

# State of the thermodynamic database for the BOFdePhos project

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# 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, Al<sub>2</sub>O<sub>3</sub>, SiO<sub>2</sub>, FeO,  
Fe<sub>2</sub>O<sub>3</sub>, MnO,(PO)<sub>2</sub>O<sub>3</sub>



# 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



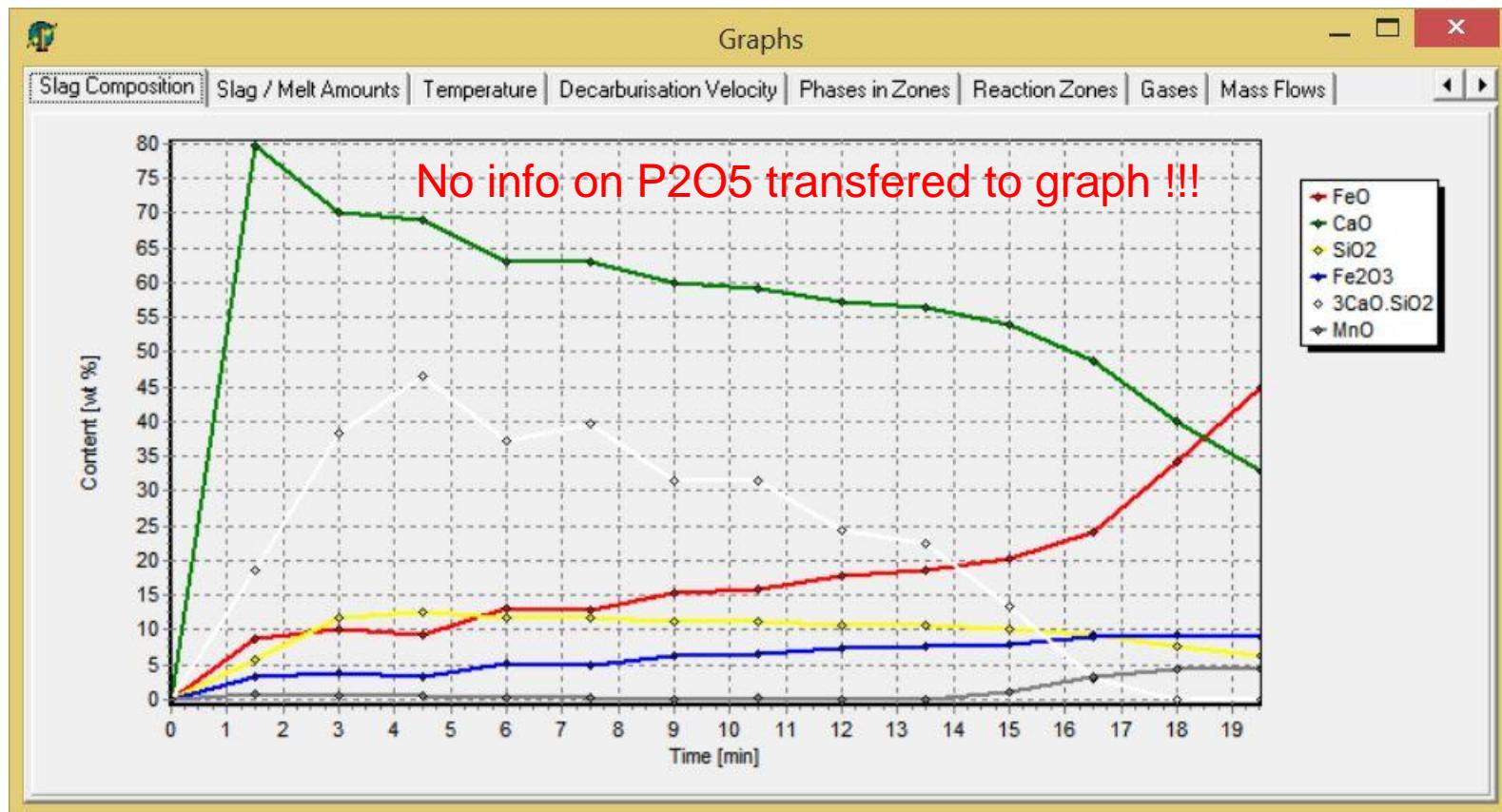
# The „old“ thermodynamic data

- **Solution phases** (continued):  
MeS (*ideal*)  
CaS,FeS,MnS
- **Stoichiometric phases**:  
100 compounds, among these P2O5 and three calcium phosphates  
CaCO<sub>3</sub>, MgCO<sub>3</sub>, dolomite as input substances



# Output from LD-Sage

## „old“ database, Jalkanen reference data



# Output from LD-Sage

## „old“ database, Jalkanen reference data

**FlowSheet**

**Report Editor**

4CaO.P2O5				
Amount:	122.8	kg		
Enthalpy:	-985390.4610	kJ		
Constituents:				
4CaO.P2O5	122.752	kg	2.994	%
Components:				
Ca	53.6824	kg	1.309	%
O	48.2927	kg	1.178	%
P	20.7765	kg	0.5067	%
SLAG#1				
Amount:	3978	kg		
Enthalpy:	-22841544.1787	kJ		
Constituents:				
SiO2	326.342	kg	7.958	%
Fe2O3	407.659	kg	9.942	%
(PO)2O3	0.00371176	kg	9.052E-5	%

Threshold Amount: 1 E -3

[kg], wt%    [Nm<sup>3</sup>], mol%    [kMol]

