Application of the FactSage in the assessment of fuel slags and the model development for suspension viscosity

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GTT Users' Meeting, 24 June 2020

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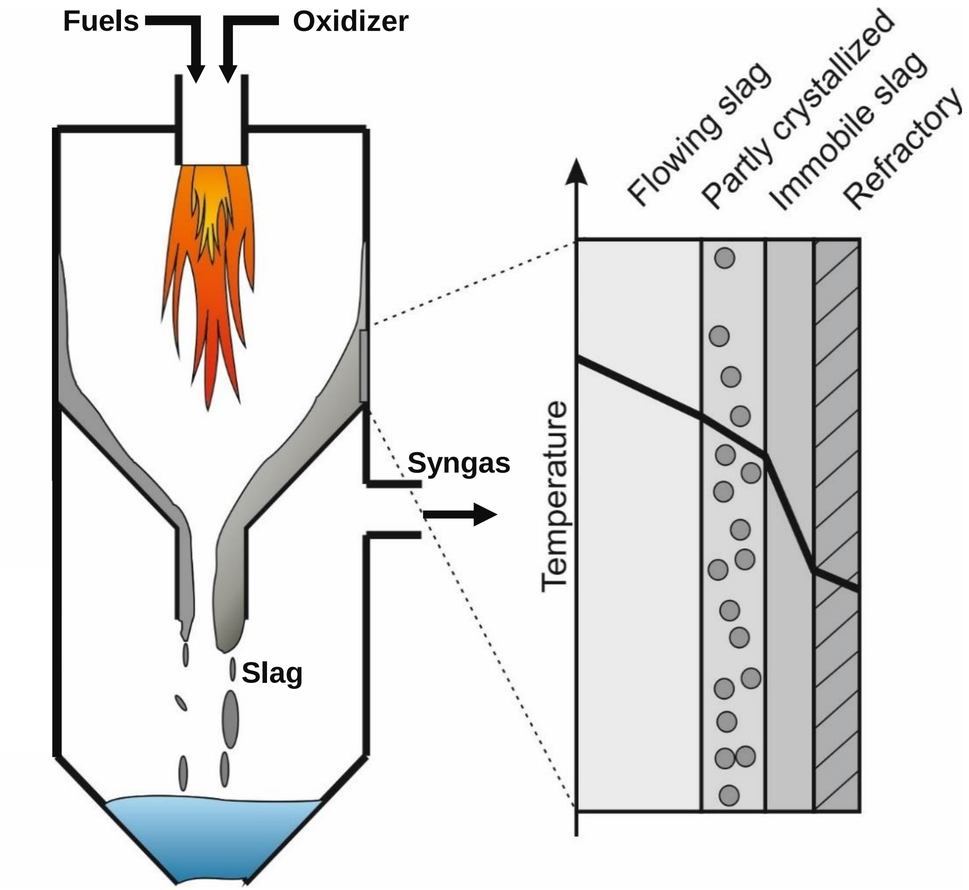
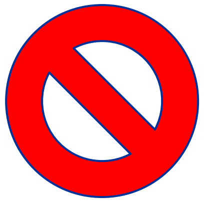
- What is an optimum slag system?
- Path to an optimum slag system
- Viscosity estimation for suspensions
- Outlook

What is an optimum slag system?

Entrained-flow slagging gasifier





Slag tapping blockage

Refractory corrosion

Design an optimum slag system

- Viscosity
- Surface tension
- Liquidus temperature
- Reactivity with refractory lining
- Thermal conductivity
- Temperature of critical viscosity

