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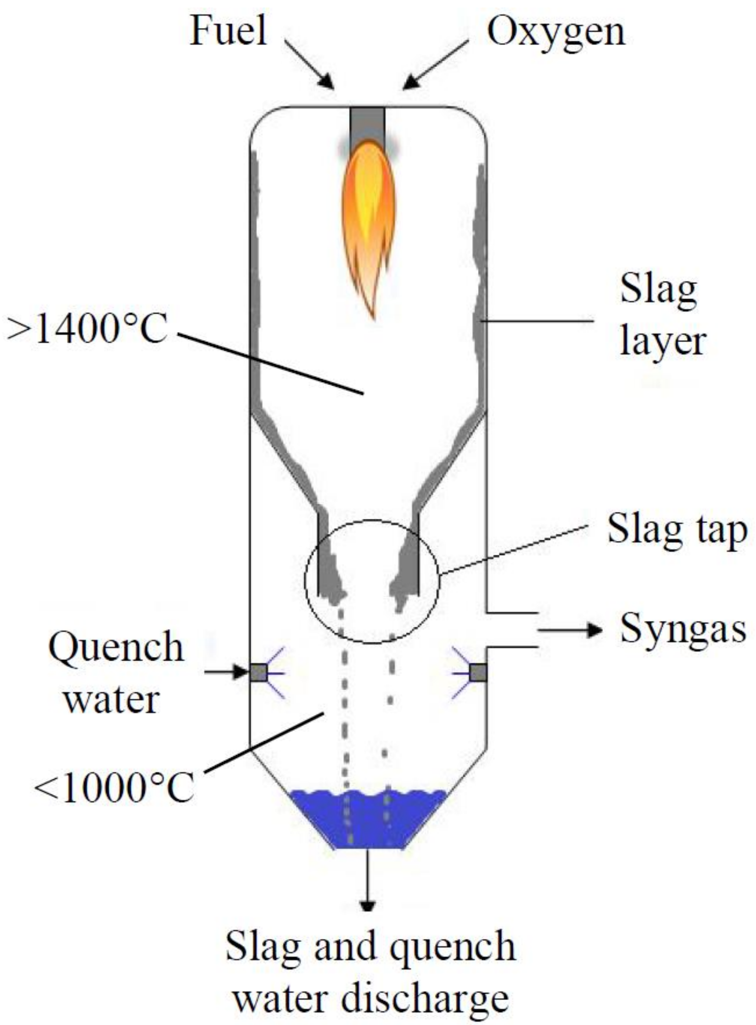
Use of the oxide database in modelling of multi-component slag viscosities

04.07.2013 Guixuan Wu

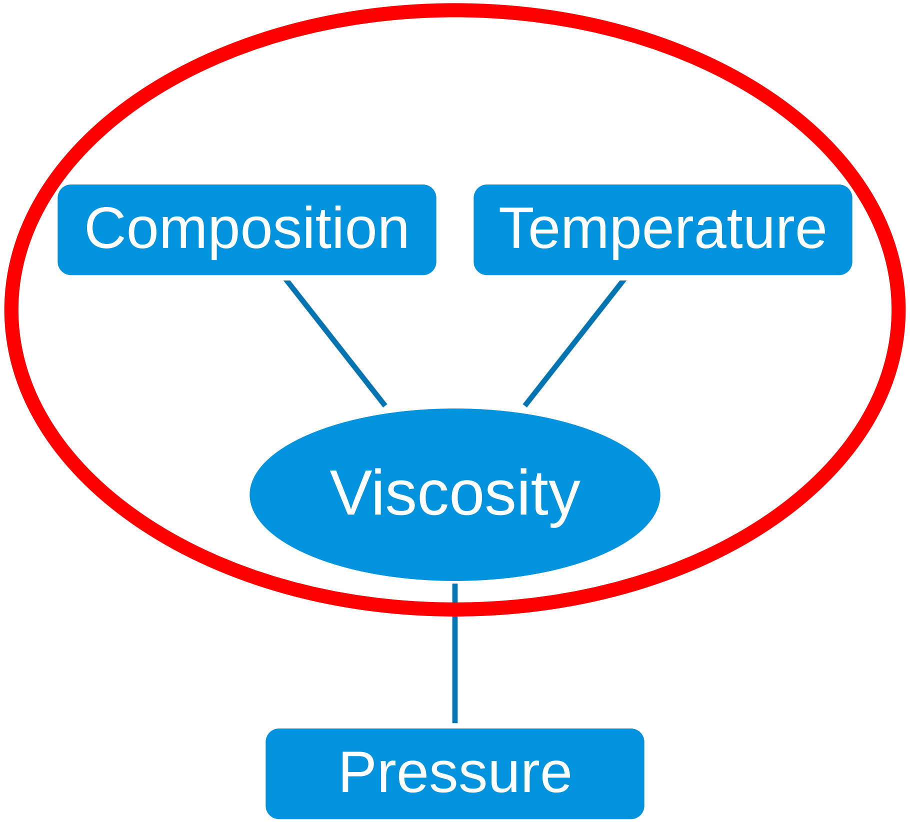
Outline

– Introduction
– Viscosity model
– Results
– Case study
– Outlook

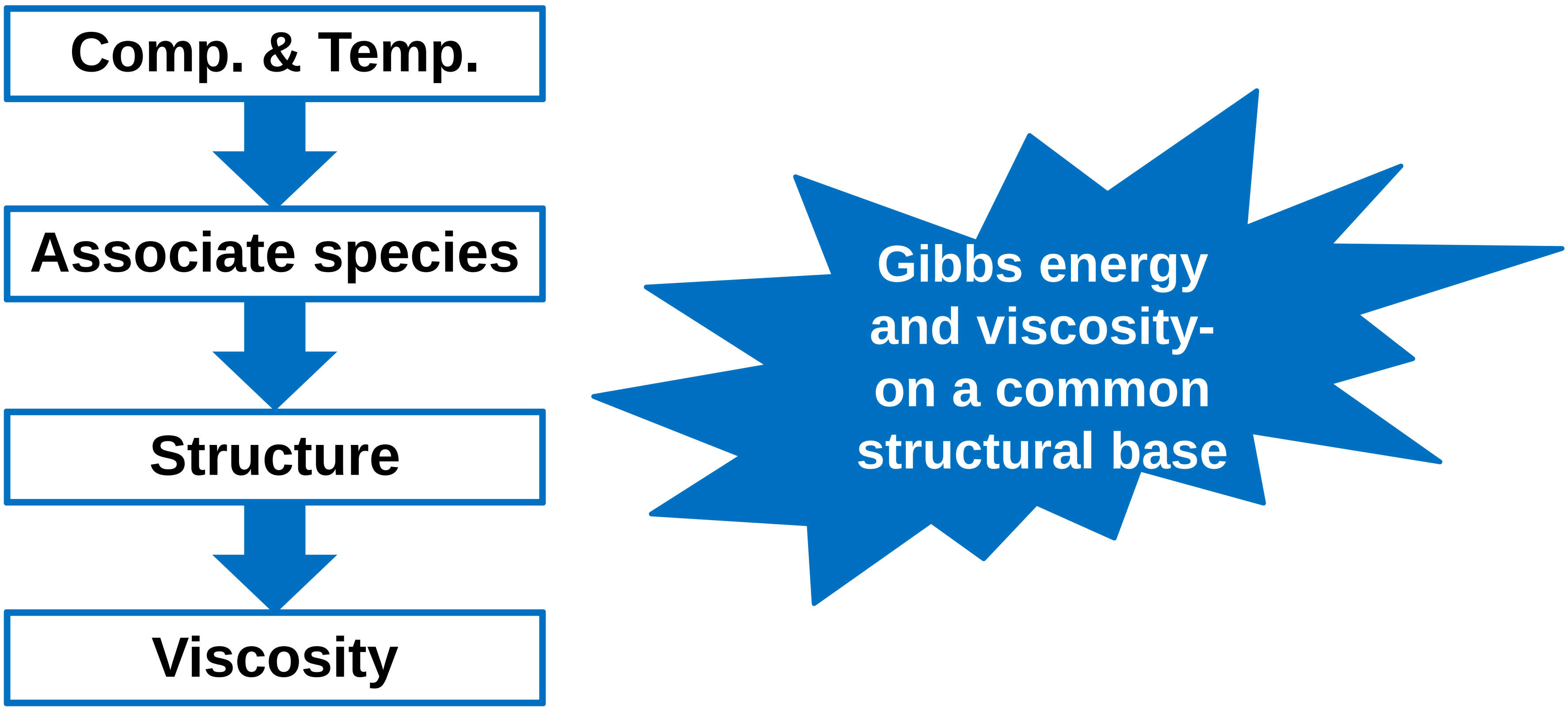
Introduction



Marc A. Duchesne: Slagging in entrained-flow gasifiers, 2012.