Save Append Exit

```

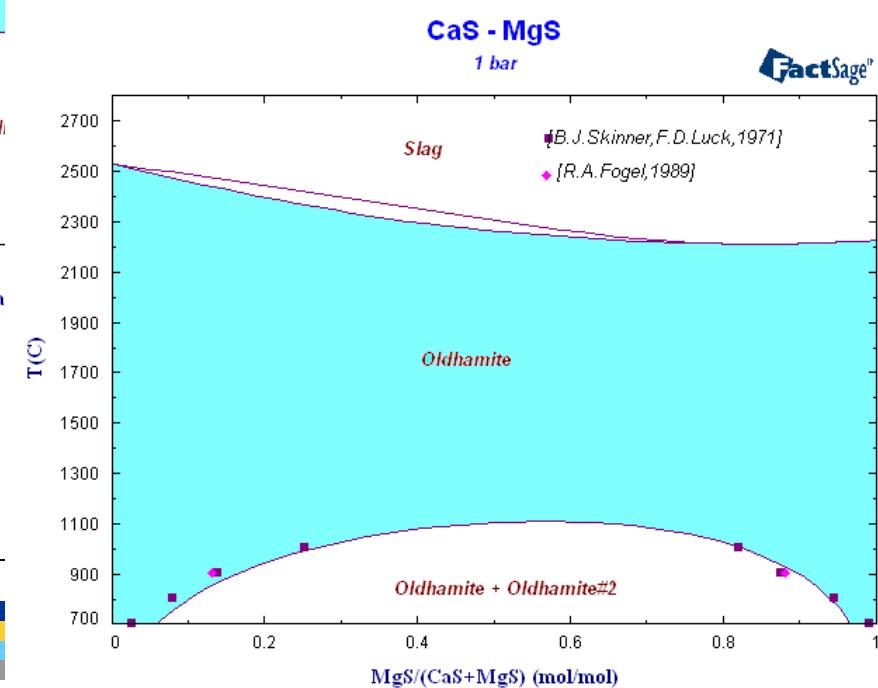
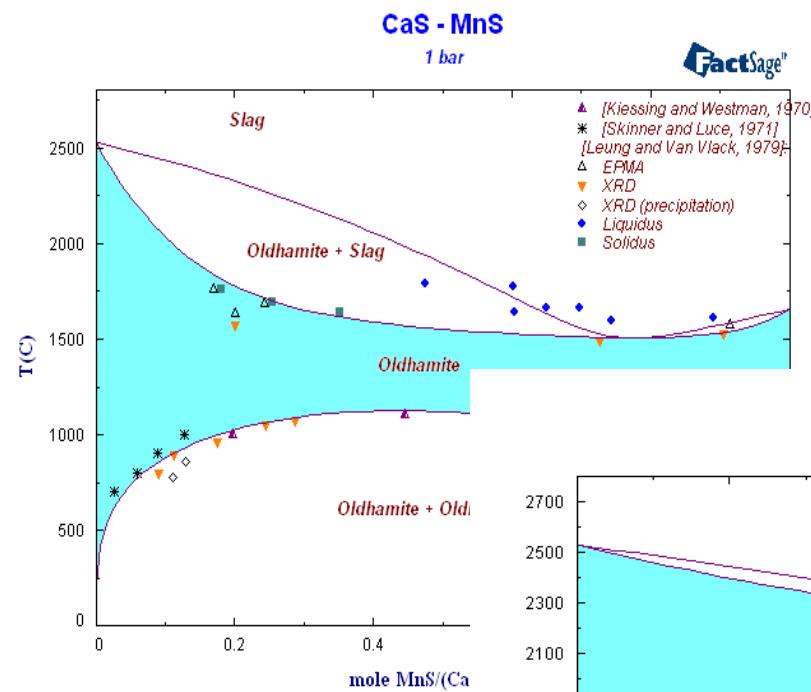
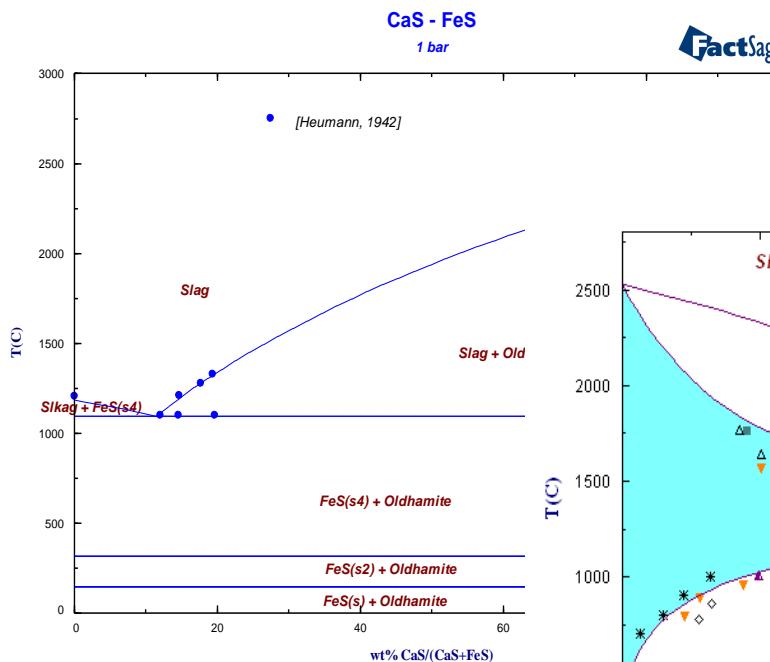
graph TD
    subgraph " "
        otSpotSplitter[otSpotSplitter] -- hssGas --> hssSr
        hssSr -- hssMelt --> hssMeltBox[ ]
        BathSplitter[BathSplitter] -- bsGas --> bsSr
        bsSr -- bsMelt --> bsMeltBox[ ]
        metalSlagSplitter[metalSlagSplitter] -- mssGas --> mssSr
        mssSr -- mssMelt --> mssMeltBox[ ]
        hssMeltBox --> OutPut[OutPut]
        bsMeltBox --> OutPut
        mssMeltBox --> SlagReactor[SlagReactor]
        SlagReactor -- srMelt --> OutPut
    end

```

Click here to obtain report !

