JÜLICH
FORSCHUNGSZENTRUM

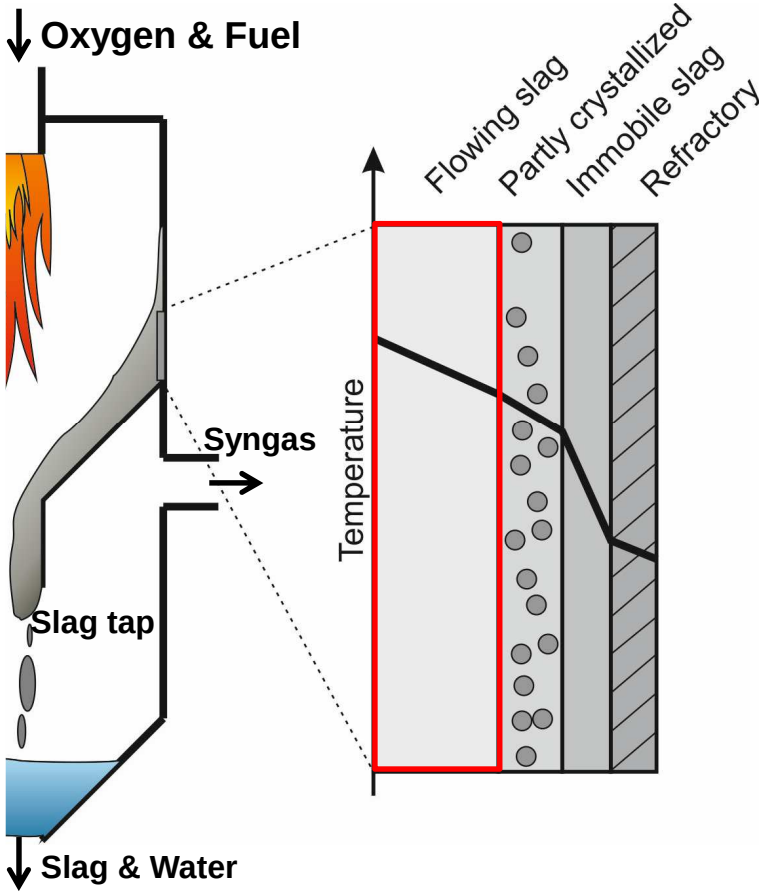
Modelling viscosity of molten oxides (HotVeGas Part III)

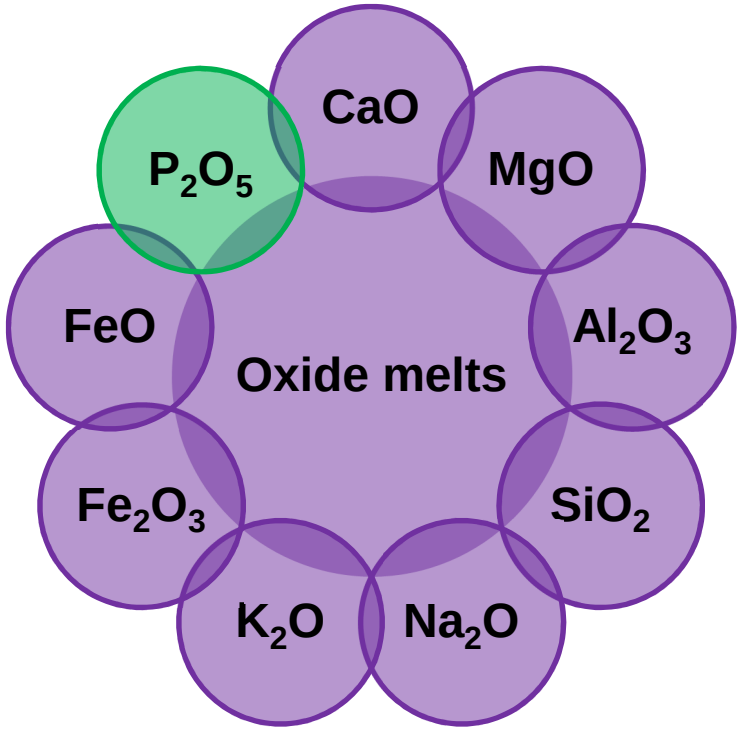
29.06.2017 Guixuan Wu

IEK-2, Forschungszentrum Jülich GmbH, Germany

GTT Annual Users' Meeting 2017

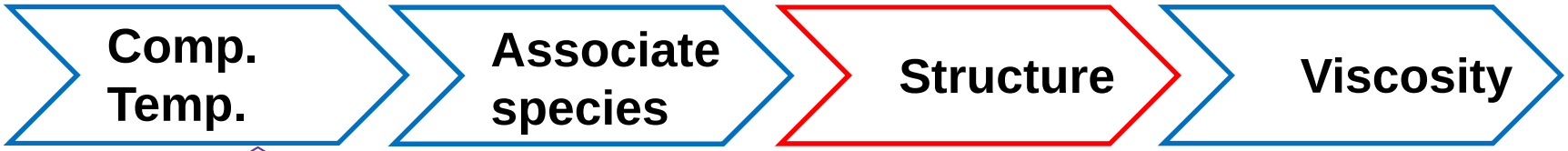
Introduction & aims





- Improvement of the viscosity model for FeO_x-containing systems
- Further development of the viscosity model for P_2O_5-containing systems

The viscosity model



$P(O_2)$ for MeO_x containing system

Modified Arrhenius model

$$\ln \eta = \ln \eta_{ideal} + \ln \eta_{excess}$$

$$= (\sum X_i \cdot \ln \eta_i) + (\ln \eta_{self-pol.} + \ln \eta_{inter-pol.})$$

