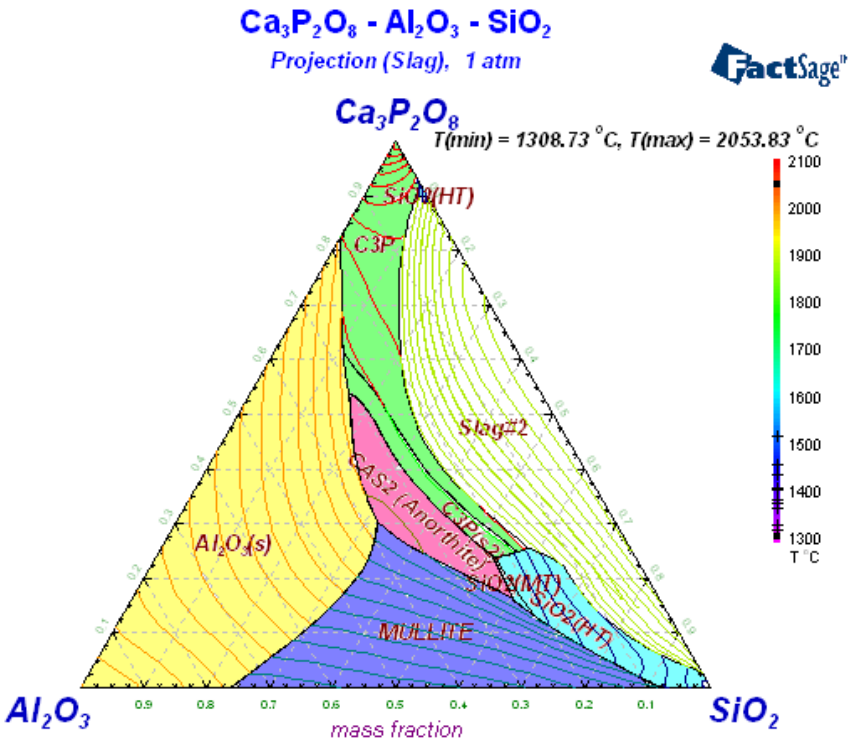
I.-H. Jung and P. Hudon, "Thermodynamic assessment of P_2O_5," *J. Am. Ceram. Soc.*, Vol. 95, No. 11, 2012.

Liquidus surface in $Ca_3P_2O_8$-Al_2O_3-SiO_2



before optimisation





P.D.S. St. Pierre, J. Am. Ceram. Soc., 39[4], (1956), pp. 147-150.