The idea of current viscosity model



Viscosity model

– **Arrhenius model (modified)**

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

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

Si-Al-based ternary associate species

Si-based associate species

where: $\ln \eta_i = A_i + B_i/T$

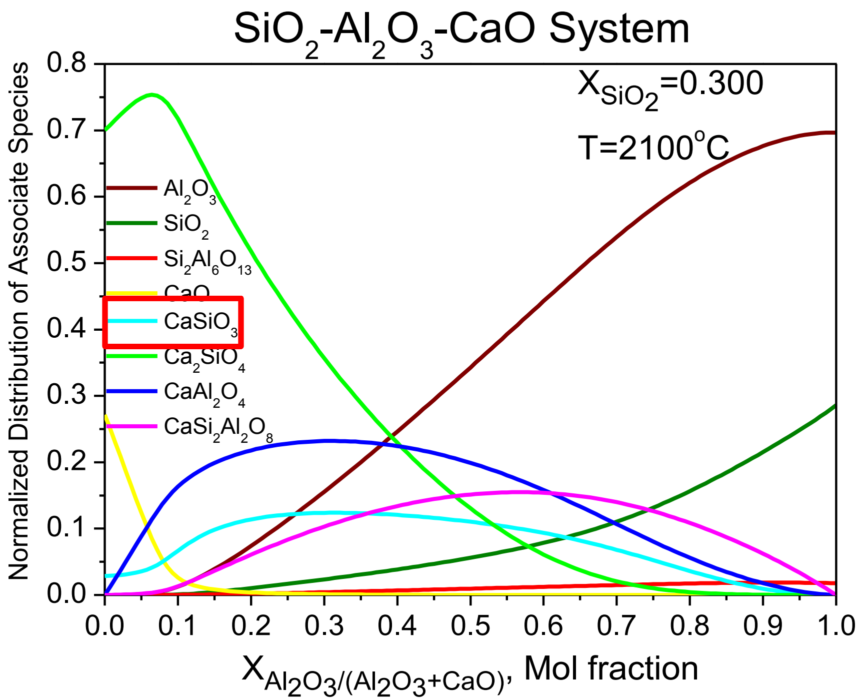
$$\ln \eta_{self-pol.} = \sum\left(A^*_{j,SiO2} + B^*_{j,SiO2}/T\right) \cdot \left(X^{n_j}_{SiO2}\right)$$

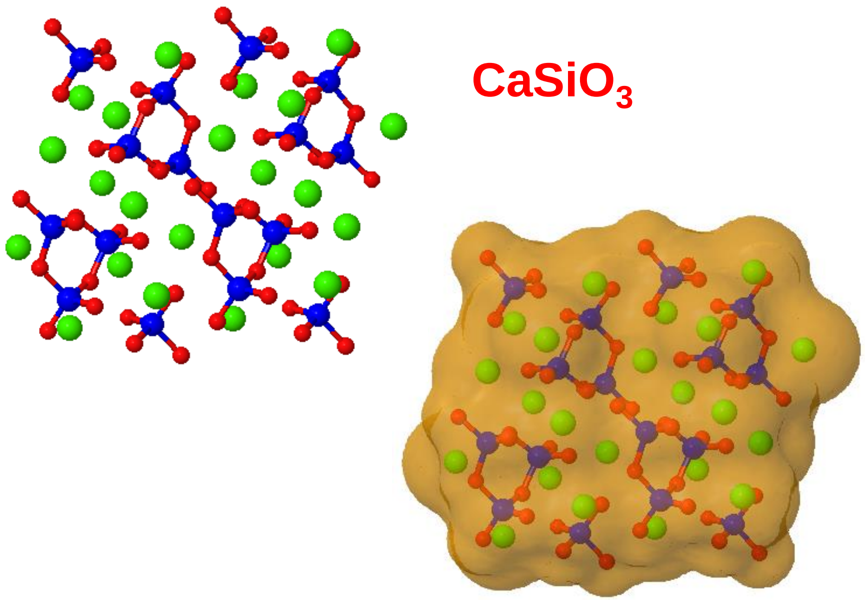
$$\ln \eta_{inter-pol.} = \sum\left(A^*_k + B^*_k/T\right) \cdot \left(X_k \cdot X^{n_k}_{SiO2}\right)$$

Probability

– System: SiO_2-Al_2O_3-CaO-MgO-Na_2O-K_2O
– 34 different associate species
– Data source: SciGlass database and FactSage references
– Data search: 62 subsystems with 32 subsystems available

Ideal viscosity part

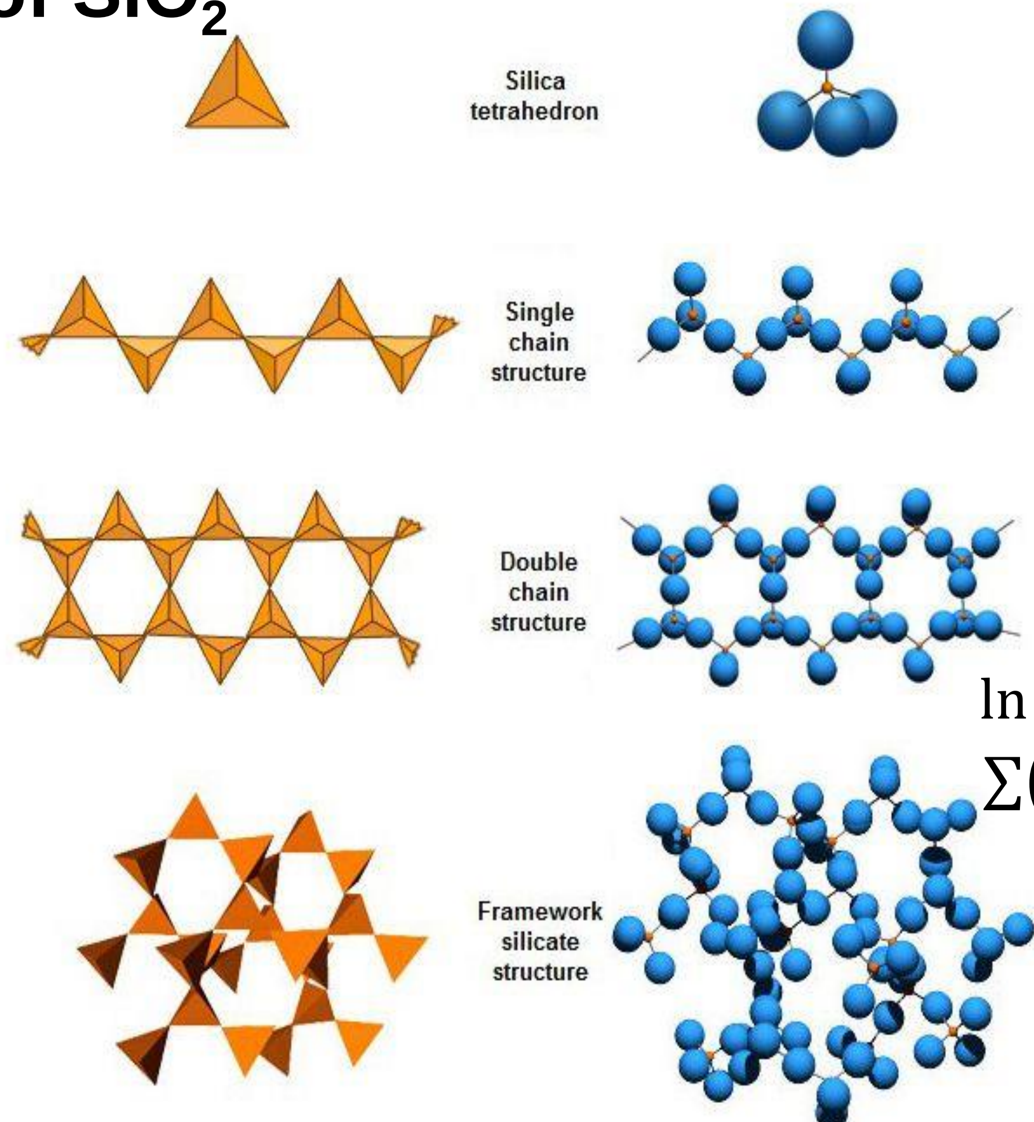




– **Associate species model** is employed to predict the **slag structure**, which can be presented by the relative concentrations of each **associate species**.