$$\ln \eta_i = A_i + B_i/T$$ → basic structural units

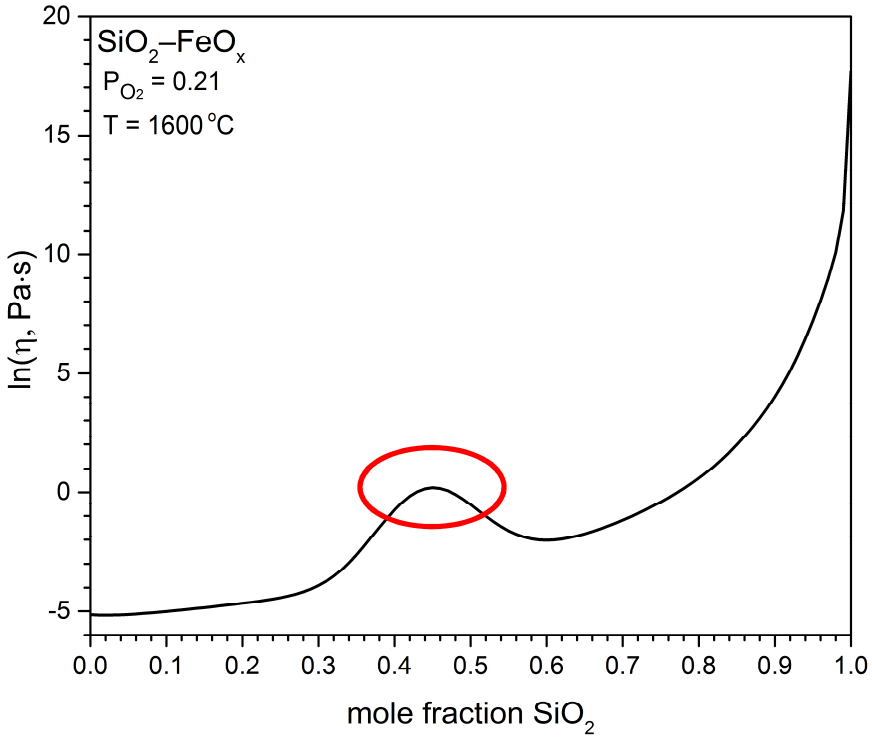
larger structural units

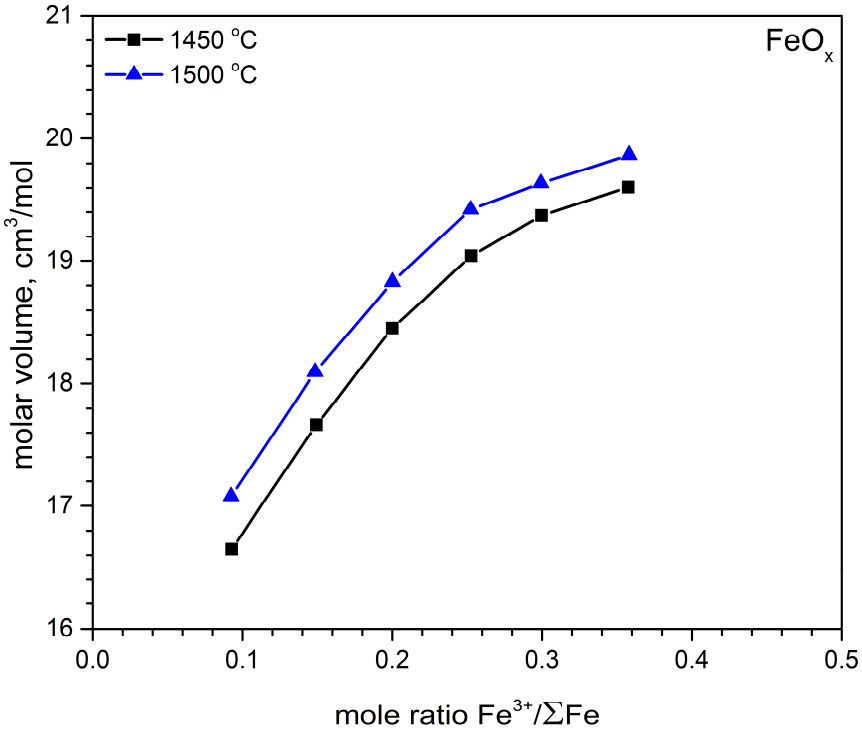
$$\ln \eta_{self-pol.} = \sum (A_{j,SiO_2} + B_{j,SiO_2}/T) \cdot (X^{n_j}_{SiO_2})$$

$$+ \sum_k \left(A_{(Si-Me^{3+})_k} + B_{(Si-Me^{3+})_k}/T \right) \cdot (X^{n_k}_{(Si-Me^{3+})})$$

$$\ln \eta_{inter-pol.} = \sum_m \left(A_{(Si-Me^{3+})_m} + B_{(Si-Me^{3+})_m}/T \right) \cdot (X_{(Si-Me^{3+})_m} \cdot X^{n_m}_{SiO_2})$$