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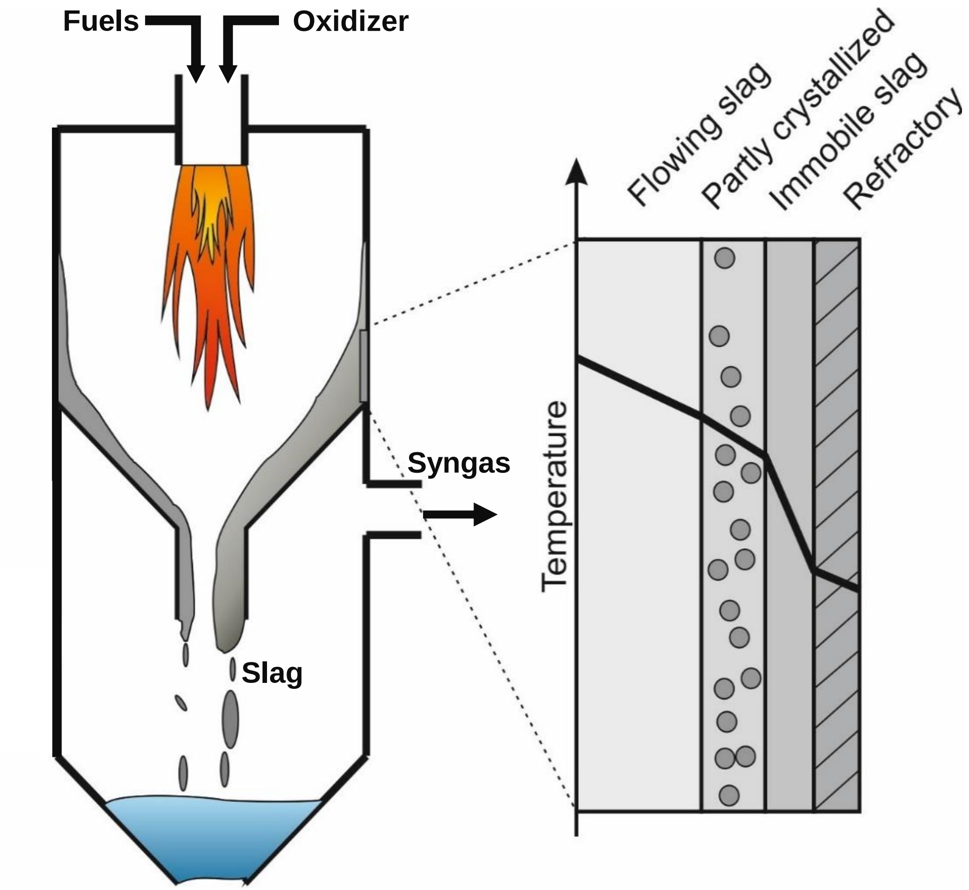
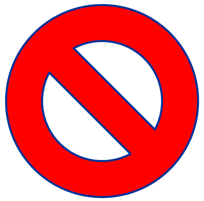
What is an optimum slag system?

Entrained-flow slagging gasifier





Slag tapping blockage

Refractory corrosion

Design an optimum slag system

- **Viscosity**
- **Surface tension**
- **Liquidus temperature**
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- **Thermal conductivity**
- **Temperature of critical viscosity**

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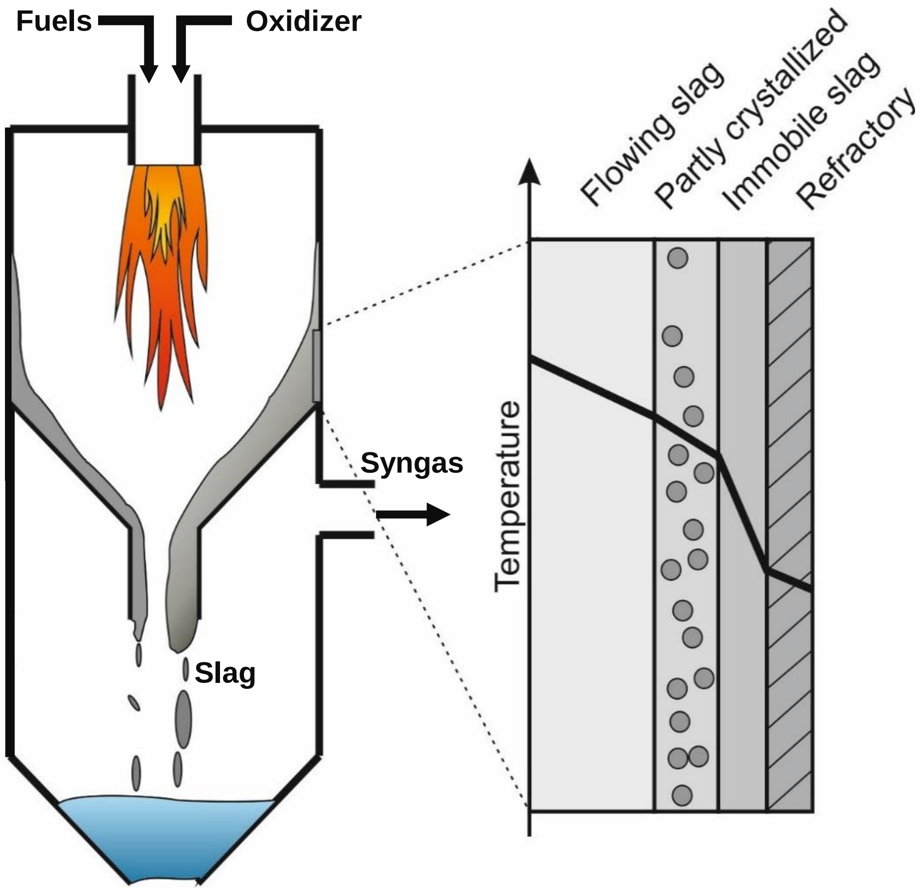
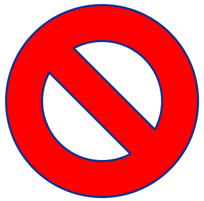
What is an optimum slag system?