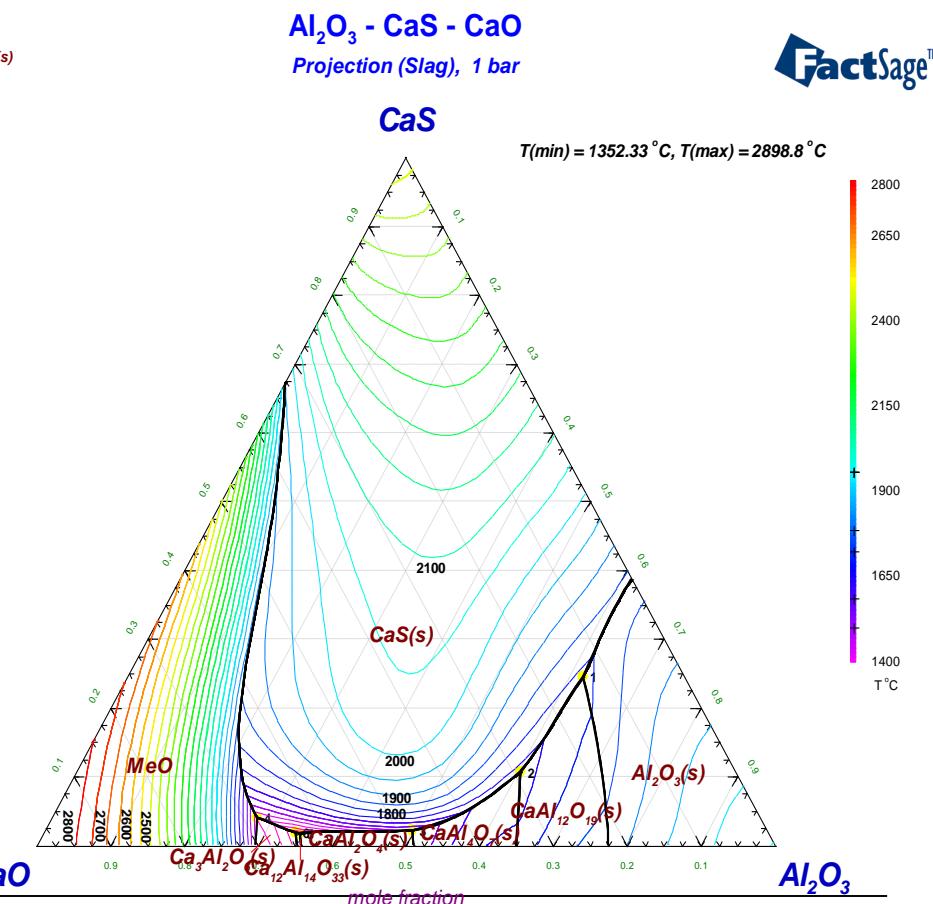
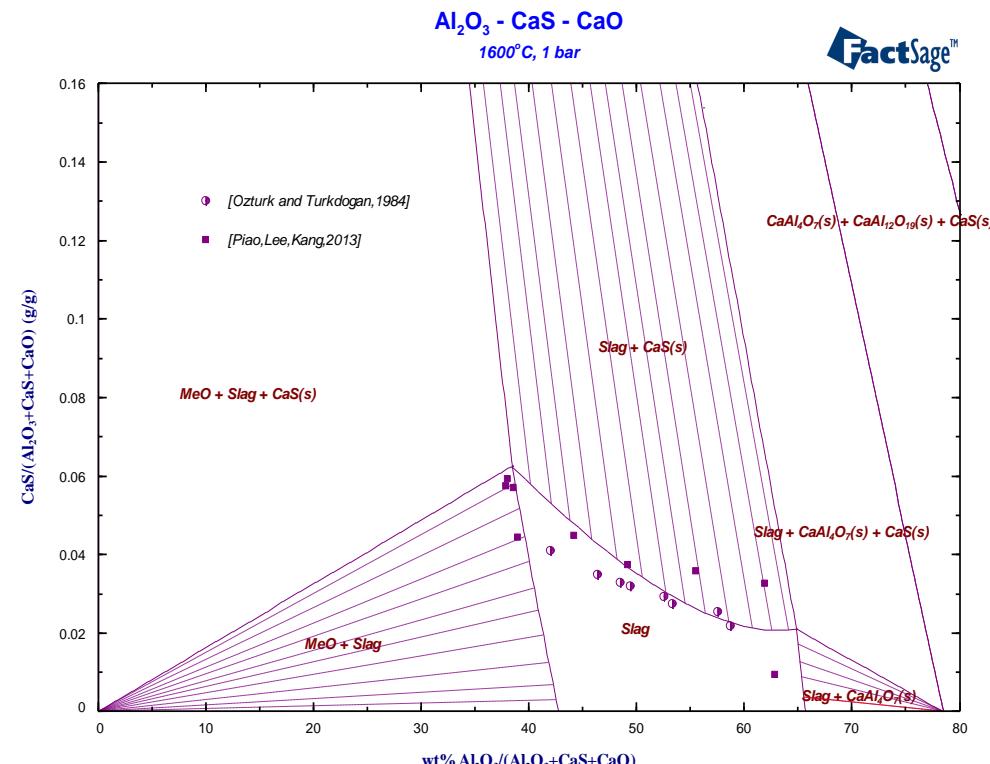
# Thermodynamic database