$$\ln \eta_{ideal} = \sum X_i \cdot (A_i + B_i/T)$$

Excess viscosity part 1: self-polymerization of SiO_2



L. Wang: Doctoral thesis, KTH, 2009.

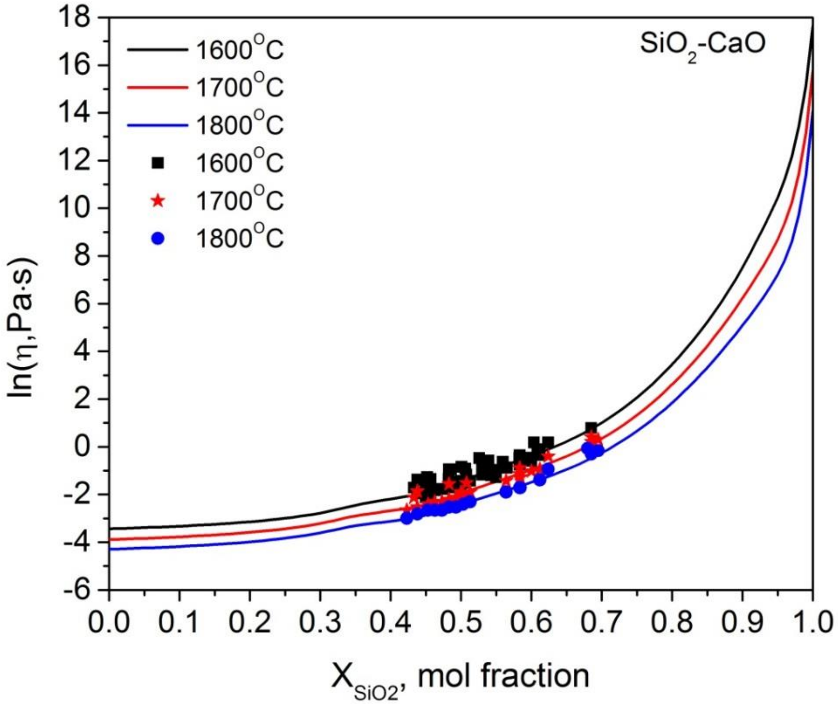
S: SiO_2

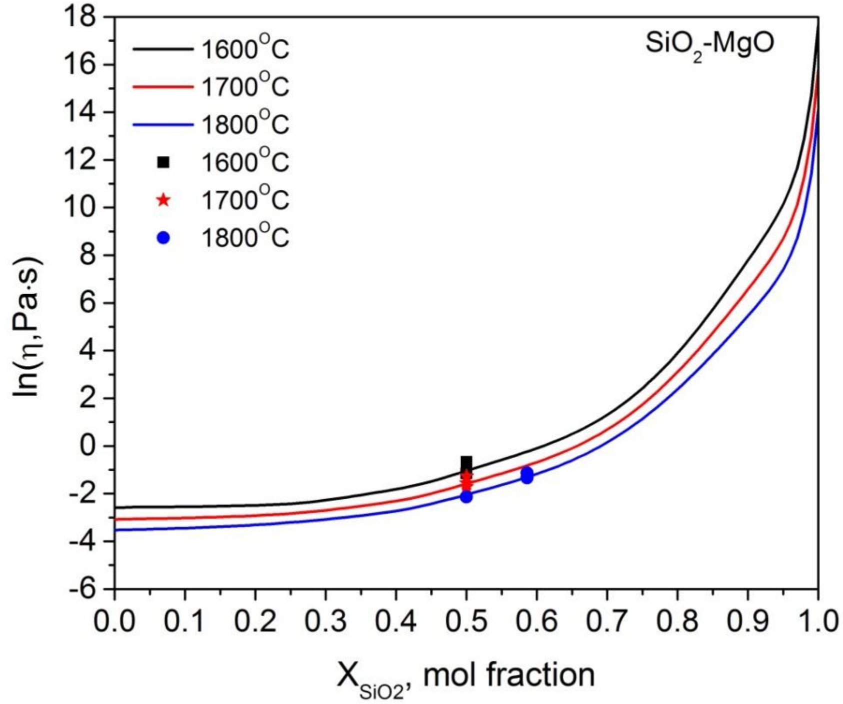
$$S_1+S_1=S_2$$
$$S_1+S_2=S_3$$
$$\ldots \ldots$$
$$S_1+S_{k-1}=S_k$$

self-pol.

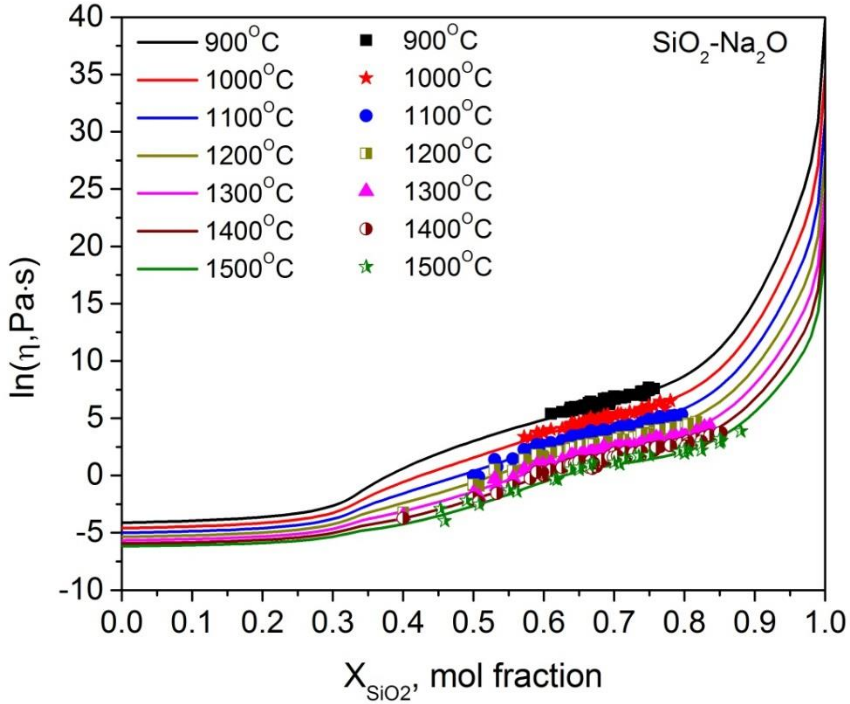
$$\ln \eta_{\mathrm{self-pol.}} = \sum\left(A^{*}_{j,SiO2} + B^{*}_{j,SiO2}/T\right) \cdot \left(X^{n_j}_{SiO2}\right)$$