Entrained-flow slagging gasifier





Slag tapping blockage

Refractory corrosion

Design an optimum slag system

- Viscosity (5-25 Pa·s)
- Surface tension
- Liquidus temperature
- Reactivity with refractory lining
- Thermal conductivity
- Temperature of critical viscosity

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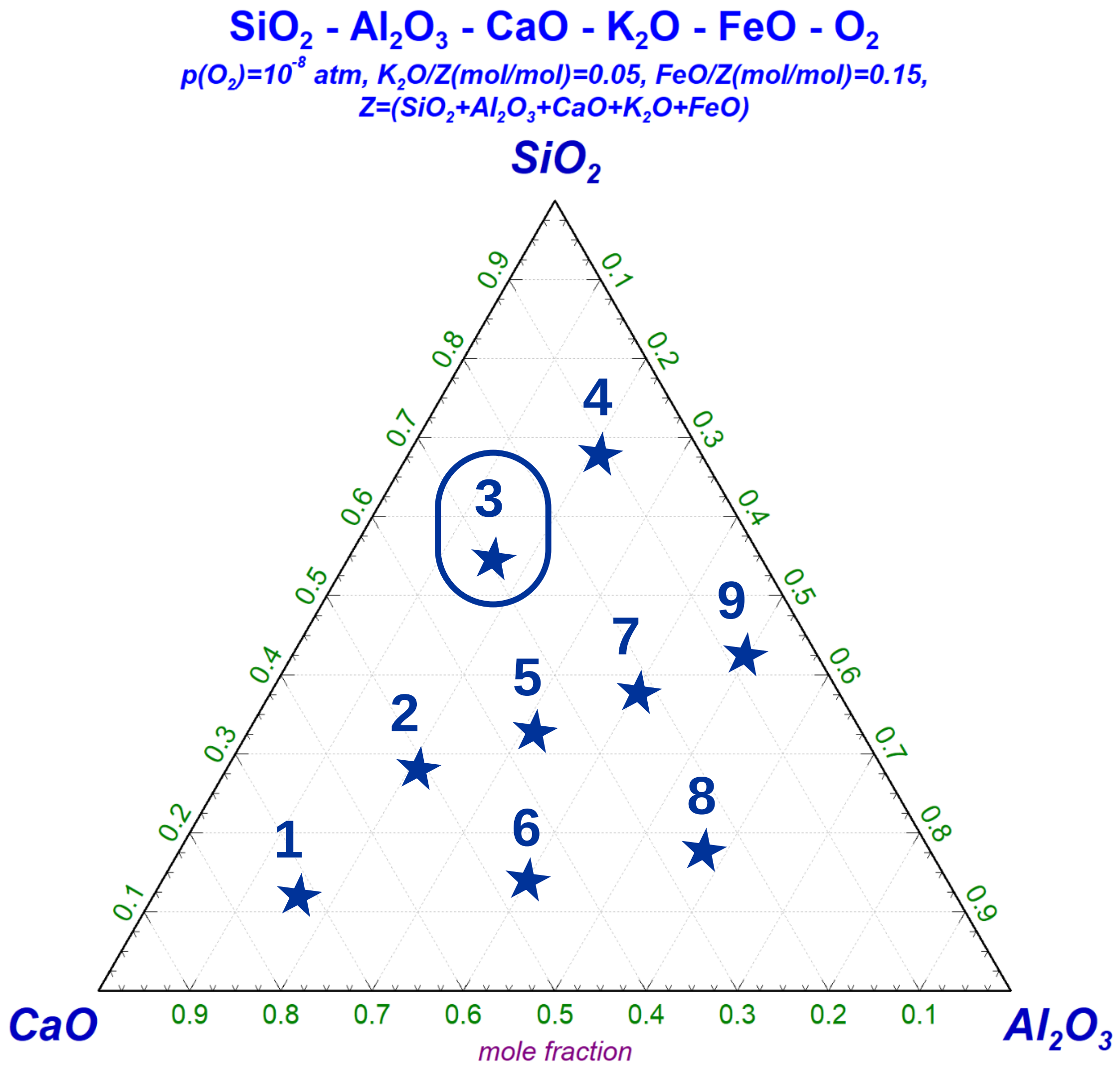
Path to an optimum slag system