## Sulphide subsystems



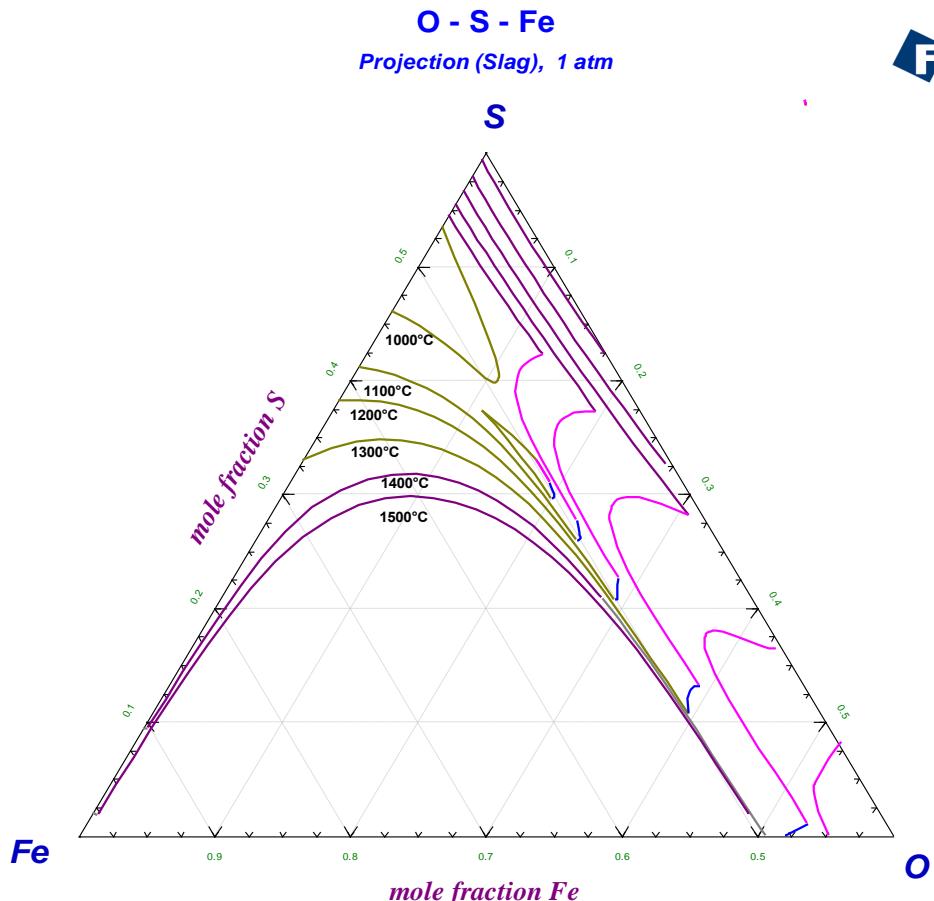
# Thermodynamic database

## Ternary systems with sulphide component

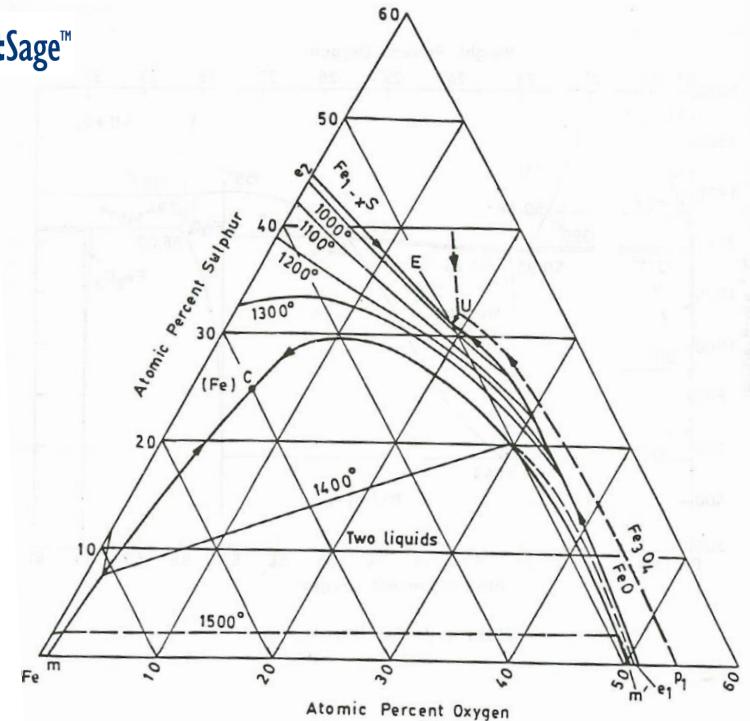


# Thermodynamic database

## The Fe-O-S system



FactSage™



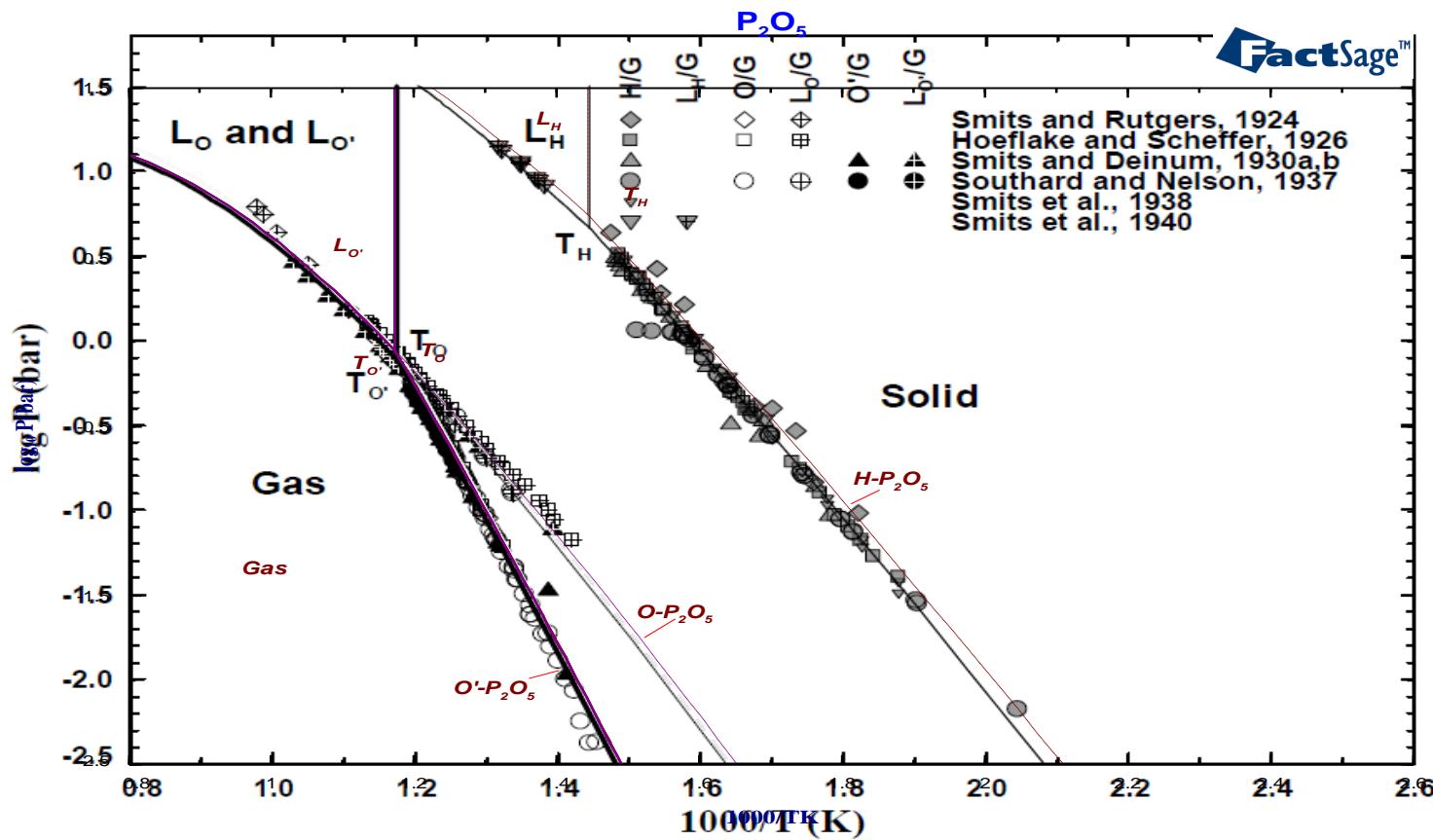
35.2a Fe-O-S Liquidus Projection in Atomic Percent

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

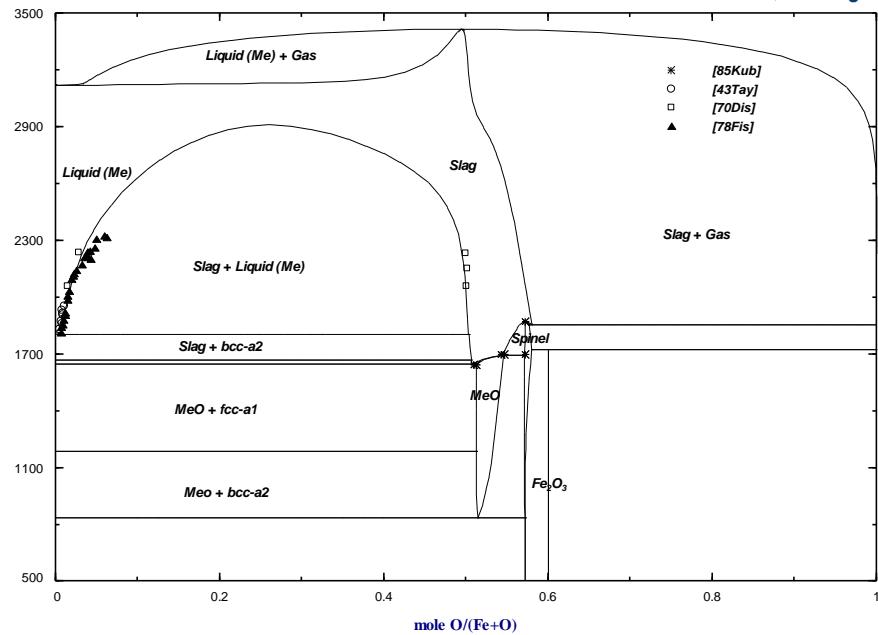
## Data for pure P<sub>2</sub>O<sub>5</sub>