The local viscosity maximum in SiO_2–FeO_x



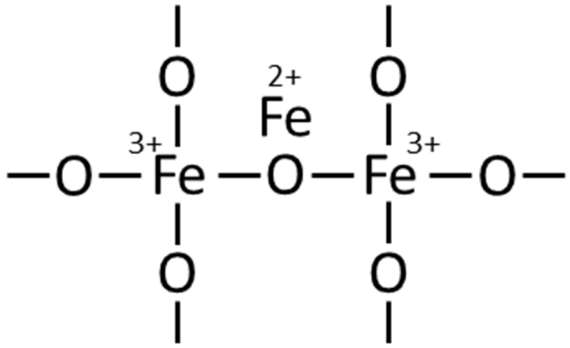


$(FeO \cdot SiO_2 \cdot Fe_2O_3)$

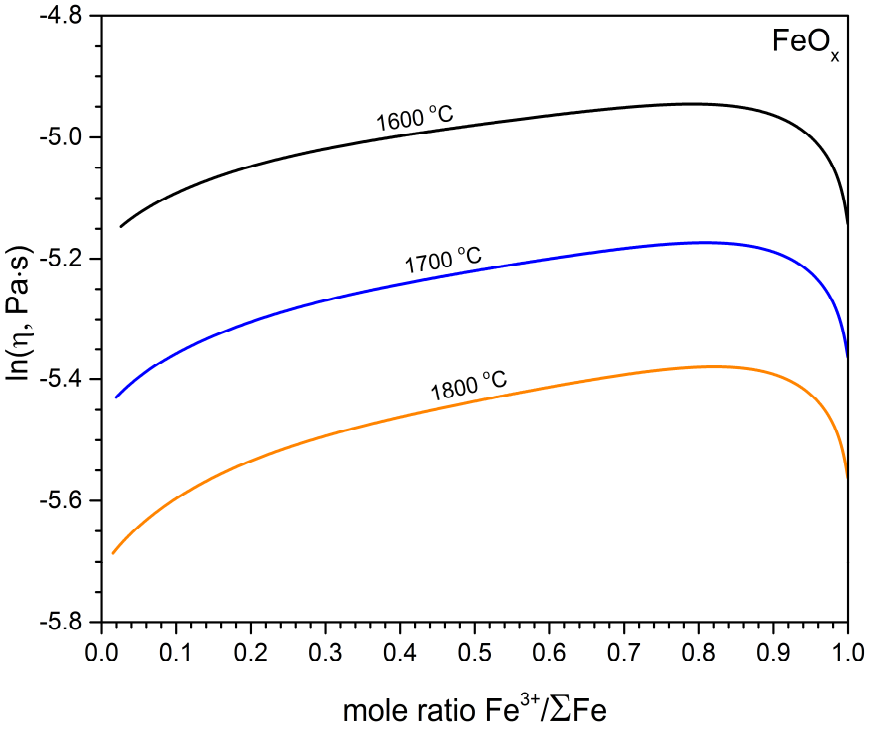
Fayalite Fe_2SiO_4 clustering

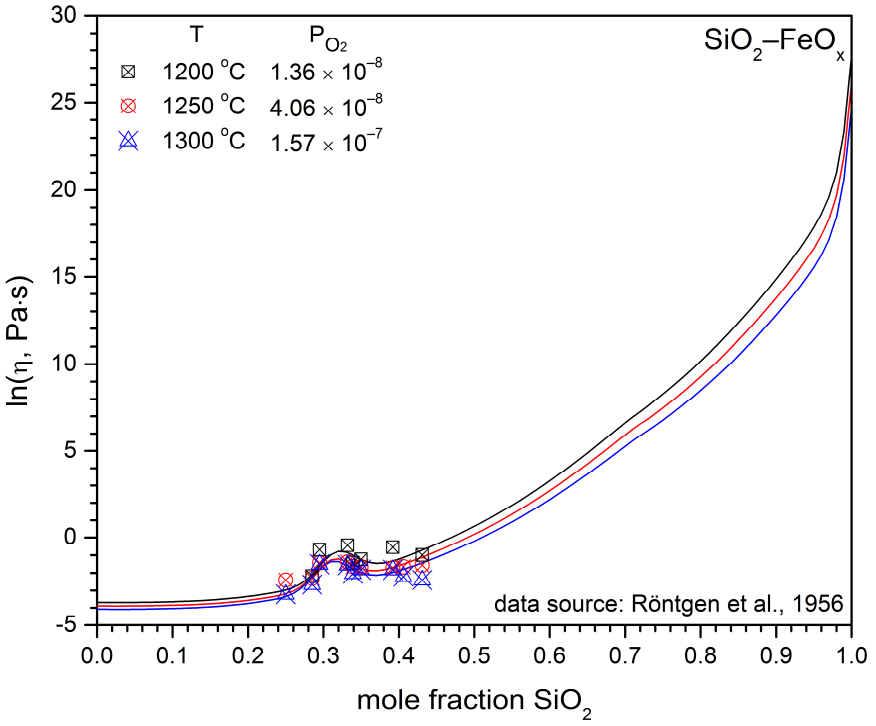
Analogous species
Ca_2SiO_4 and Mg_2SiO_4

Species
Fe_3O_4



The local viscosity maximum in SiO_2–FeO_x

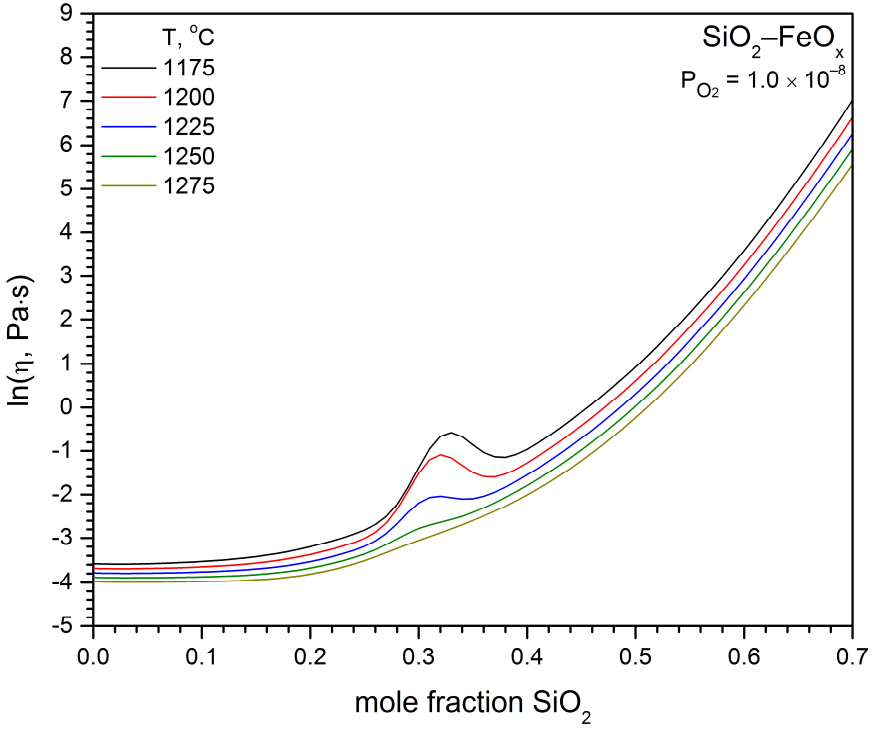


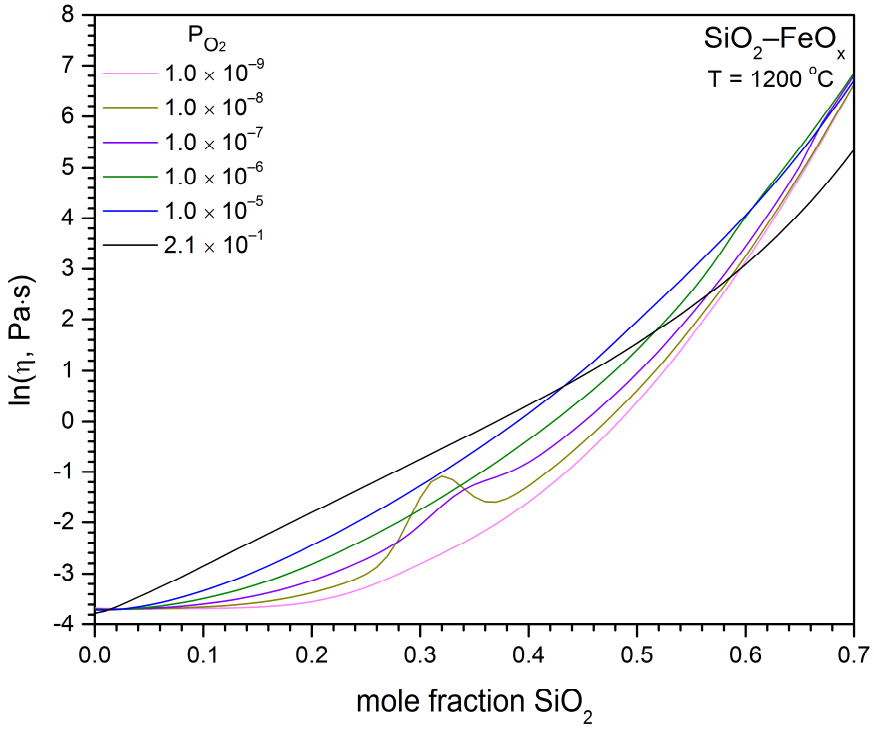


- the charge compensation of FeO_2^- and Fe^{2+}
- the presence of Fe^{2+} in tetrahedral coordination

(Fe_3O_4·Fe_2SiO_4)

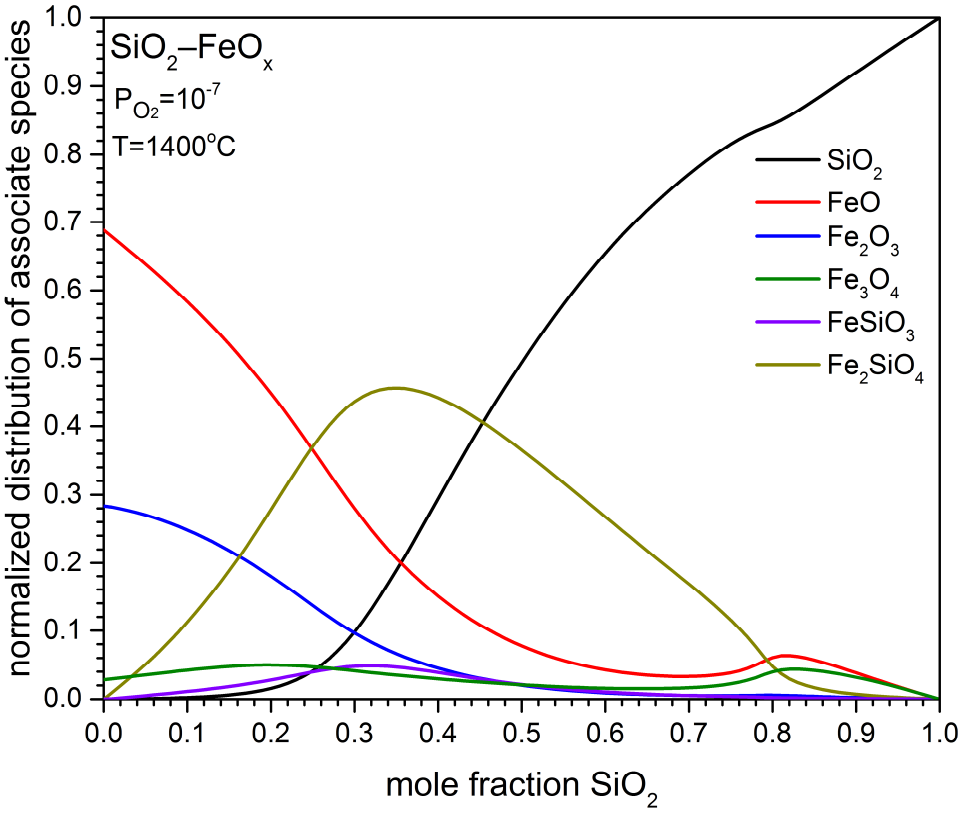
The local viscosity maximum in SiO_2–FeO_x