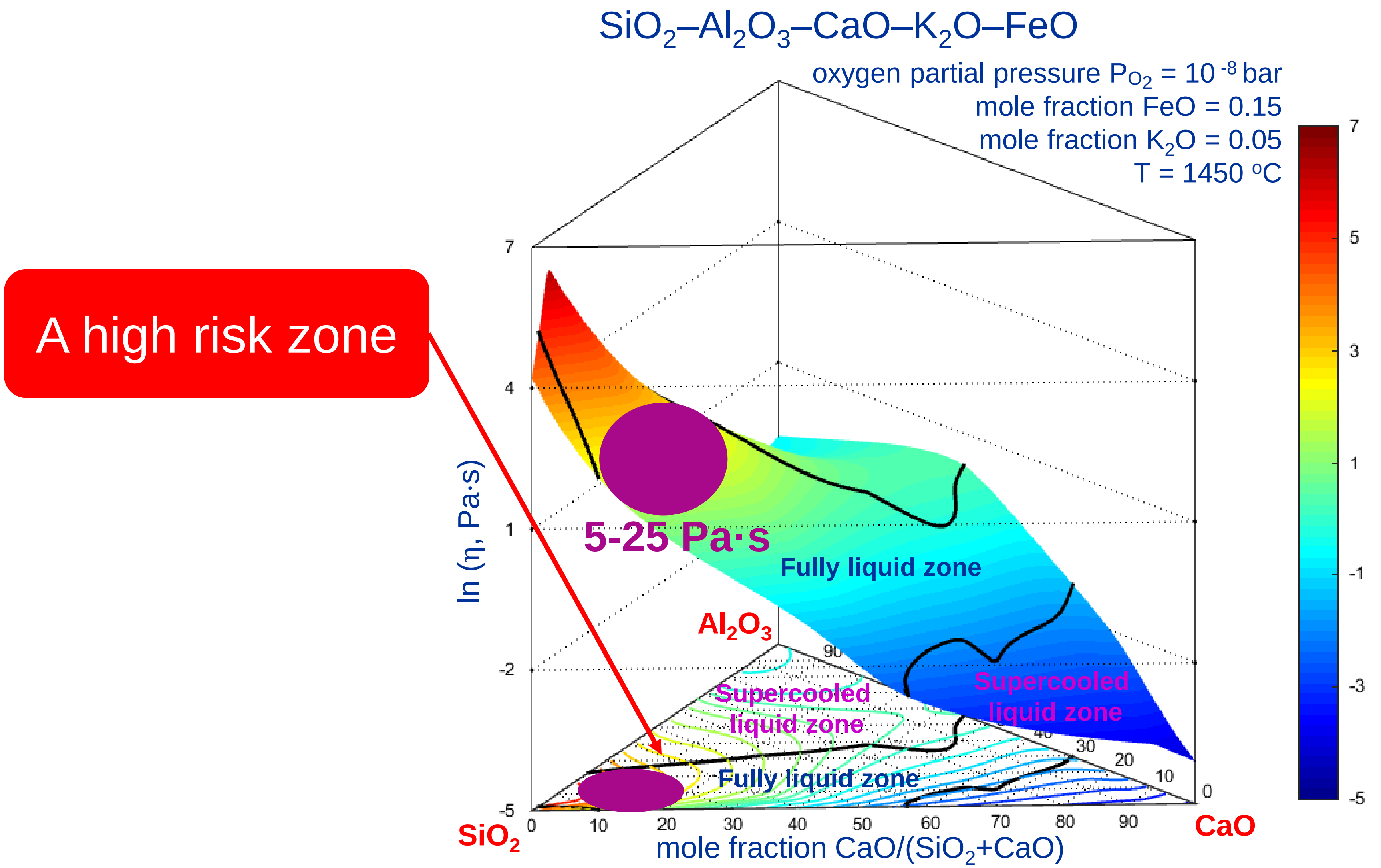


Operating temperature of 1450 ^oC

Via experimental approach?