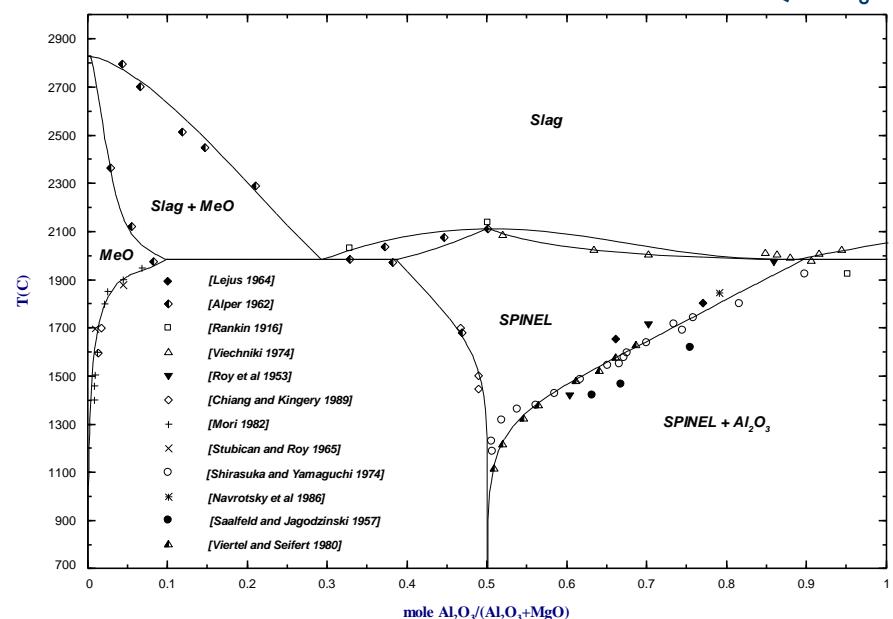
# Thermodynamic database

## Binary systems, including Fe-X

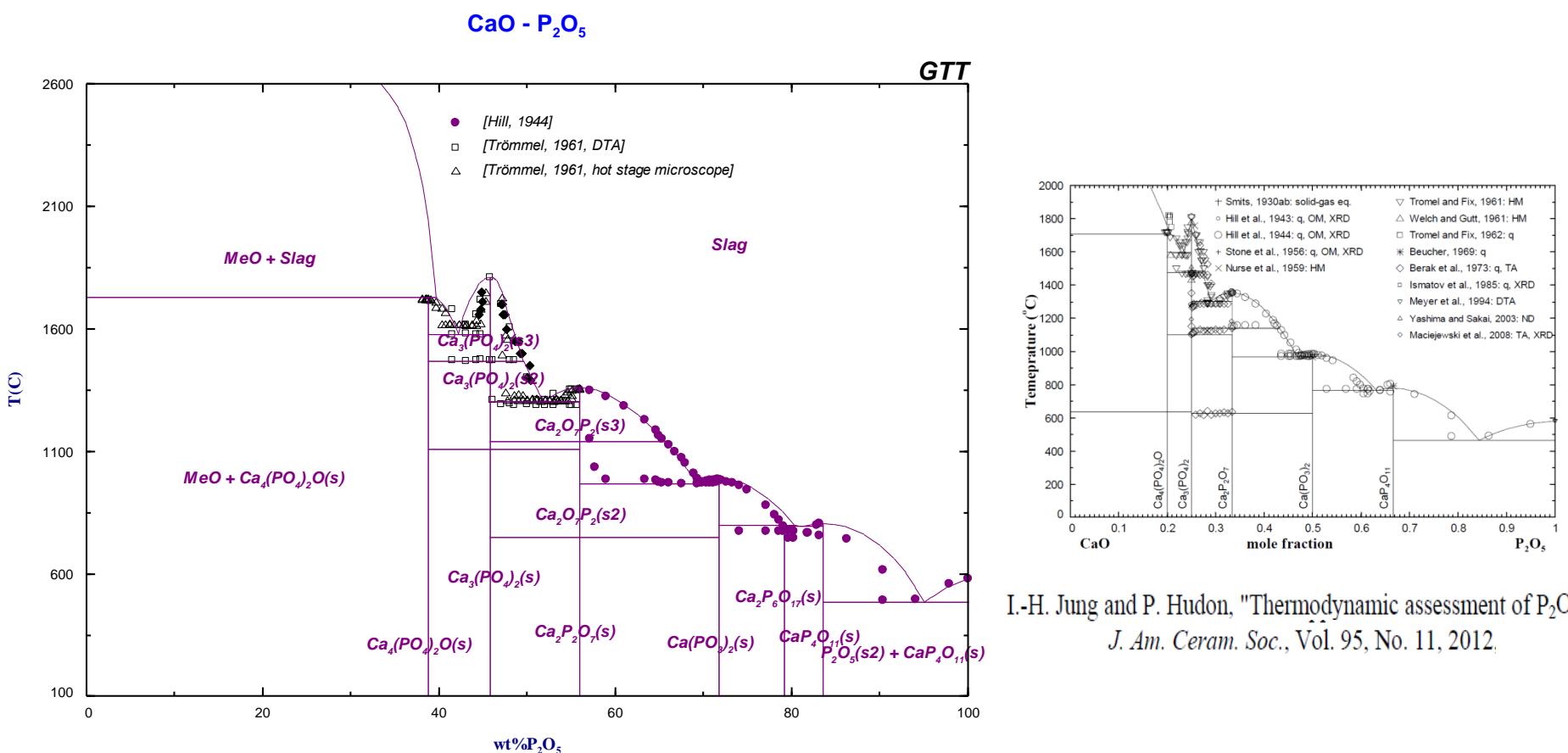
### Fe - O



### MgO – $\text{Al}_2\text{O}_3$

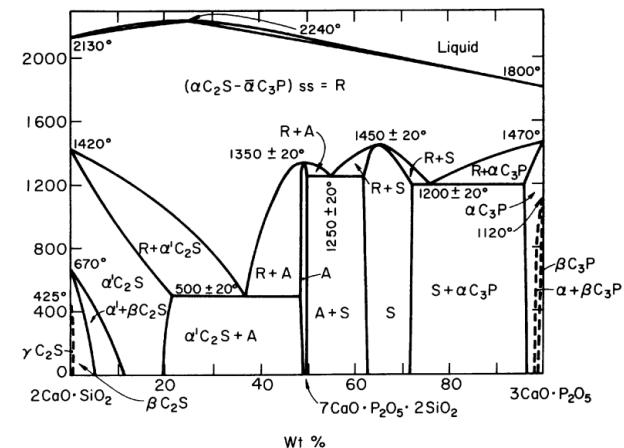
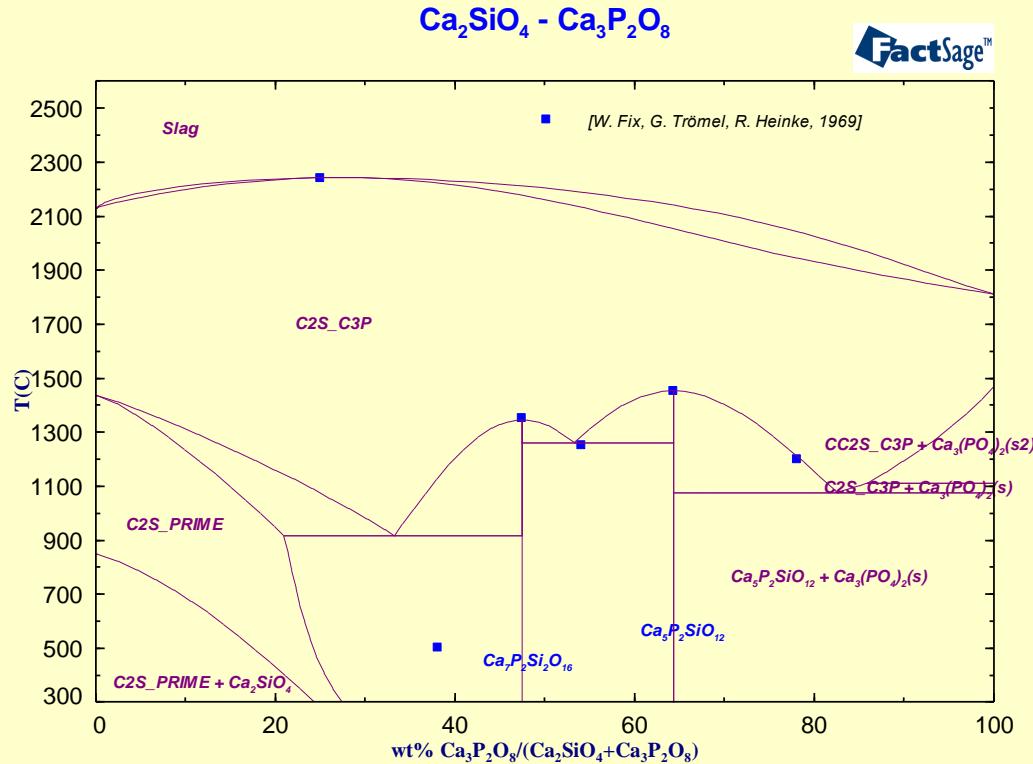