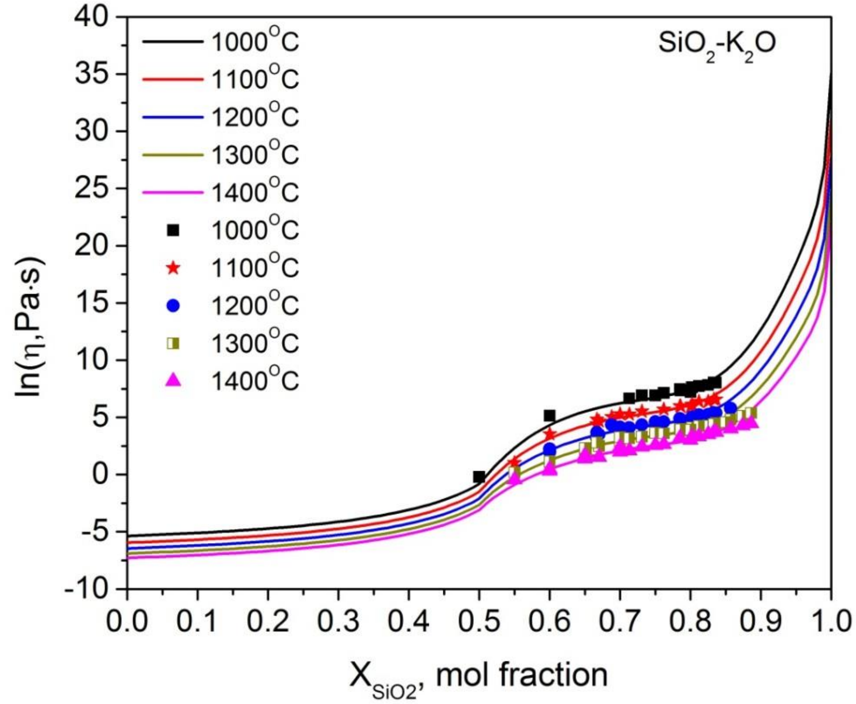
Binary system SiO_2-CaO or MgO





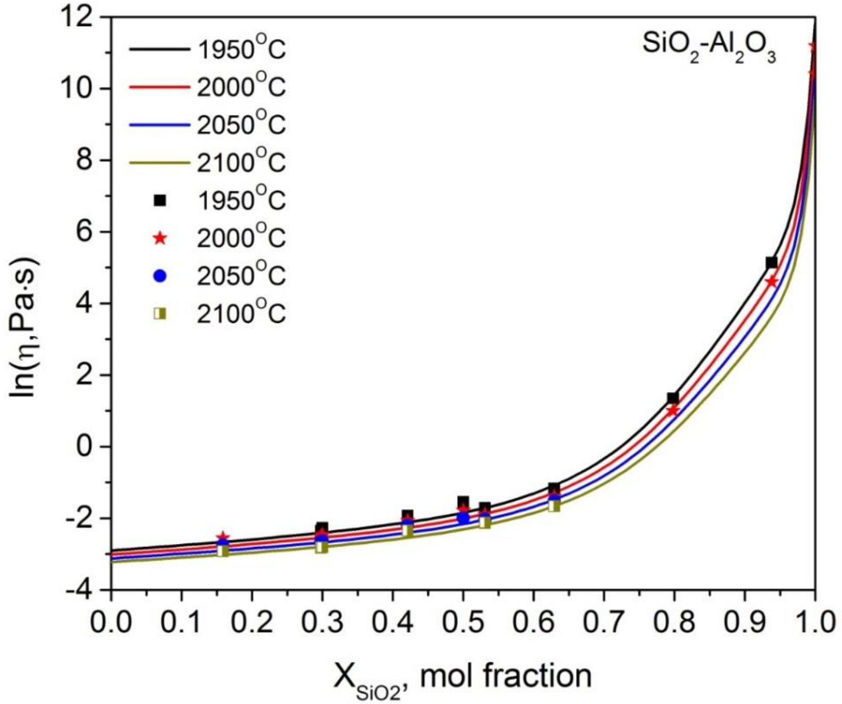
Binary system SiO_2-Na_2O or K_2O

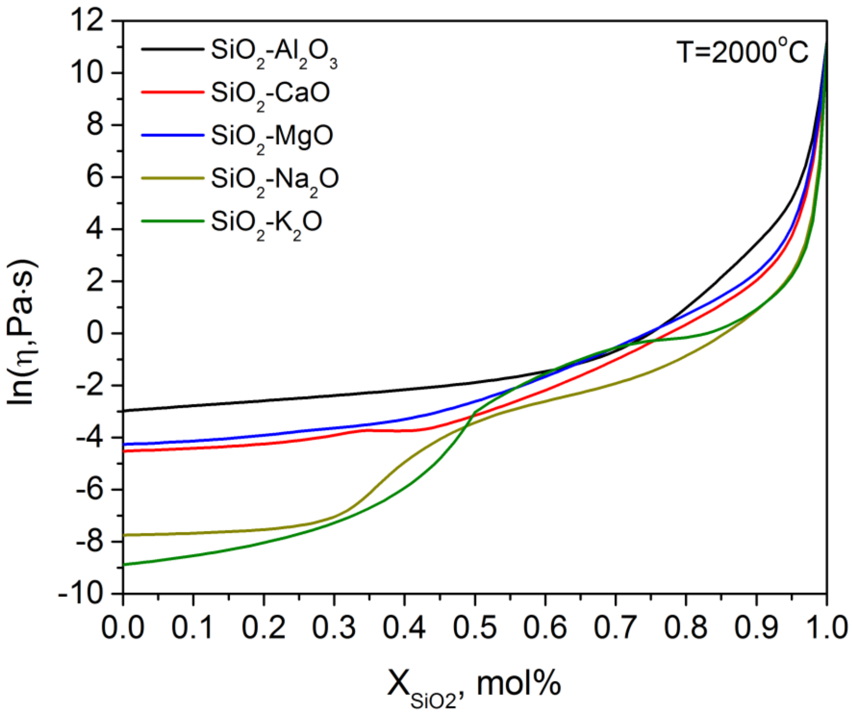




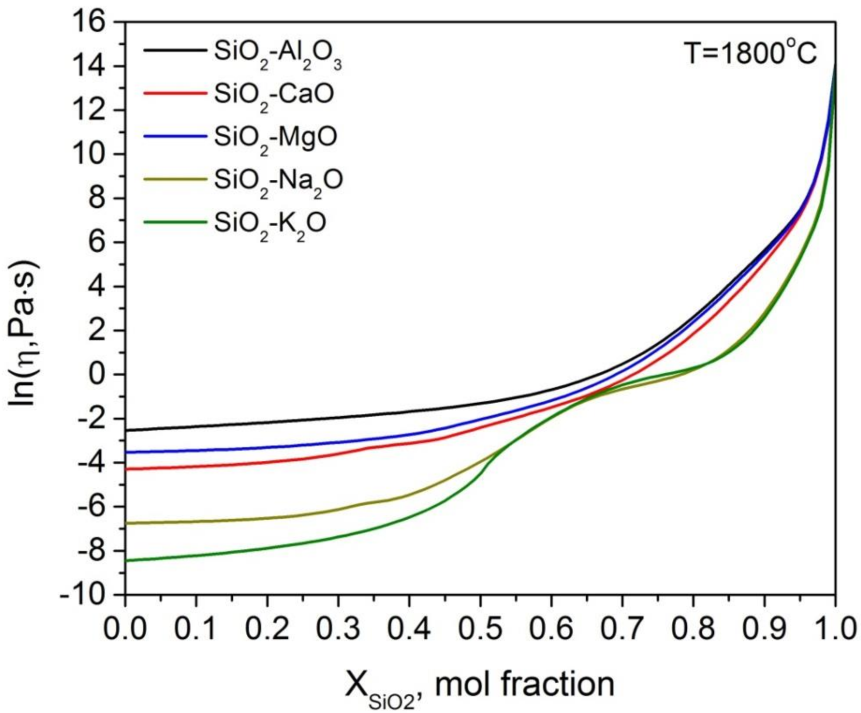
Na_4SiO_4 V.S. Na_2O

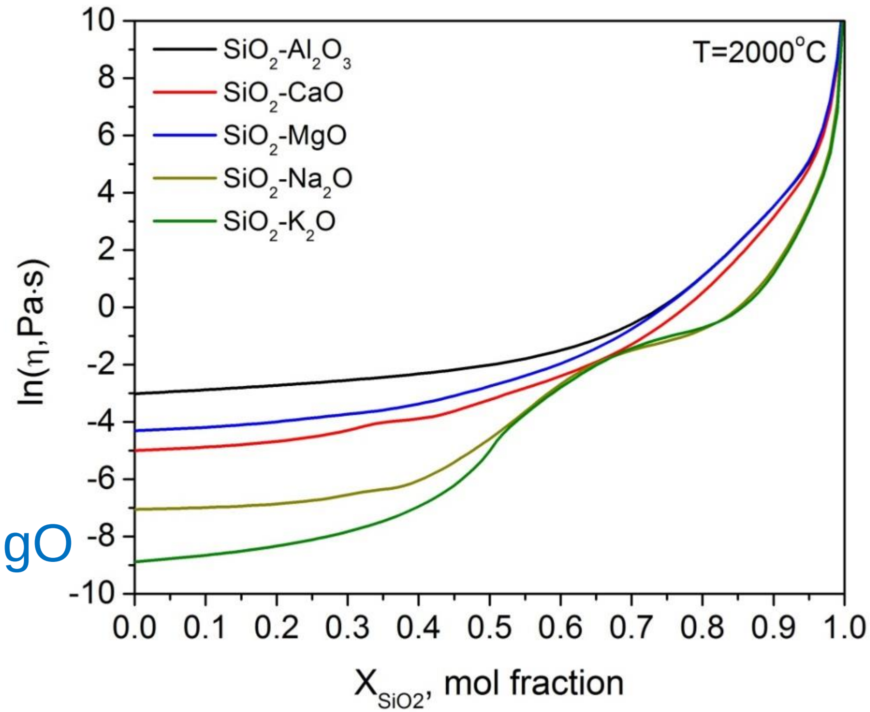
Binary system SiO_2-Al_2O_3





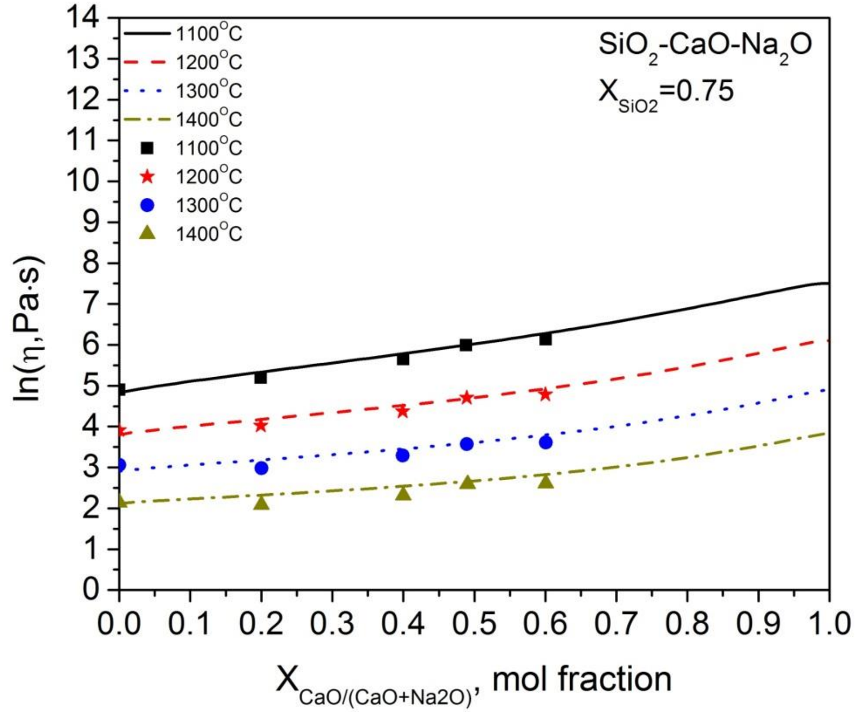
Comparison of SiO_2-based binary systems