Model parameters for SiO_2–FeO_x

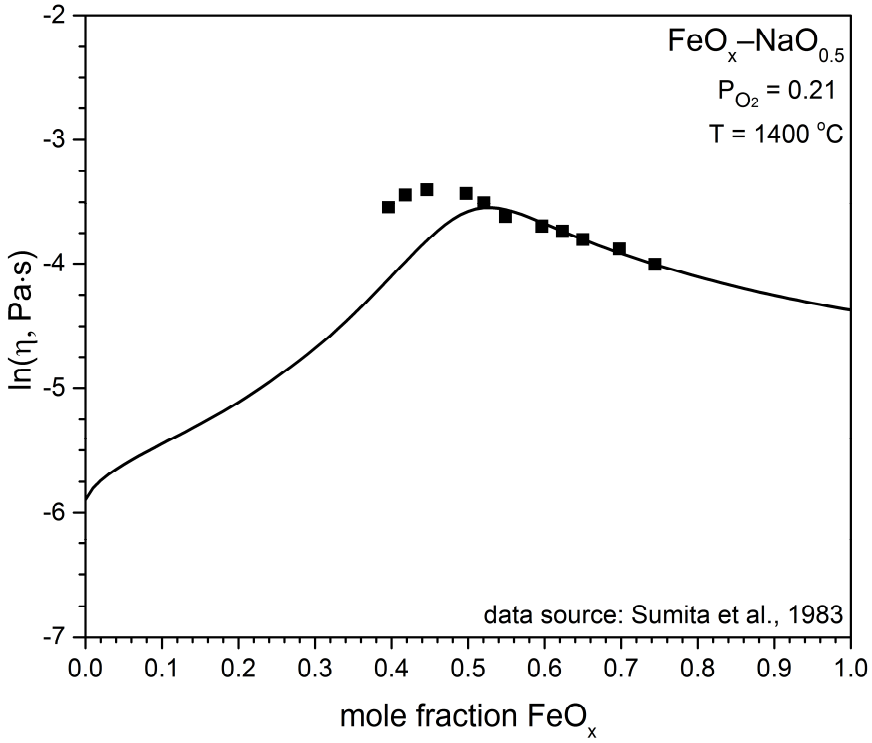
Associate species	Model parameters	
	A_i	B_i
$FeSiO_3$ (original)	–3.48	109.57
$FeSiO_3$	–9.25	20.86



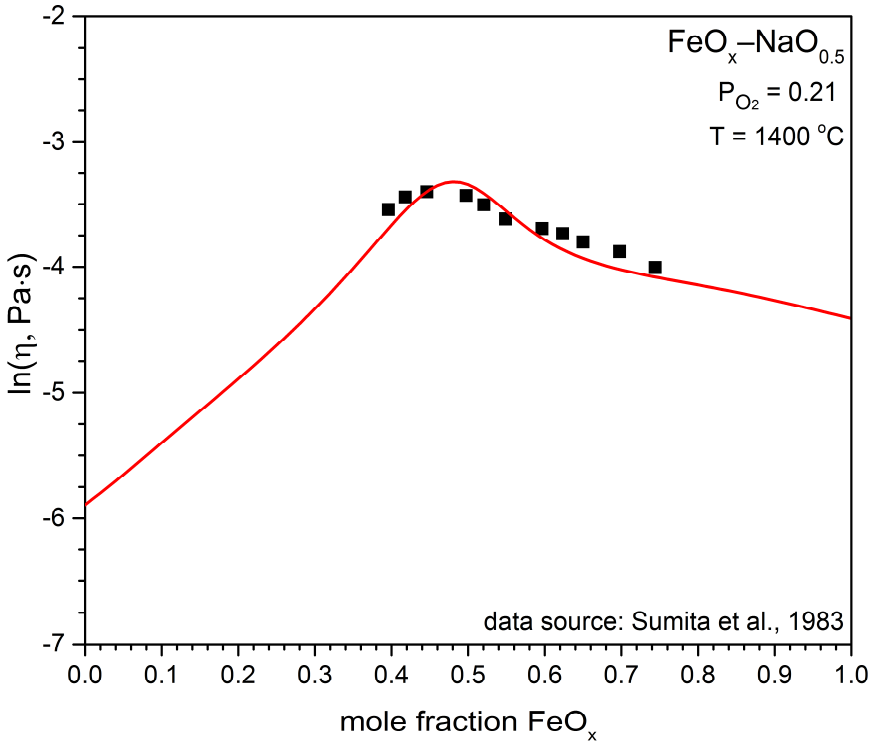
Fe_2SiO_4…?…$FeSiO_3$…?…SiO_2

($FeSiO_3 \cdot SiO_2$) and ($FeSiO_3)_2$

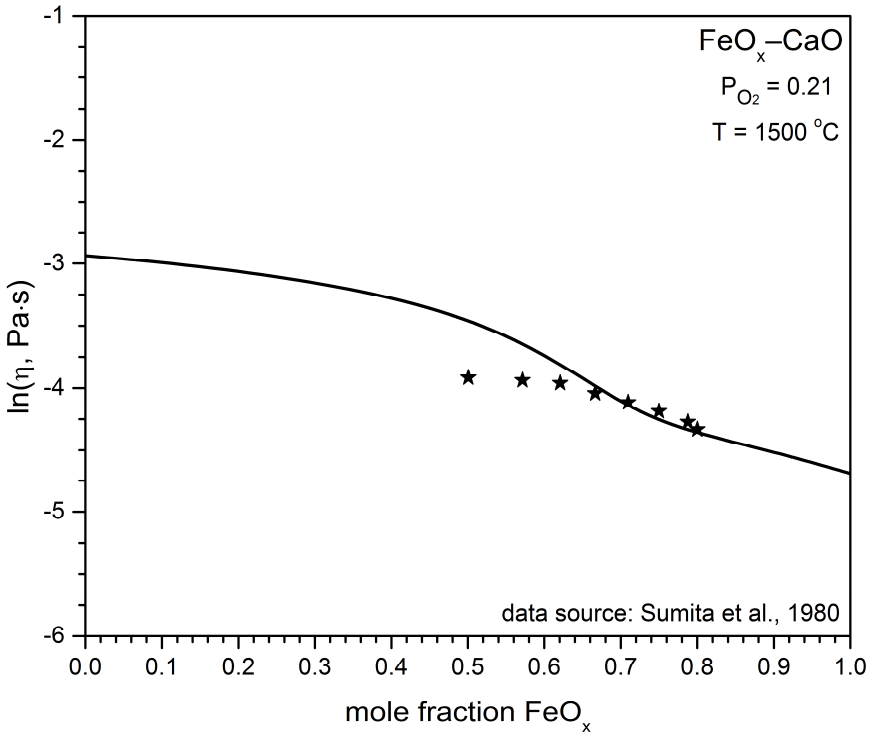
The viscosity maximum in FeO_x–$NaO_{0.5}$