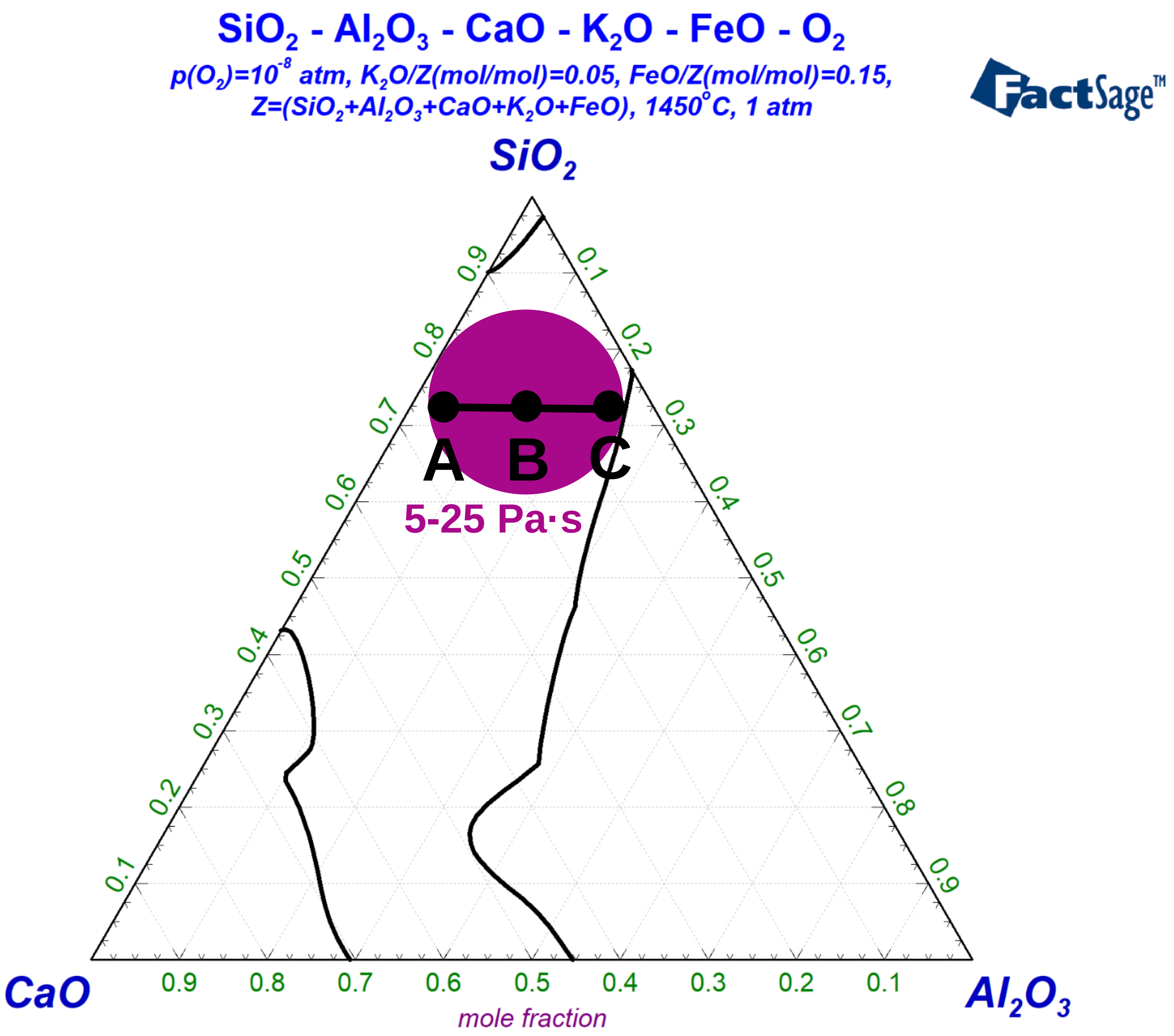
Slag 3 is assumed to be the optimum slag system **but locally.**