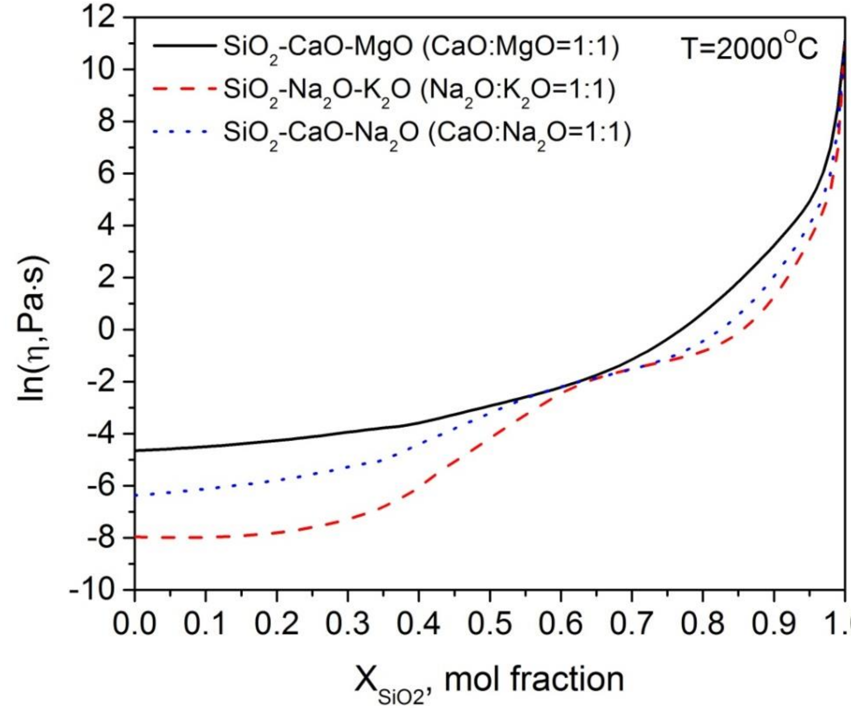




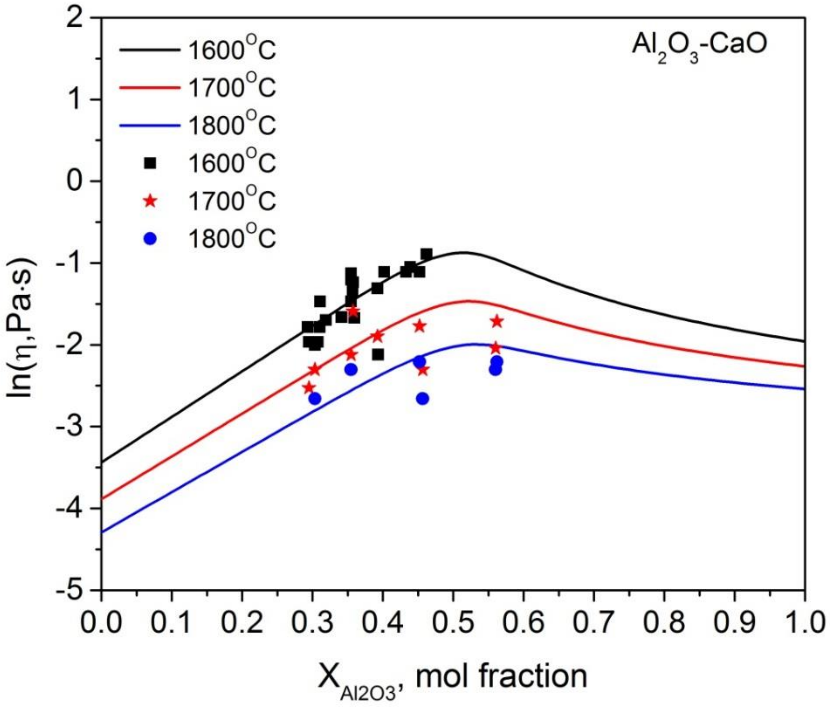
Viscosity sequence: SiO_2-Al_2O_3> SiO_2-MgO >SiO_2-CaO>SiO_2-Na_2O>SiO_2-K_2O