Thermodynamic database

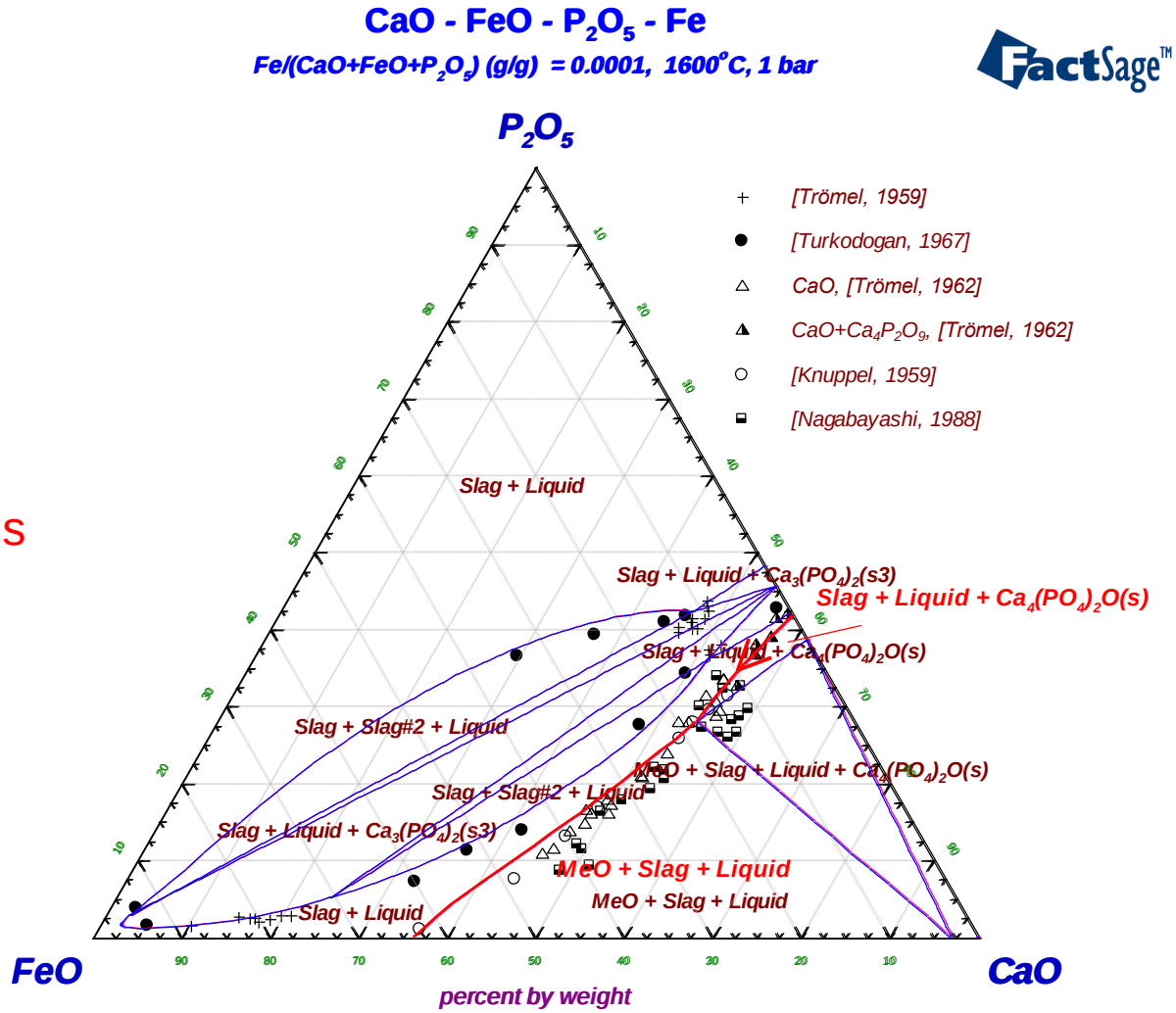
Phosphorous containing phases in present database:

Gas:	P, P2O5 as well as N2,O2,CO,CO2,SiO and many others
Liquid oxide:	P2O5 as well as 23 P2O5-containing associate species
Solid solutions:	7 phosphates 1 silicate-phosphate (C2S-C3P) 4 phosphates with limited SiO2 solubility 4 silicates with limited P2O5 (PO4) solubility
Stoichiometric compounds:	P and P2O5 as well as 56 phosphides, phosphates or silico-phosphates
Liquid-Fe:	Mg, Mn, Ca, O, S, P