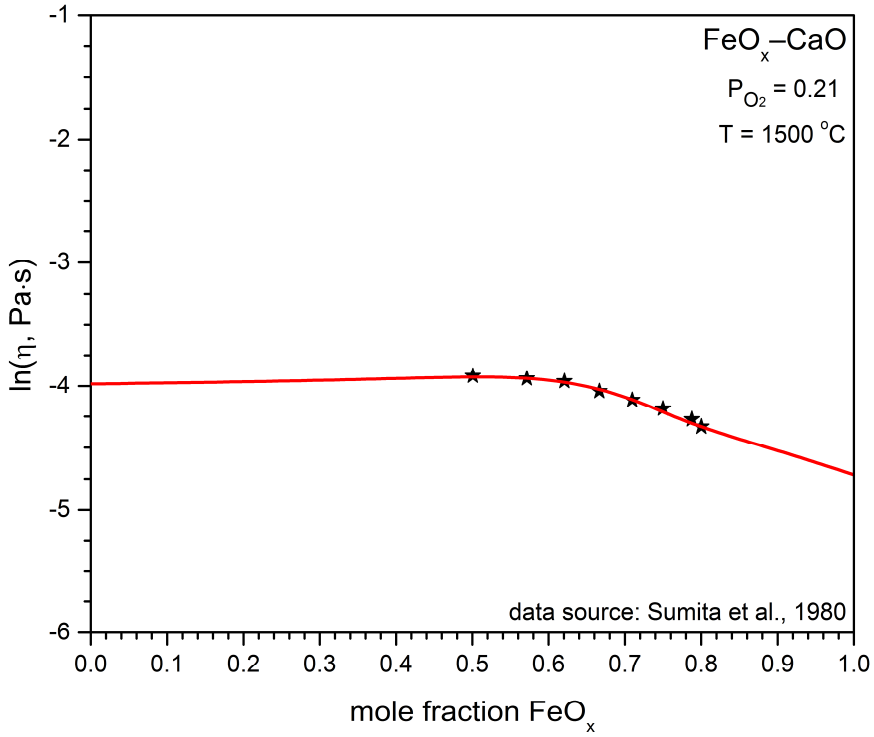


$(NaFeO_2 \cdot Na_2FeO_2)$



The viscosity maximum in FeO_x–CaO





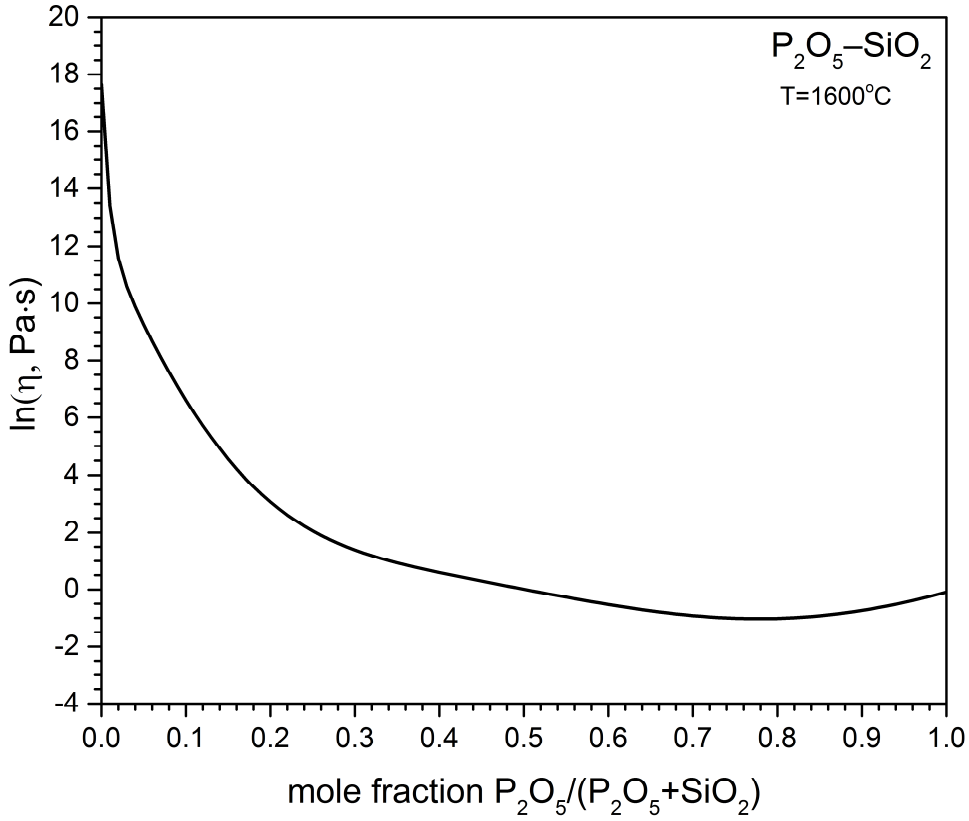
Associate species	Model parameters	
	A_i	B_i
CaO (original)	–12.30	16.59
CaO	–12.28	14.72