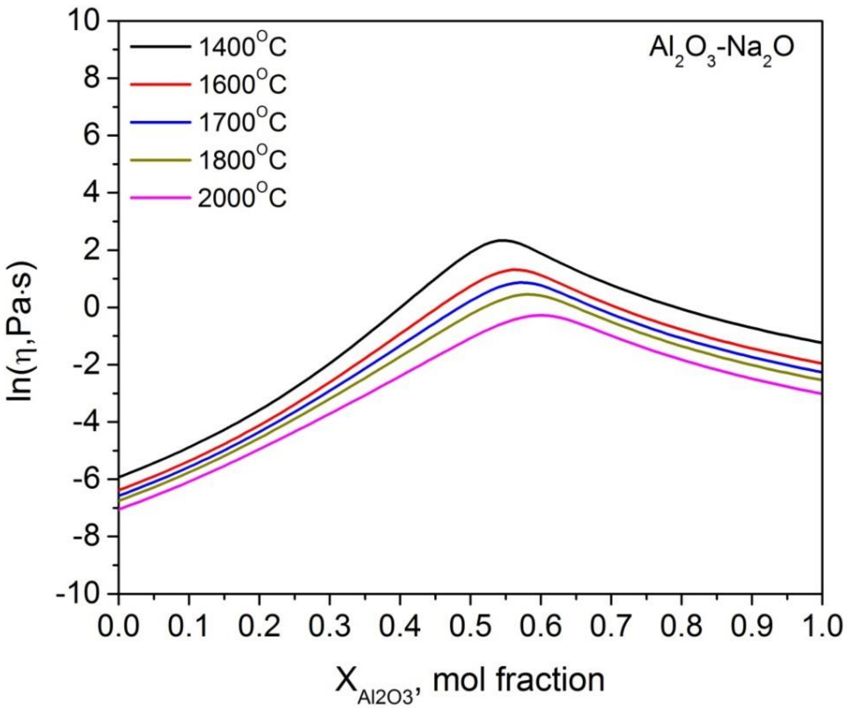
Ternary system SiO_2-CaO-Na_2O



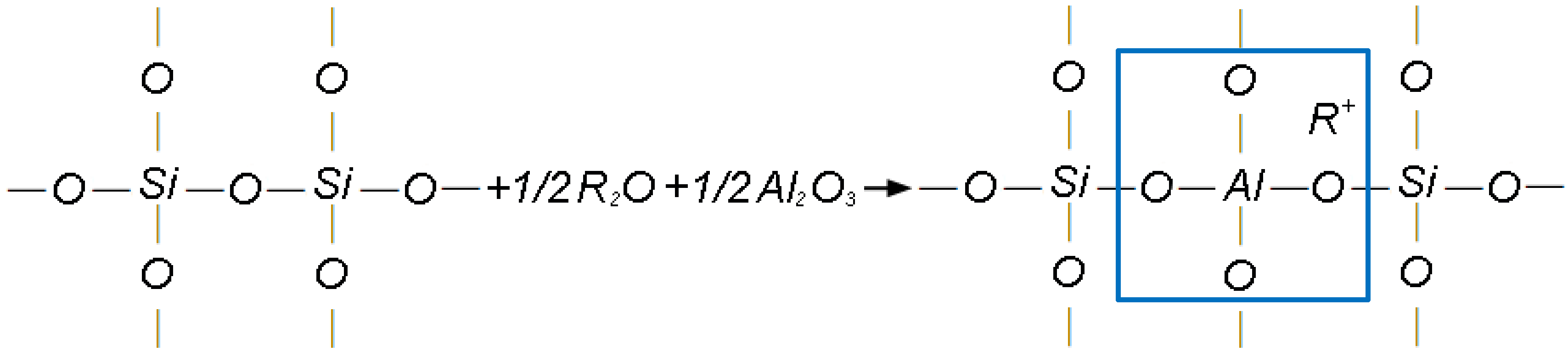


Binary system Al_2O_3-CaO or Na_2O

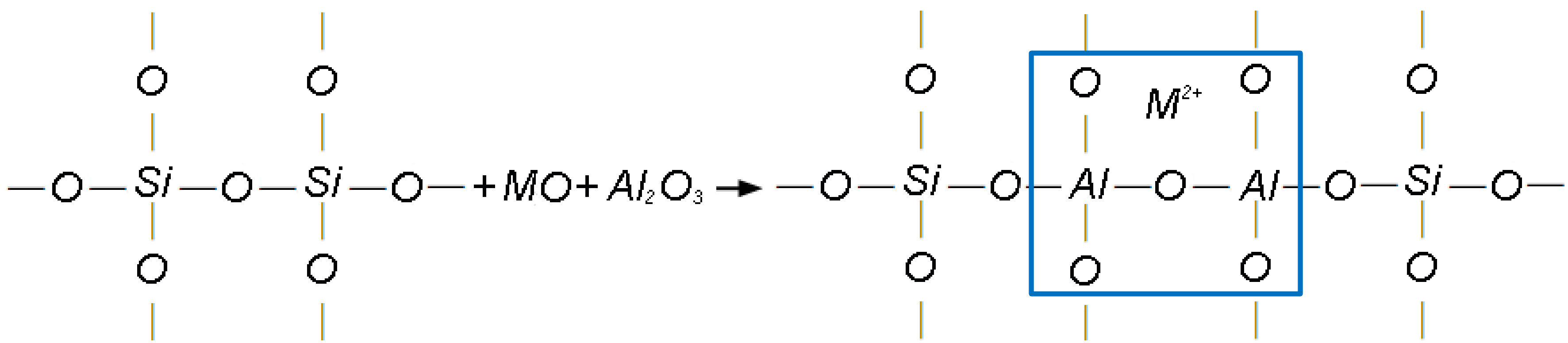




Compensation effect of Al_2O_3

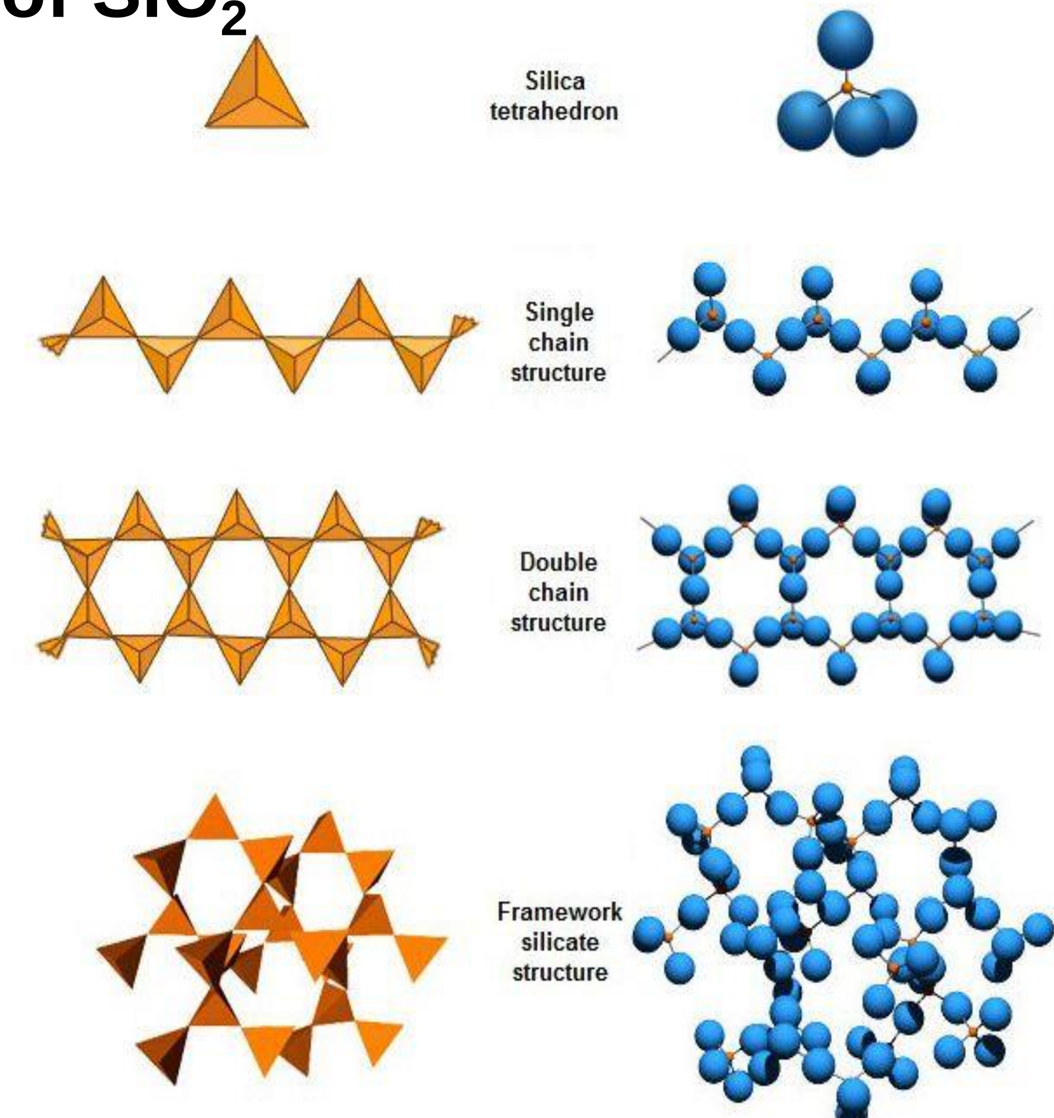


$RAlO_2$, $RAlSiO_4$, $RAlSi_3O_8$ or $RAlSi_2O_6$
R: Na, K



MAl_2O_4, $MSi_2Al_2O_8$ or $M_2Al_4Si_5O_{18}$
M: Ca, Mg

Excess viscosity part 2: inter-polymerization of SiO_2



L. Wang: Doctoral thesis, KTH, 2009.

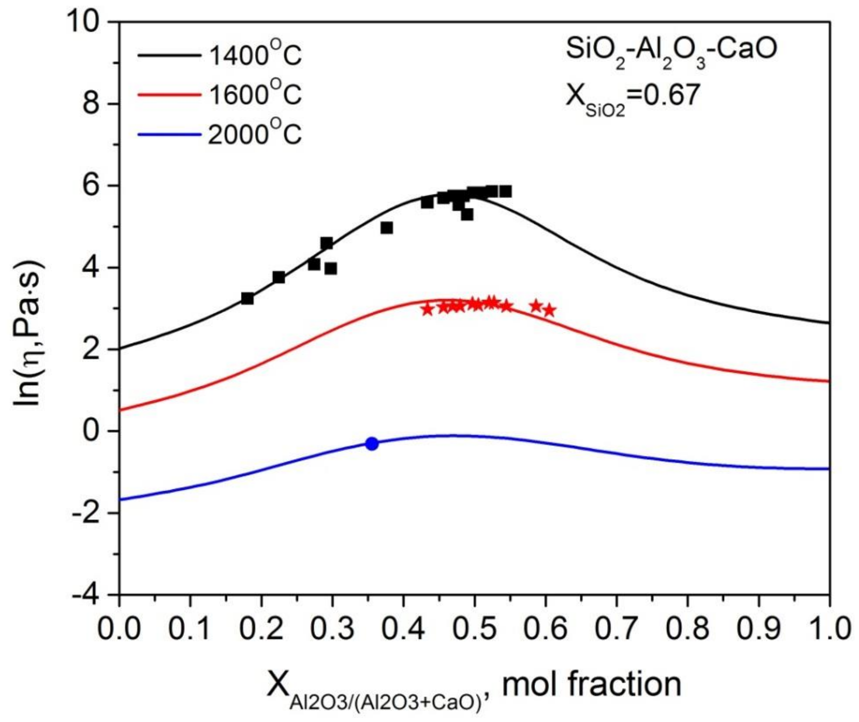
S: SiO_2, A: Al_2O_3, N: Na_2O

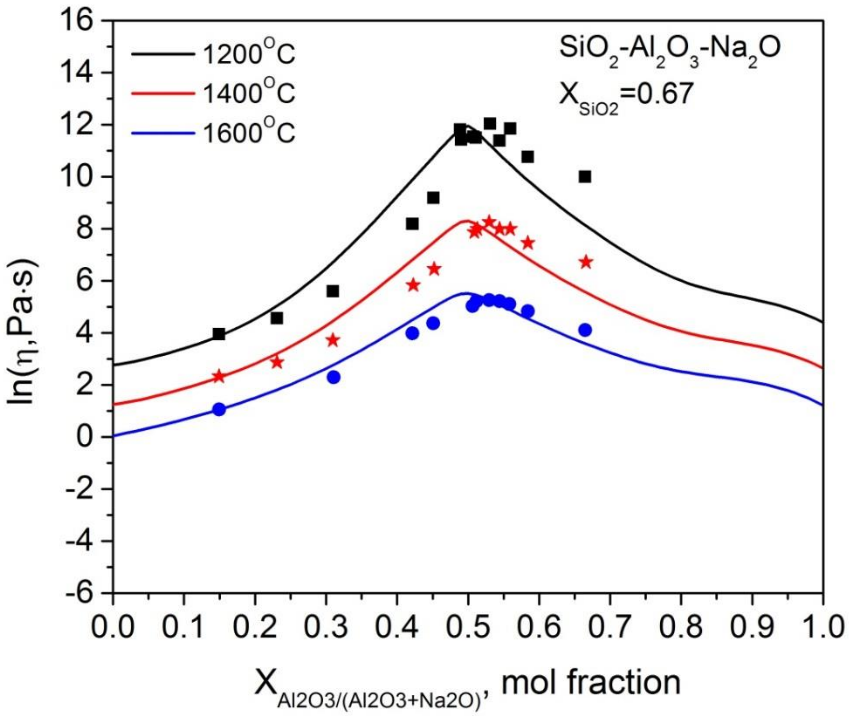
$$A_1N_1S_1 + S_1 = A_1N_1S_2$$
$$A_1N_1S_1 + S_2 = A_1N_1S_3$$
… …
$$A_1N_1S_1 + S_{k-1} = A_1N_1S_k$$

inter-pol.