Path to an optimum slag system



Combine information on the phase relationships with the viscosity values

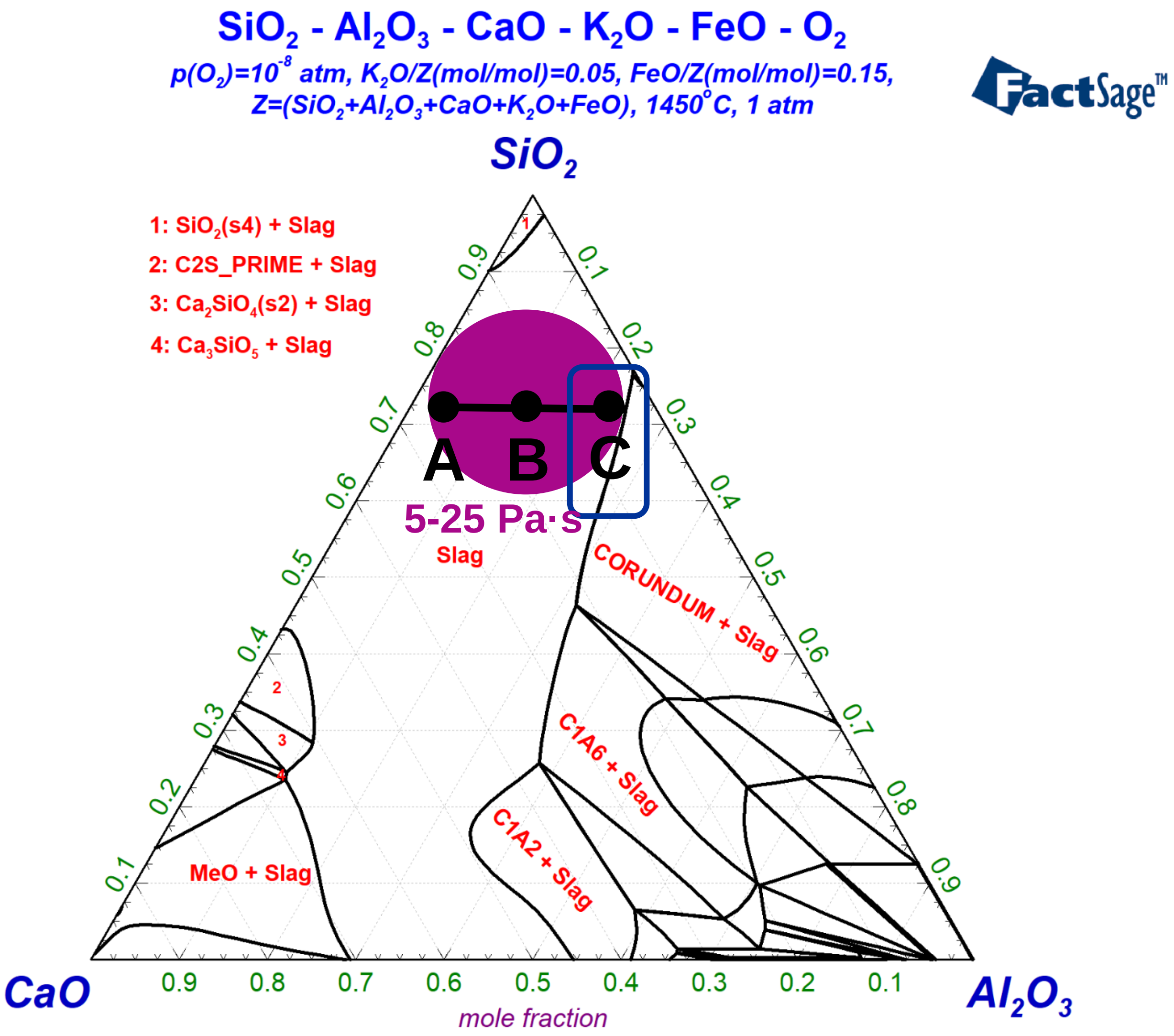
Path to an optimum slag system



Which slag (A, B, or C) is the best candidate?