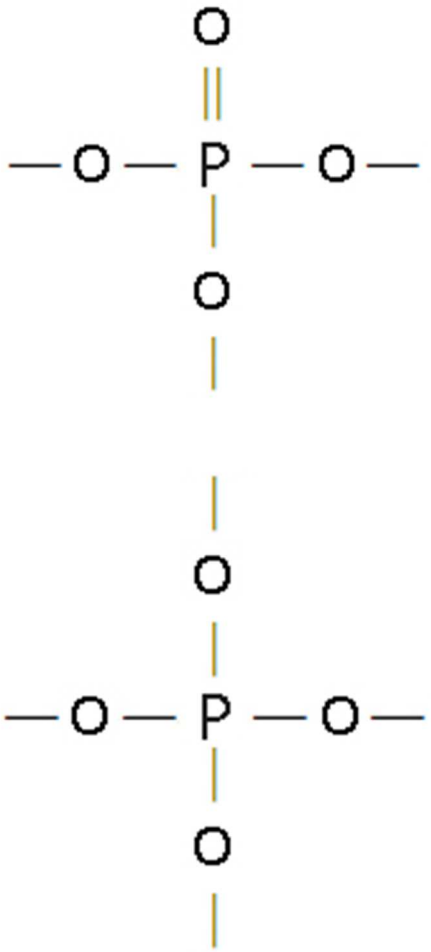
P_2O_5-containing systems

JÜLICH FORSCHUNGSZENTRUM

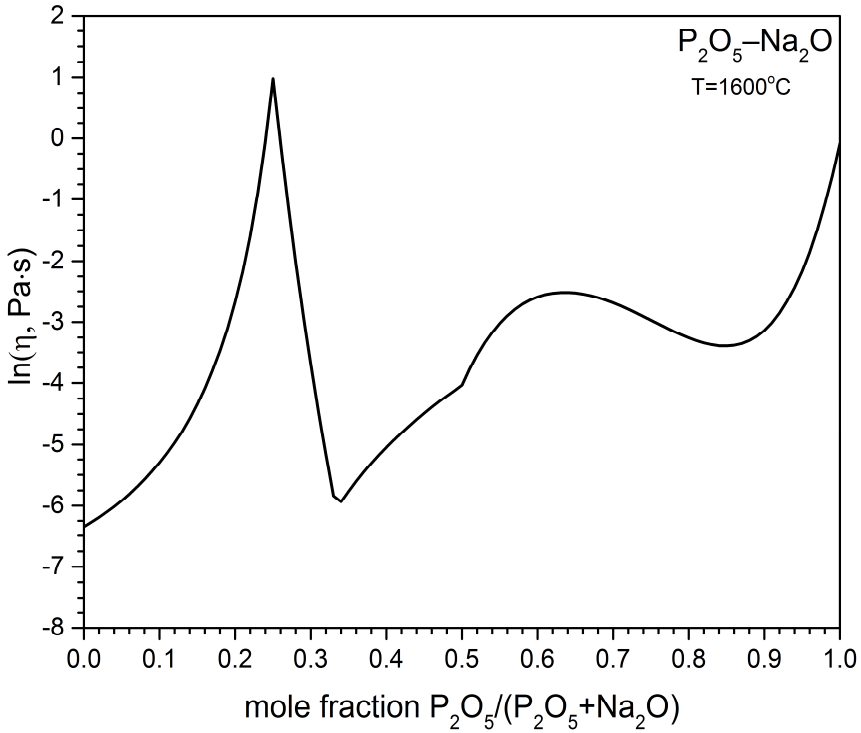
Associate species	Structural units	Associate species	Structural units
P_2O_5	$PO_{2.5}$	$Na_4P_2O_7$	$Na_2PO_{3.5}$
P_2SiO_7	P_2SiO_7	$NaPO_3$	$NaPO_3$
$P_4Si_3O_{16}$	$P_{4/3}SiO_{16/3}$	Na_3PO_4	Na_3PO_4
$AlPO_4$	$AlPO_4$	KPO_3	KPO_3
CaP_2O_6	$Ca_{0.5}PO_3$	K_3PO_4	K_3PO_4
$Ca_2P_2O_7$	$CaPO_{3.5}$	$K_4P_2O_7$	$K_2PO_{3.5}$
$Ca_3P_2O_8$	$Ca_{1.5}PO_4$	$FePO_4$	$FePO_4$
$Mg_3P_2O_8$	$Mg_{1.5}PO_4$	$Fe_2P_2O_7$	$FePO_{3.5}$
$Mg_2P_2O_7$	$MgPO_{3.5}$	FeP_2O_6	$Fe_{0.5}PO_3$
MgP_2O_6	$Mg_{0.5}PO_3$	$Fe_3P_2O_8$	$Fe_{1.5}PO_4$

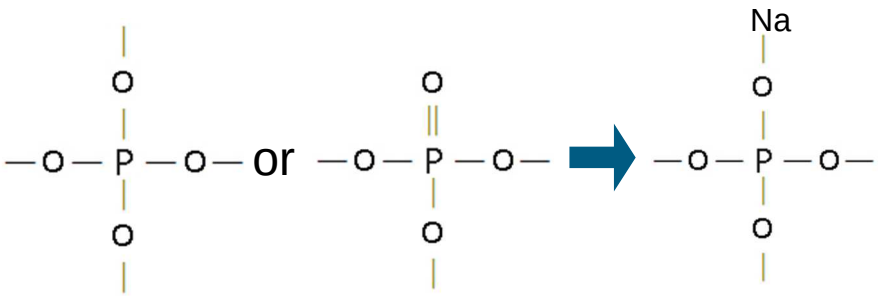
P_2O_5–SiO_2


P2O5–SiO2
T=1600°C
ln(η, Pa·s)
20
18
16
14
12
10
8
6
4
2
0
-2
-4
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0
mole fraction P2O5/(P2O5+SiO2)