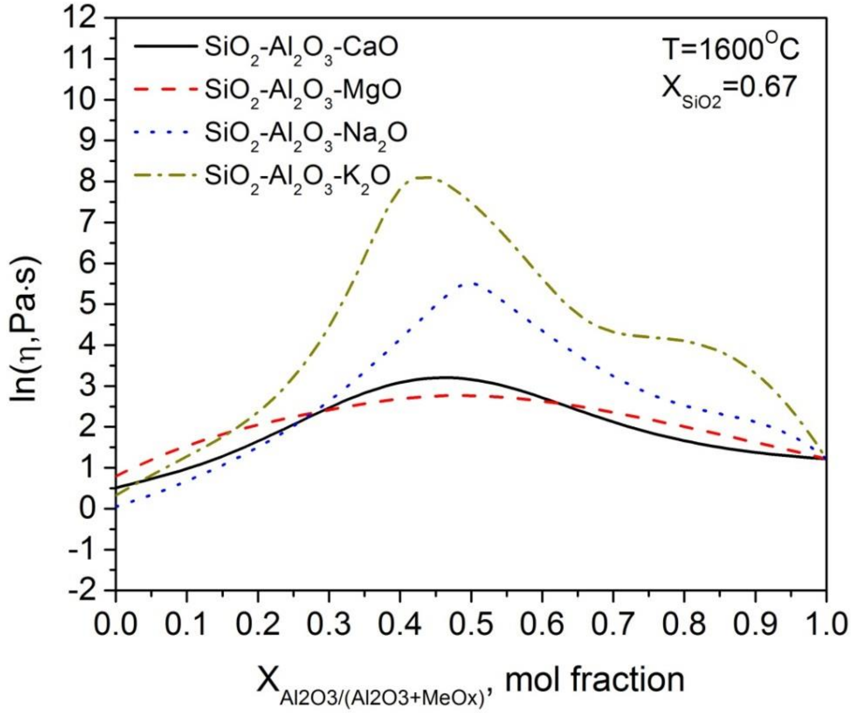
$$\ln \eta_{\text{inter-pol.}} = \sum \left(A^{*}_{k} + B^{*}_{k}/T \right) \cdot \left(X_k \cdot X^{n_k}_{SiO2} \right)$$

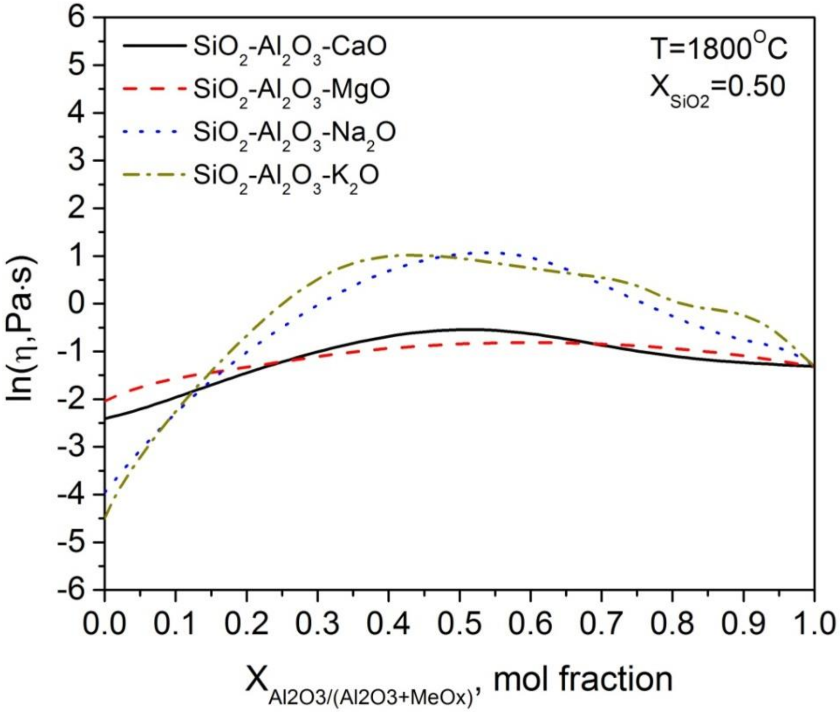
Ternary system SiO_2-Al_2O_3-CaO or Na_2O





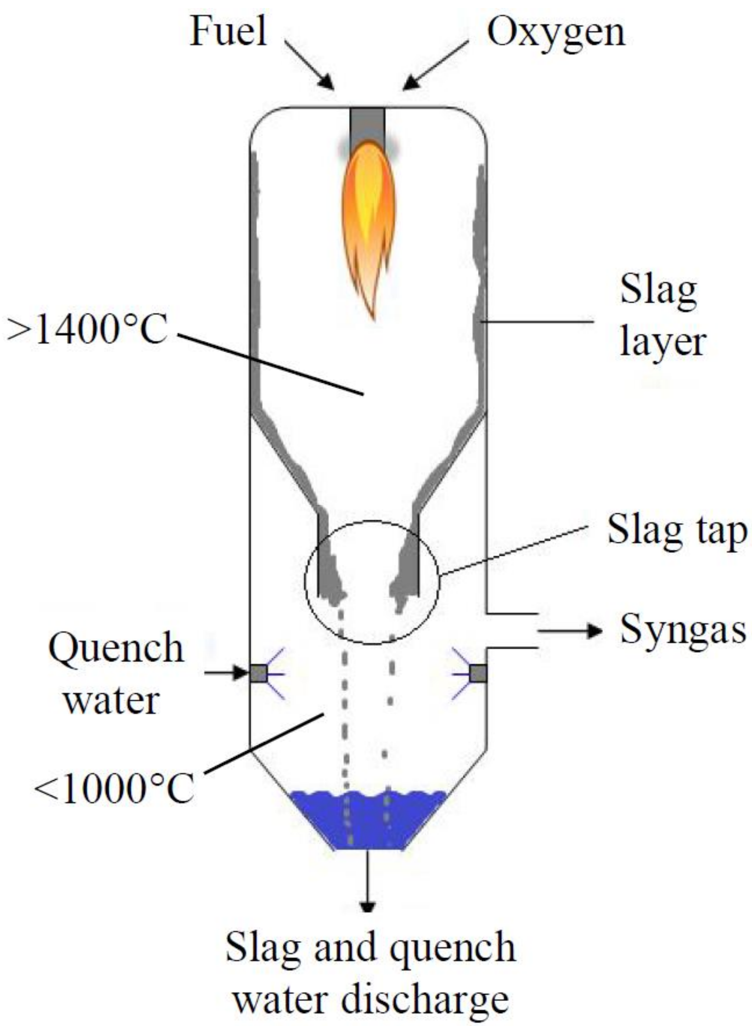
Comparison of SiO_2-Al_2O_3-based ternary systems

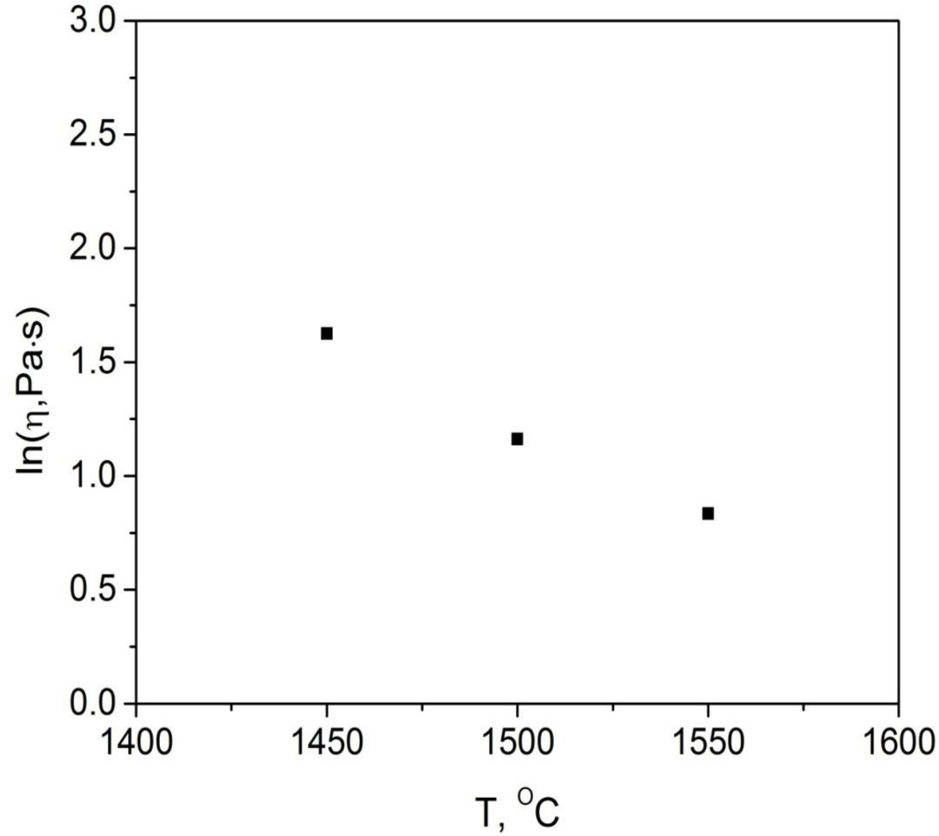




Viscosity maximum sequence:
SiO_2-Al_2O_3-K_2O>SiO_2-Al_2O_3-Na_2O
>SiO_2-Al_2O_3-CaO>SiO_2-Al_2O_3-MgO