# Thermodynamic database

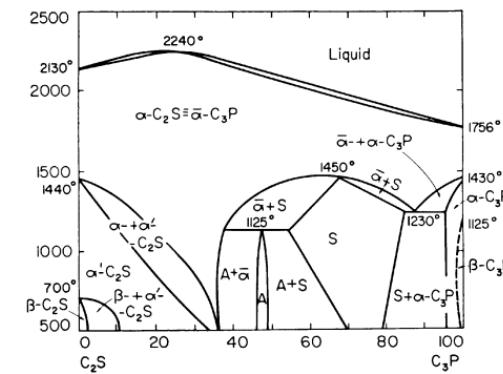


# Thermodynamic database

# Isopleth section $\text{Ca}_2\text{SiO}_4$ - $\text{Ca}_3\text{P}_2\text{O}_8$



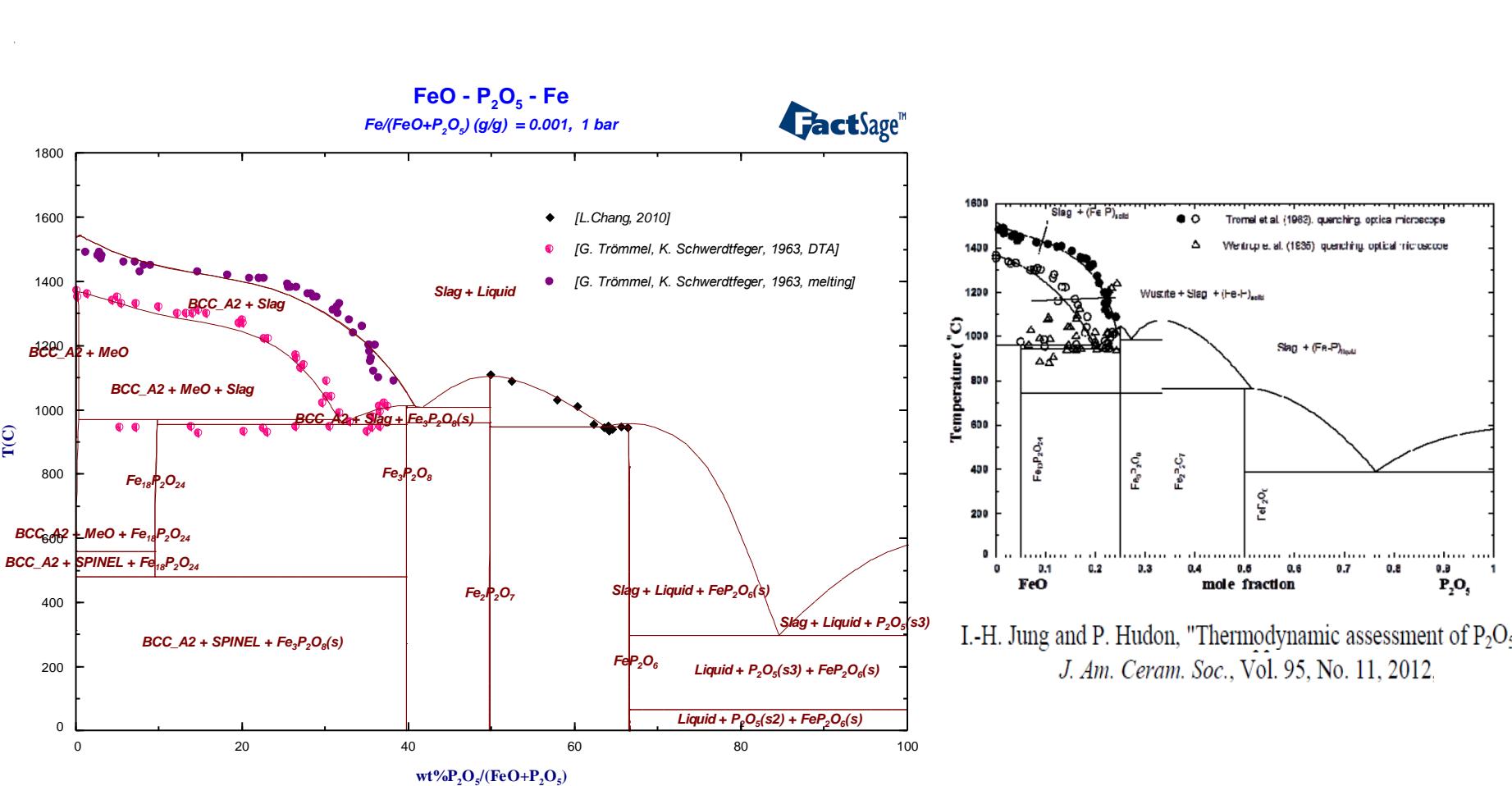
*W. Fix, H. Heymann, and R. Heinke, J. Am. Ceram. Soc., 52 [6] 346-347 (1969).*