P_2O_5–Na_2O

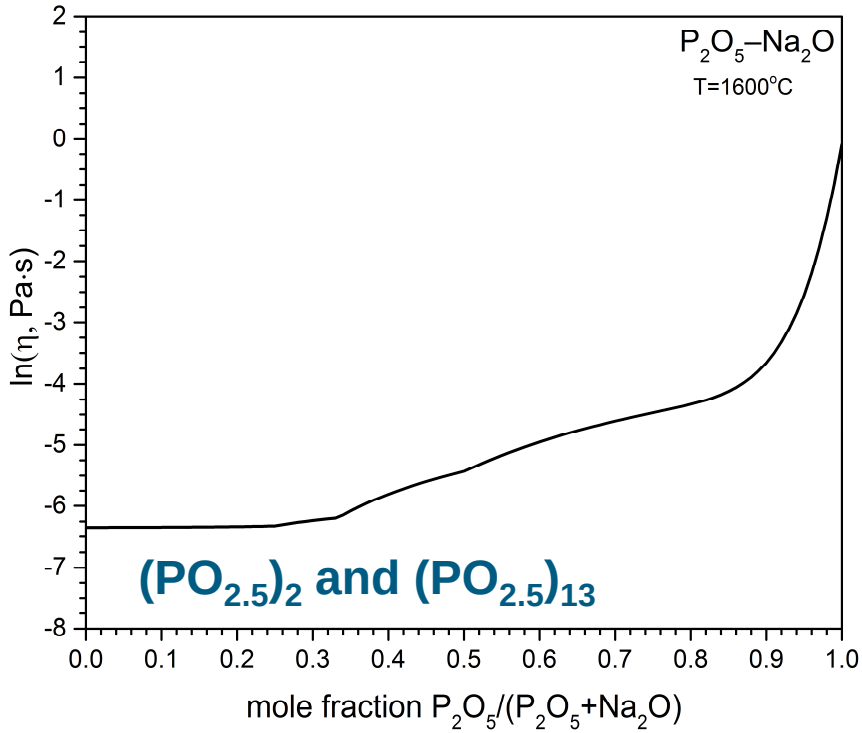




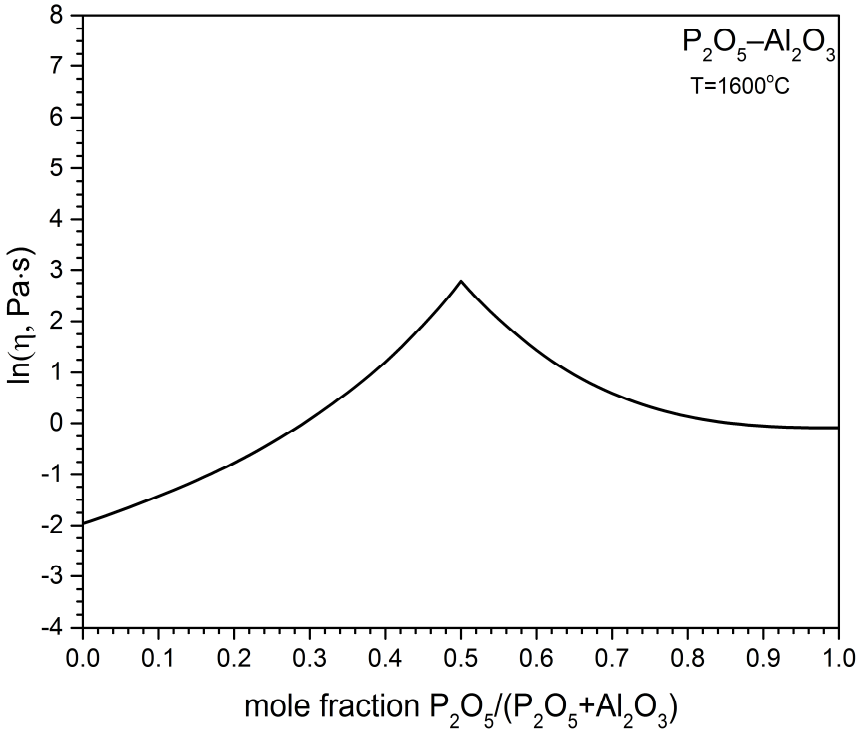
$Na_4P_2O_7$

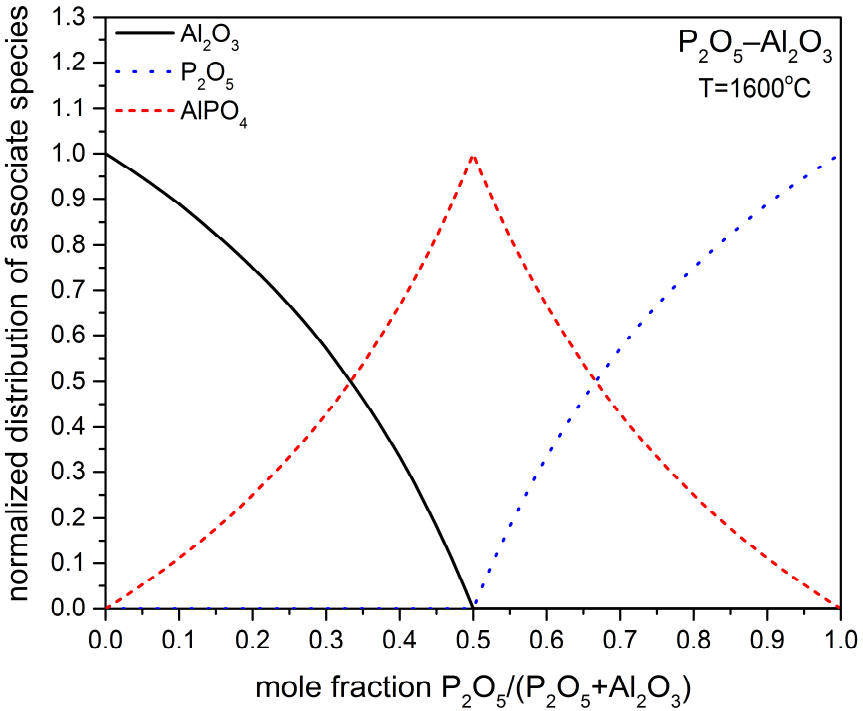
$NaPO_3$

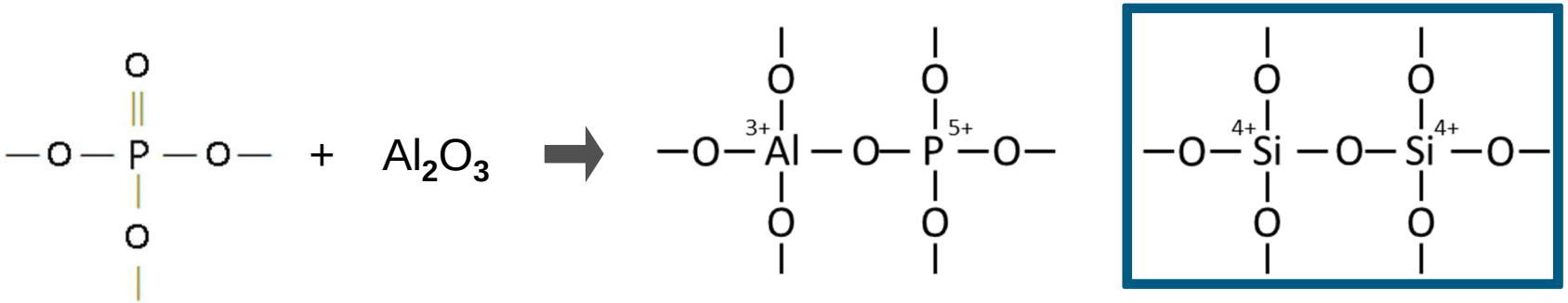
Na_3PO_4



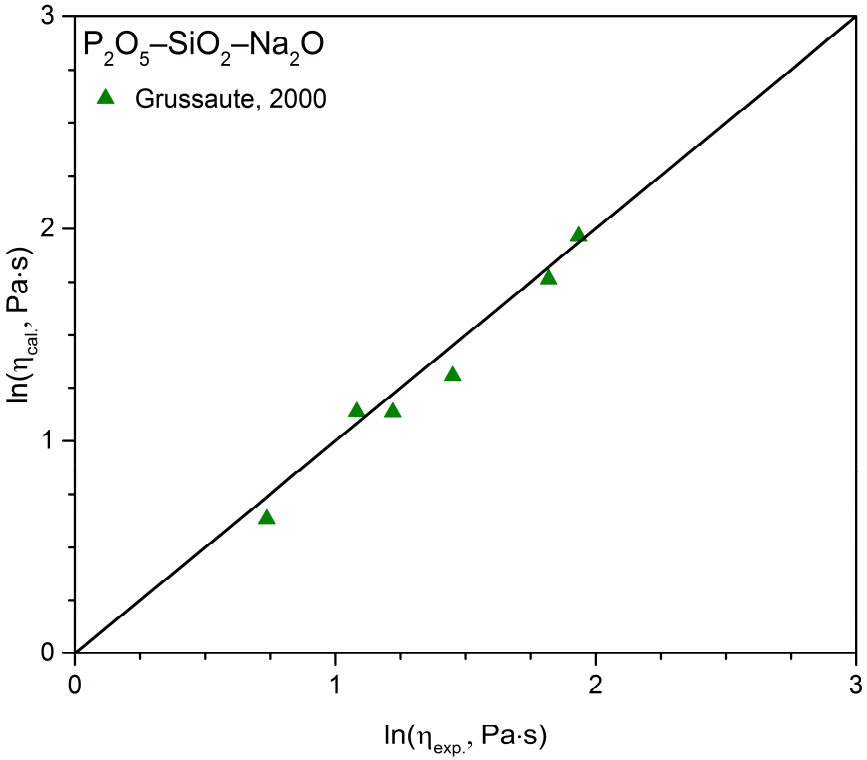
P_2O_5–Al_2O_3

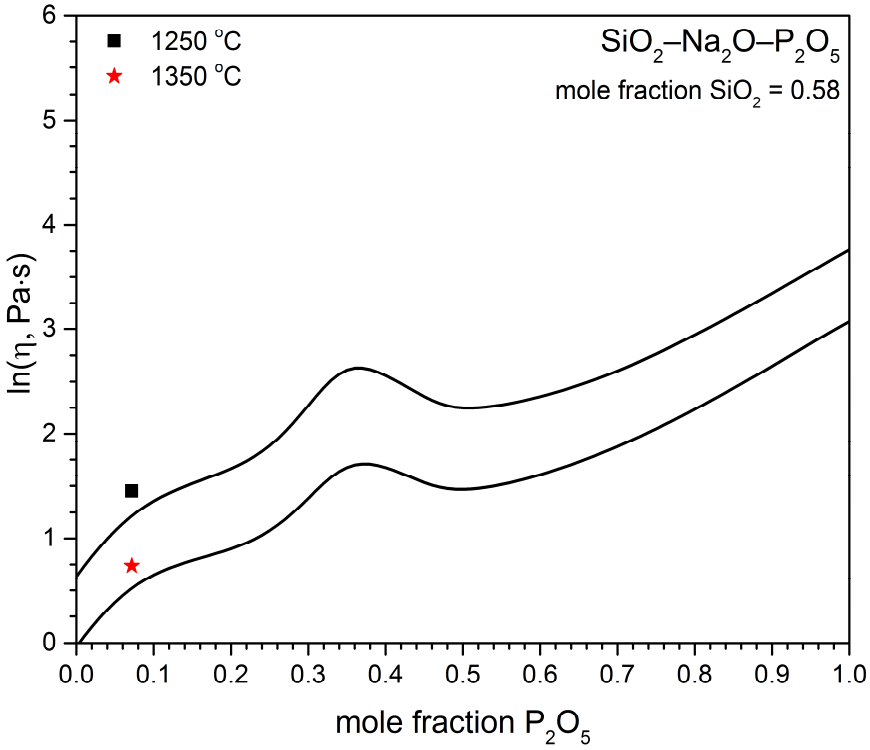

P2O5–Al2O3
T=1600°C
ln(η, Pa·s)
mole fraction P2O5/(P2O5+Al2O3)


Al2O3
P2O5
AlPO4
P2O5–Al2O3
T=1600°C
normalized distribution of associate species
mole fraction P2O5/(P2O5+Al2O3)

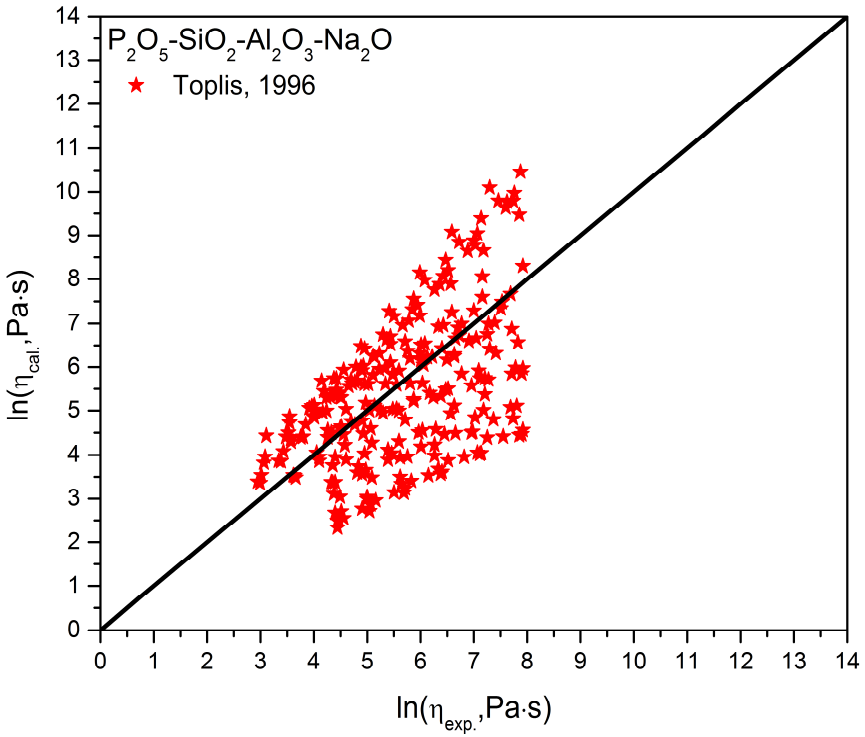

+
Al2O3
3+
5+
4+
4+

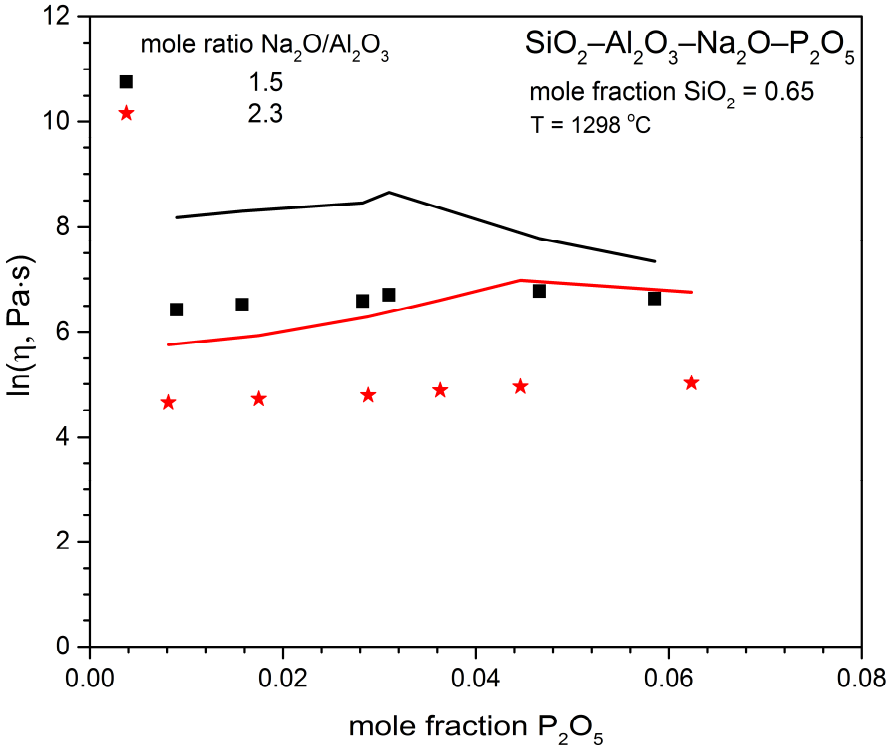
P_2O_5–SiO_2–Na_2O





P_2O_5–SiO_2–Al_2O_3–Na_2O





Conclusions & outlook

- The model performance for FeO_x-containing systems has been improved
- A new mechanism is proposed to describe the local viscosity maximum around the fayalite compound in the binary system SiO_2–FeO_x
- The presence of the local viscosity maximum is dependent on temperature and oxygen partial pressure
- The model has been further developed for P_2O_5-containing systems in conjunction with the structural dependence of viscosity
- More experimental data are needed for the further assessment of model parameters of P_2O_5-containing systems

JÜLICH
FORSCHUNGSZENTRUM

Thank you very much for your attention!