Alumina based refractory lining

Path to an optimum slag system

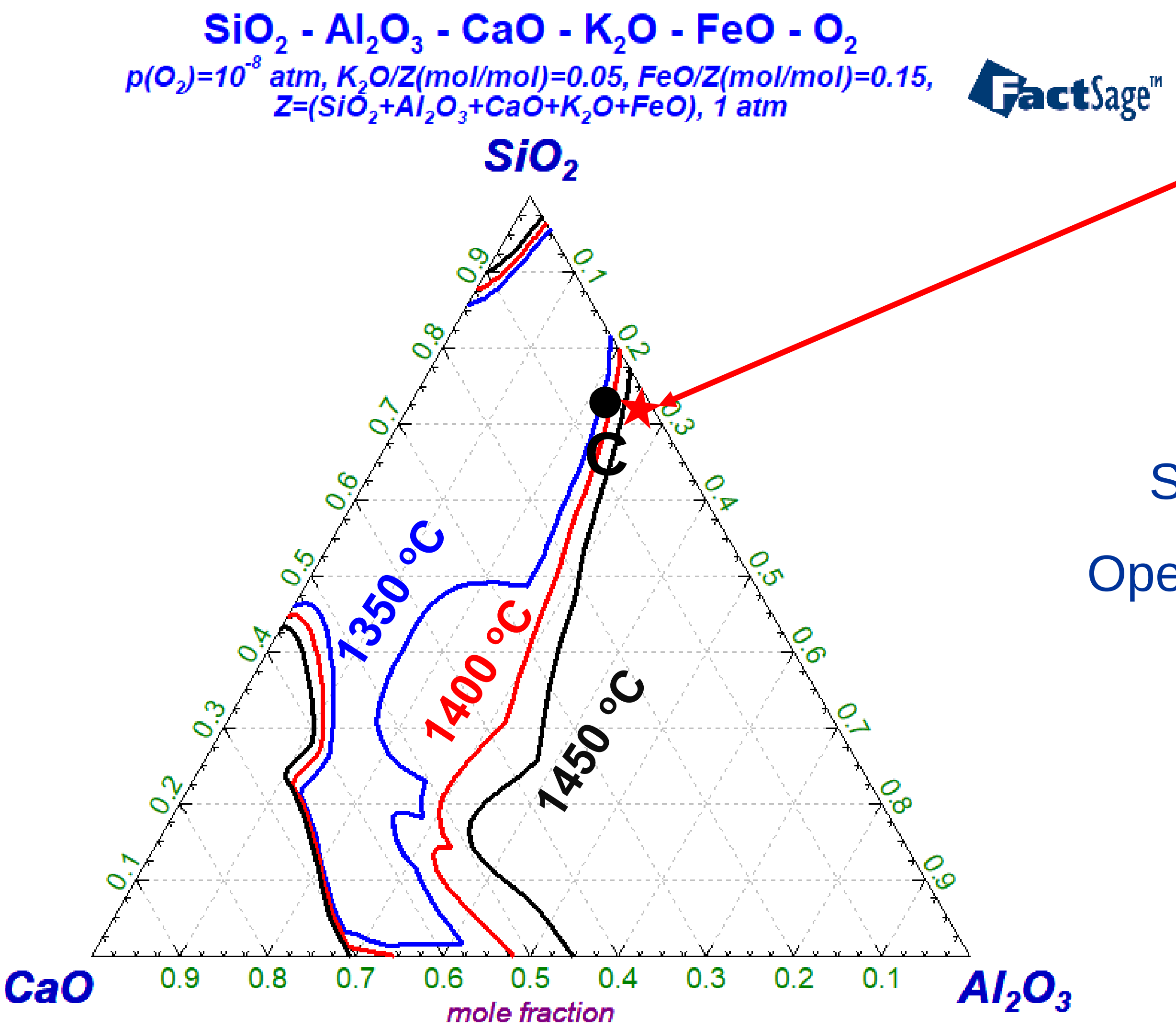


Which slag (A, B, or C) is the best candidate?