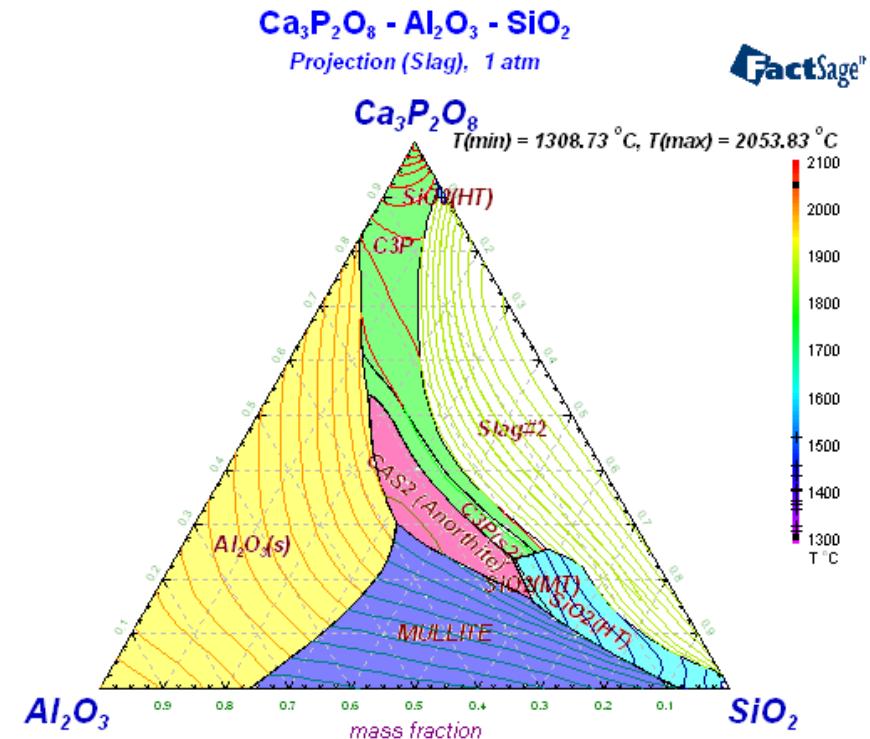
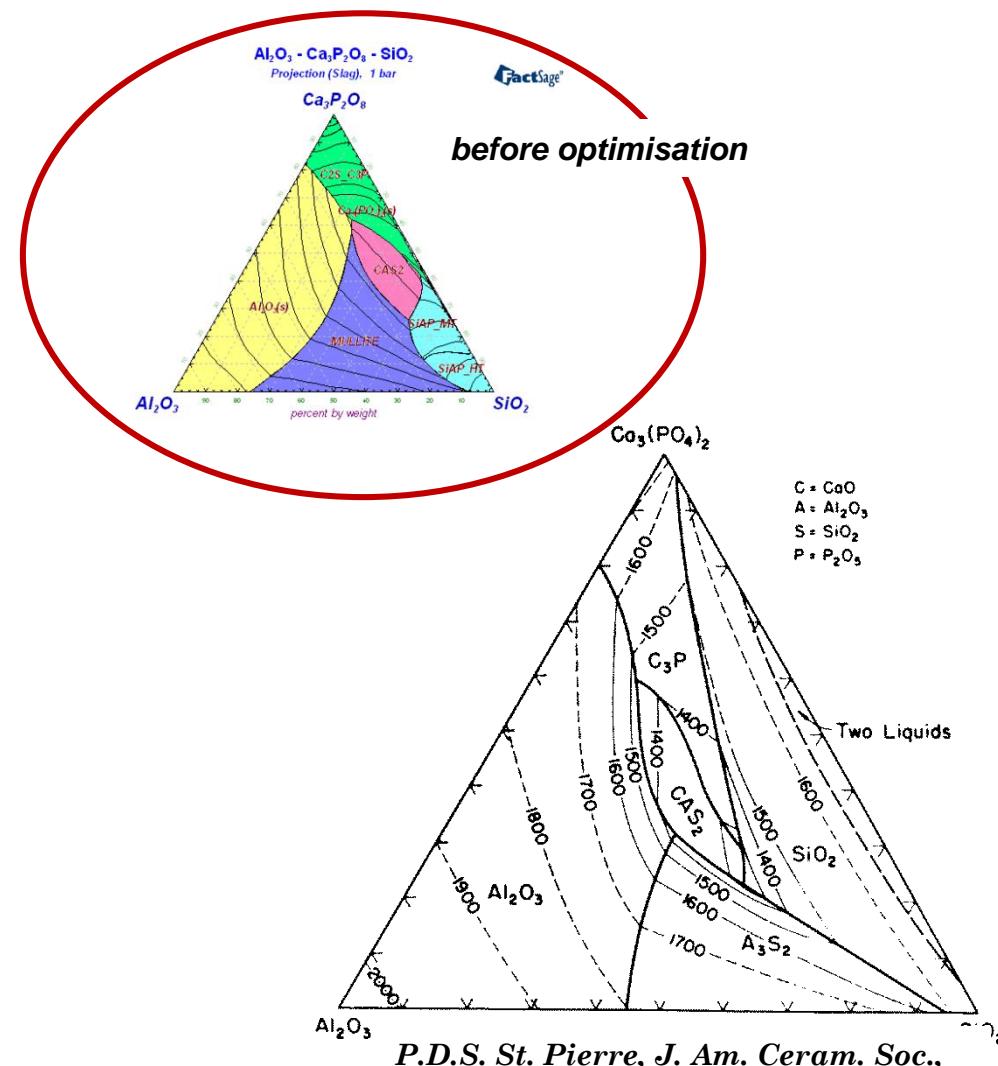
*R. W. Nurse, J. H. Welch, W. H. Gutt,  
J. Chem. Soc., 1077-1083 (1959).*



# Thermodynamic database



# Liquidus surface in $\text{Ca}_3\text{P}_2\text{O}_8$ - $\text{Al}_2\text{O}_3$ - $\text{SiO}_2$



# Thermodynamic database

## Phosphorous containing phases in present database:

Gas: P, P<sub>2</sub>O<sub>5</sub> as well as N<sub>2</sub>, O<sub>2</sub>, CO, CO<sub>2</sub>, SiO and many others

Liquid oxide: P<sub>2</sub>O<sub>5</sub> as well as 23 P<sub>2</sub>O<sub>5</sub>-containing associate species

Solid solutions: 7 phosphates  
1 silicate-phosphate (C<sub>2</sub>S-C<sub>3</sub>P)  
4 phosphates with limited SiO<sub>2</sub> solubility  
4 silicates with limited P<sub>2</sub>O<sub>5</sub> (PO<sub>4</sub>) solubility

Stoichiometric compounds: P and P<sub>2</sub>O<sub>5</sub> 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-SiO<sub>2</sub>-Al<sub>2</sub>O<sub>3</sub>-FeO-Fe<sub>2</sub>O<sub>3</sub>-P<sub>2</sub>O<sub>5</sub> (CaS, FeS, MgS, MnS)