Case study: viscosity behavior in gasifier



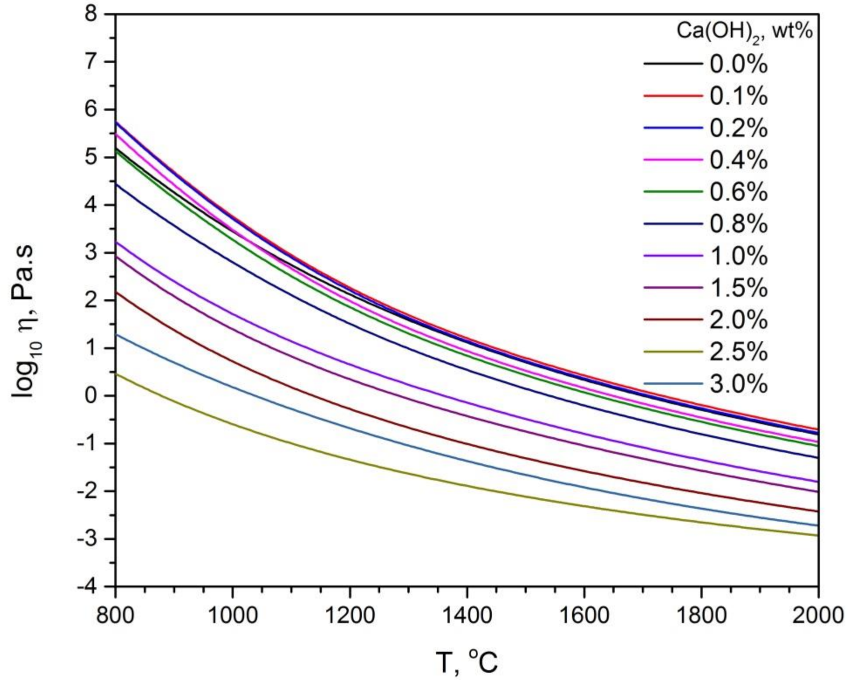


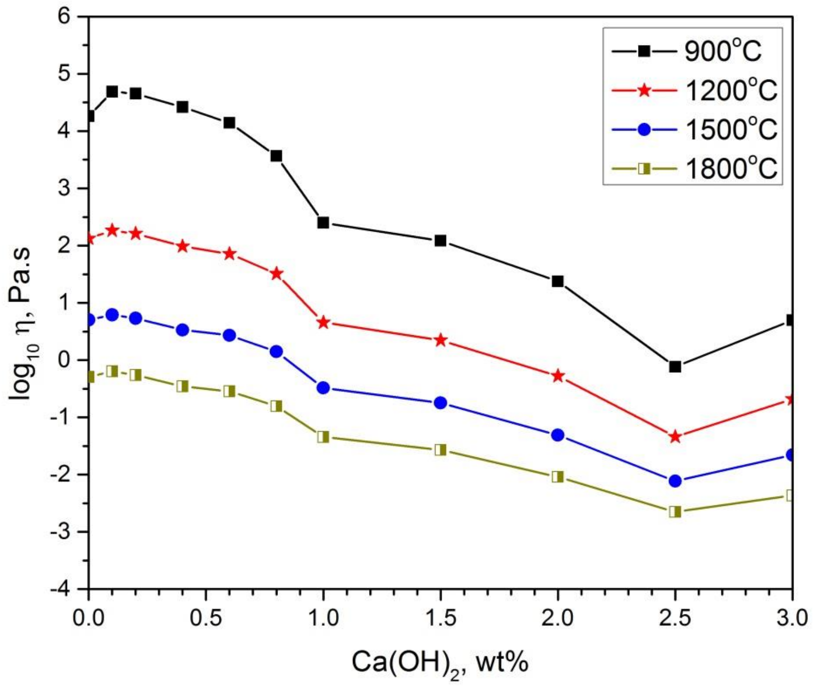
Marc A. Duchesne: Slagging in entrained-flow gasifiers, 2012.

Case study: introduction of $Ca(OH)_2$

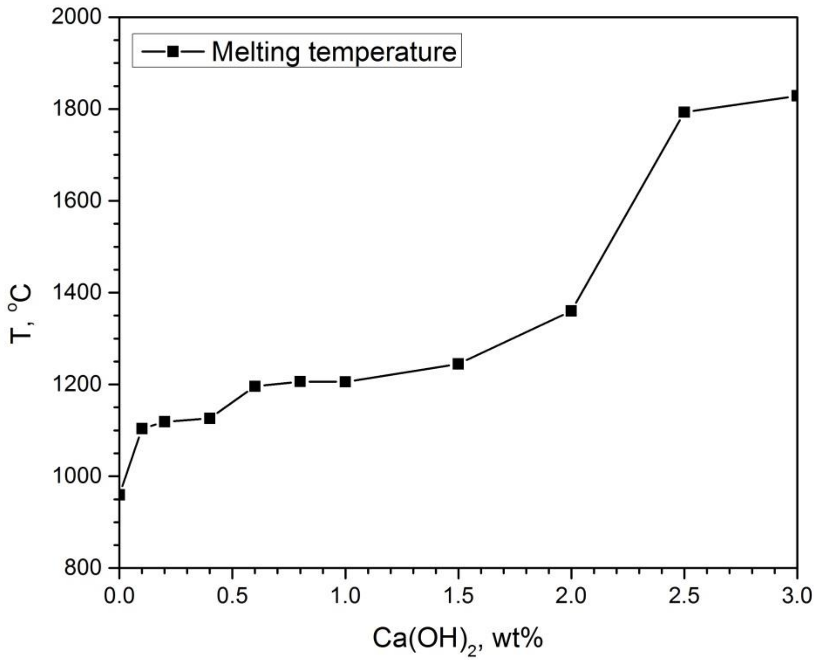
Nr. Of sample	Components, wt%			
	Glycol	Wood charcoal	Straw ash	$Ca(OH)_2$
1	70%	25%	5.0%	0.0%
2	70%	25%	4.9%	0.1%
3	70%	25%	4.8%	0.2%
4	70%	25%	4.6%	0.4%
5	70%	25%	4.4%	0.6%
6	70%	25%	4.2%	0.8%
7	70%	25%	4.0%	1.0%
8	70%	25%	3.5%	1.5%
9	70%	25%	3.0%	2.0%
10	70%	25%	2.5%	2.5%
11	70%	25%	2.0%	3.0%

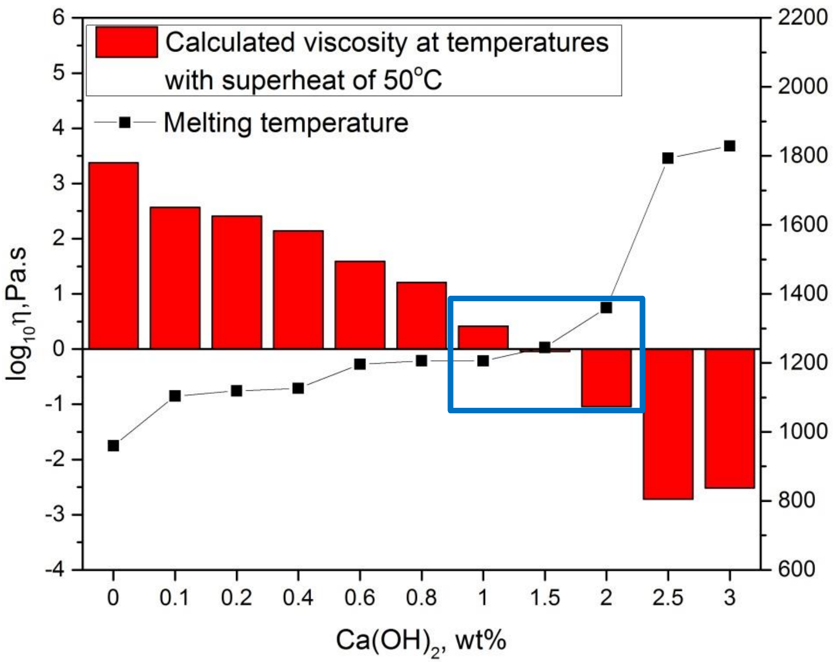
Case study: calculated viscosity





Case study: the optimum charge of $Ca(OH)_2$





Introduction of new components FeO and Fe_2O_3

- System: SiO_2-Al_2O_3-CaO-MgO-Na_2O-K_2O-**FeO-Fe_2O_3**
- **49** different associate species
- Data source: SciGlass database (version 7.2)
- Data search: **254** subsystems with **114** subsystems available

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Thank you very much for your attention!