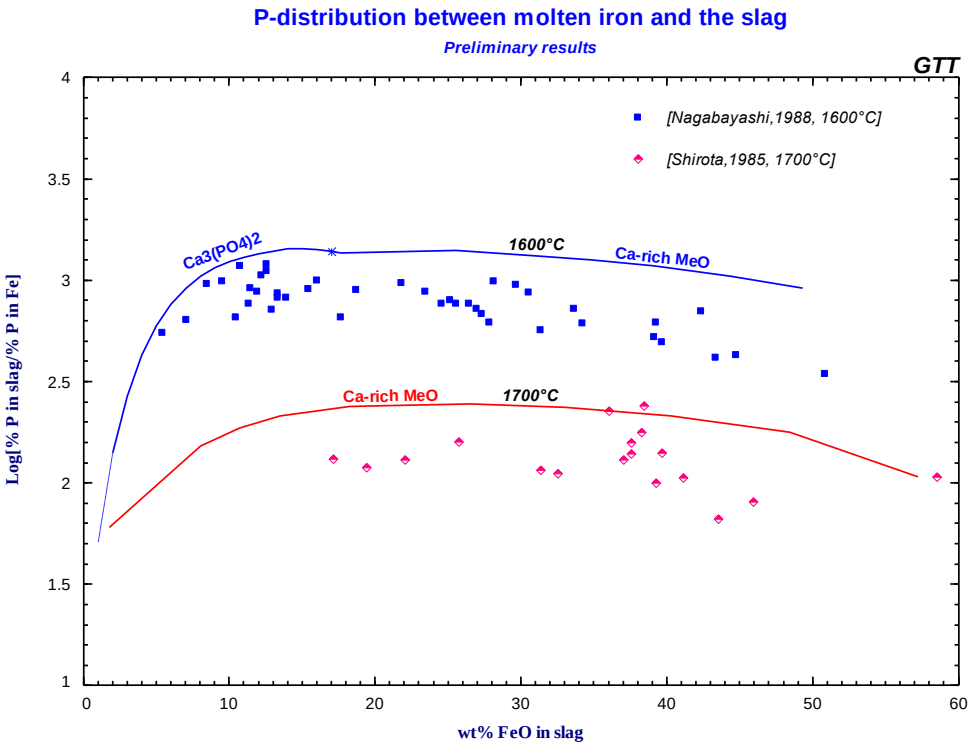
Wish-lists ?????
Fe-liq: Fe-P-C-Si-Mn-O (Mg,S,Al,Cr)
Slag: CaO-MgO-MnO-SiO2-Al2O3-FeO-Fe2O3-P2O5 (CaS,FeS,MgS,MnS)

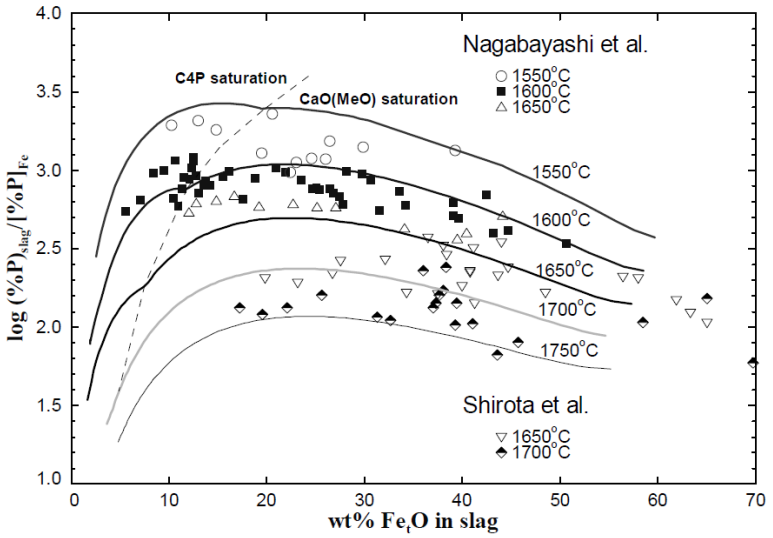
Phosphorous Distribution

Red line → Phosphorous Capacity



Phosphorous Distribution





In-Ho Jung et al.

High Temp. Mater. Proc. 2013; 32(3): 247–254

Summary and Outlook

A self-consistent thermodynamic database for the system

CaO-MgO-Al_2O_3-FeO-Fe_2O_3-MnO-Mn_2O_3-P_2O_5-SiO_2
with inclusion of S in form of
CaS-MgS-FeS-MnS as well as Al_2S_3, Na_2S, K_2S

is underway. The GTT Oxide database is a useful source for standard systems. BOFdePhos-specific data are being assessed.

The new database will be used to generate an application oriented datafile that is compatible with the ChemApp Programmers Library which is used in SimuSage and subsequently in the converter model LD-Sage.

Thank you for your attention !