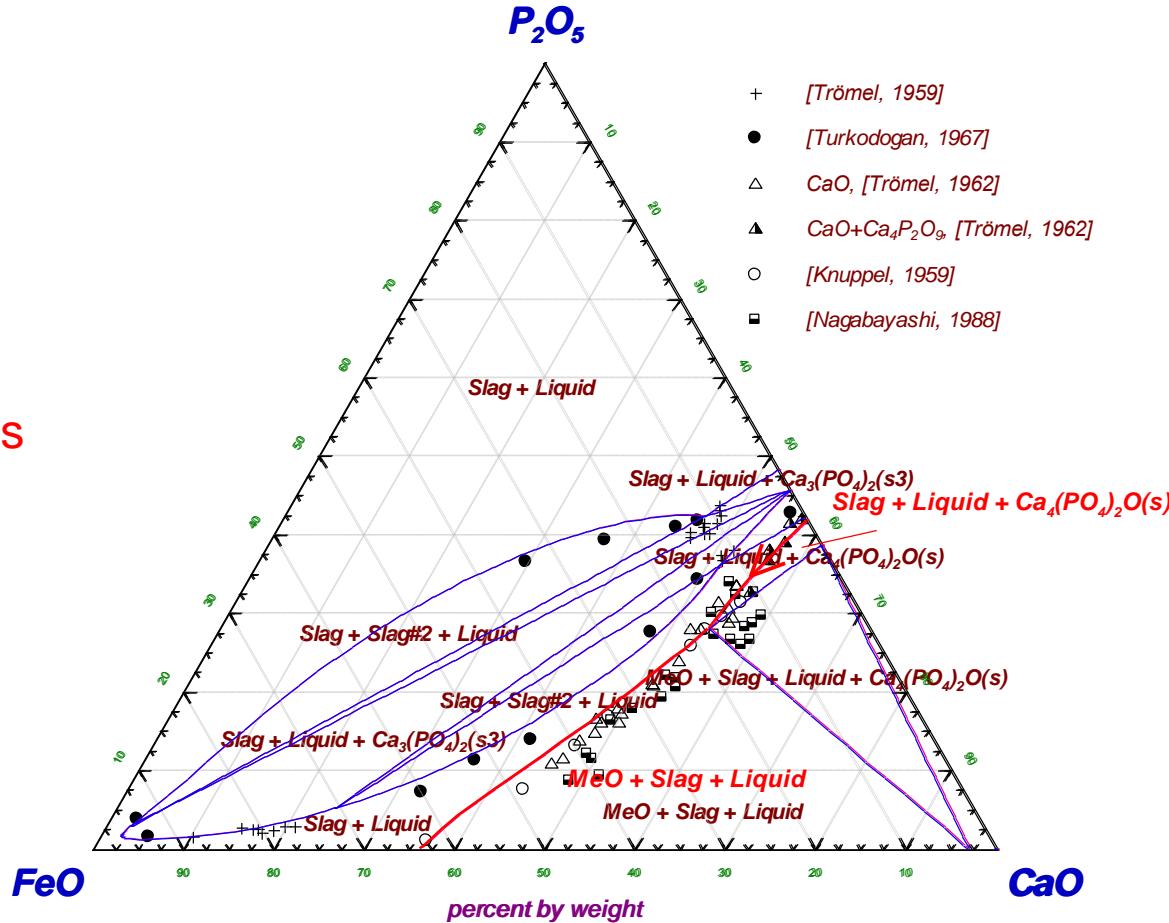


# Phosphorous Distribution

**CaO - FeO - P<sub>2</sub>O<sub>5</sub> - Fe**  
 $Fe/(CaO+FeO+P_2O_5) \text{ (g/g)} = 0.0001, 1600^\circ C, 1 \text{ bar}$



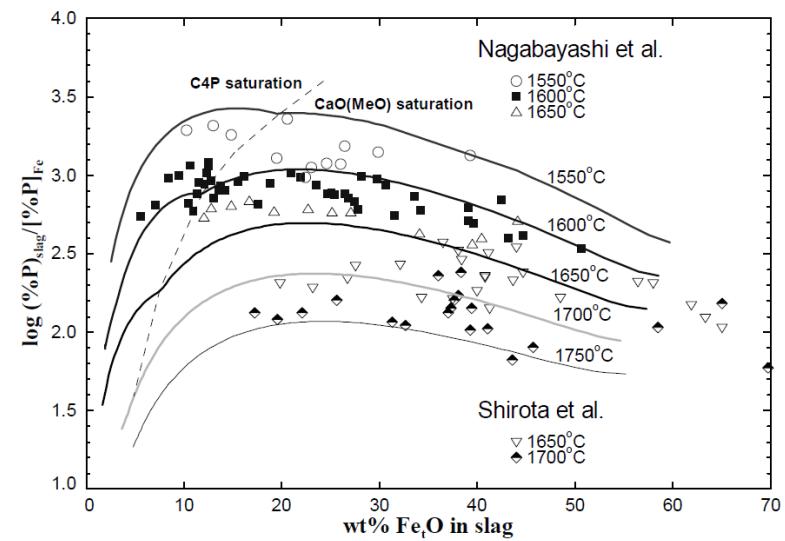
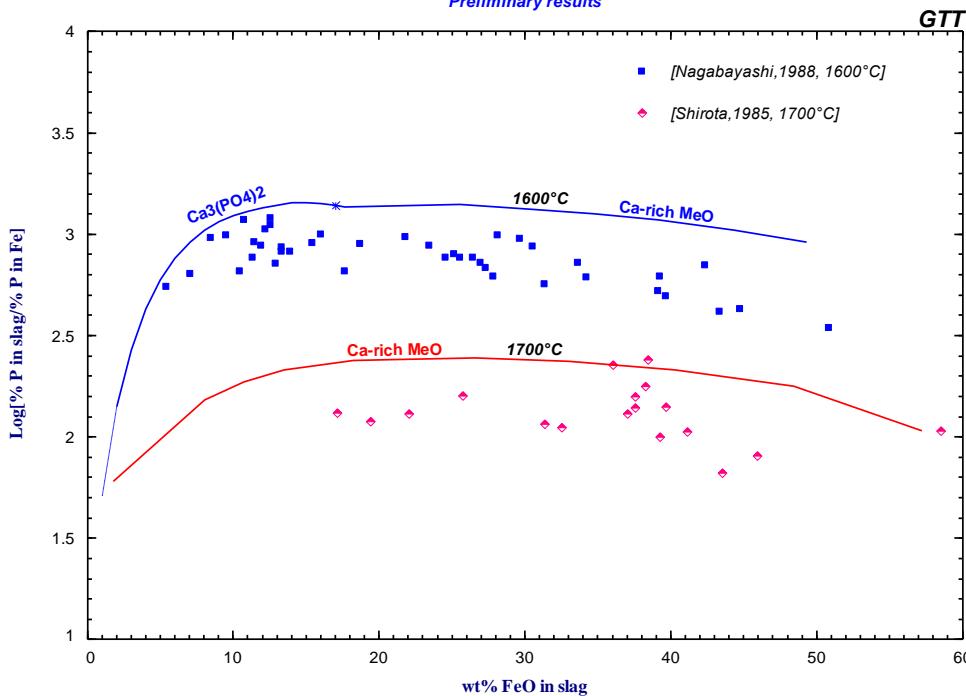
Red line →  
Phosphorous  
Capacity



# Phosphorous Distribution

P-distribution between molten iron and the slag

Preliminary results



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<sub>2</sub>O<sub>3</sub>-FeO-Fe<sub>2</sub>O<sub>3</sub>-MnO-Mn<sub>2</sub>O<sub>3</sub>-P<sub>2</sub>O<sub>5</sub>-SiO<sub>2</sub>**  
with inclusion of S in form of  
**CaS-MgS-FeS-MnS as well as Al<sub>2</sub>S<sub>3</sub>, Na<sub>2</sub>S, K<sub>2</sub>S**

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 !**