Alumina based refractory lining

$\boxed{C}$

Path to an optimum slag system



A high risk zone

Fluctuations

in

Slag composition

Operation temperature

Atmosphere

…

Experimental validation

Goal

Viscosity estimation for suspensions

Einstein-Roscoe model: $\boldsymbol{\eta_r = (1 - \alpha \cdot \varphi)^{-2.5}}$

where: $\boldsymbol{\alpha}$ is the empirical parameter depending on crystal morphology; $\boldsymbol{\varphi}$ is the volume fraction of crystalline phases.

Thermodynamic database

↓

Mass fraction of crystals

↓

Einstein-Roscoe model

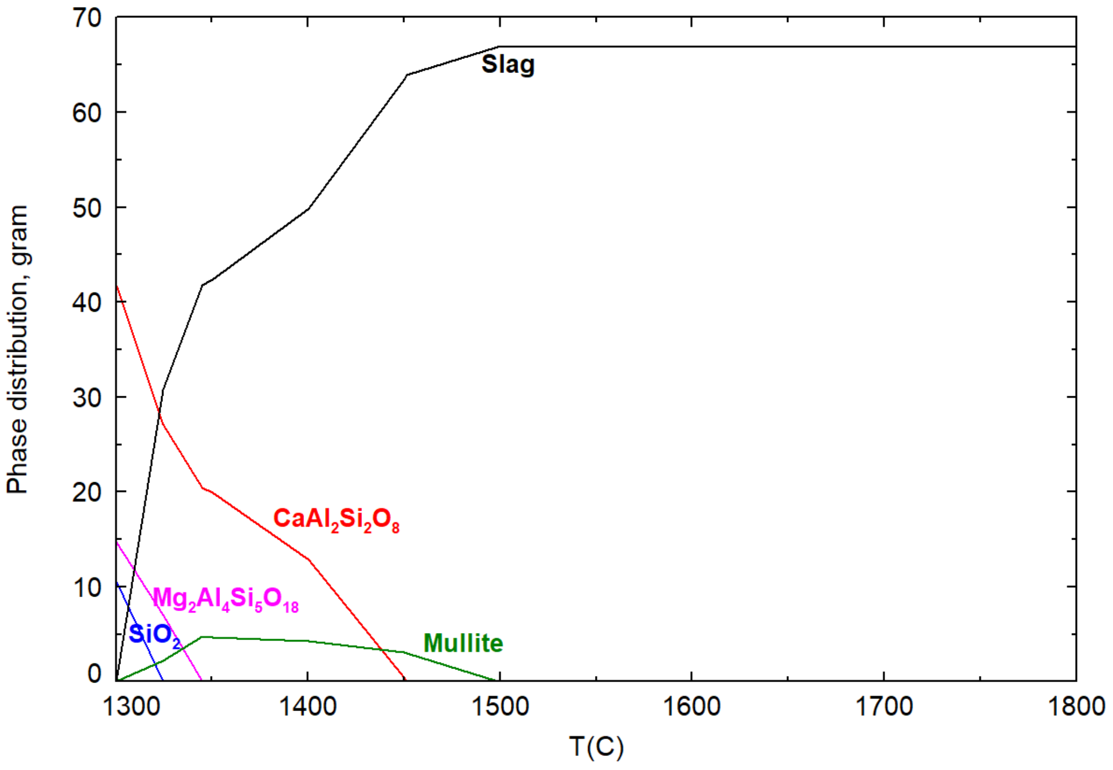
↓

$$\boldsymbol{\eta_s = \eta_l \cdot \eta_r}$$

$\boldsymbol{\eta_s}$: the viscosity of crystal-melt suspensions
$\boldsymbol{\eta_l}$: the viscosity of the remaining liquid slag
$\boldsymbol{\eta_r}$: the relative viscosity

Viscosity estimation for suspensions

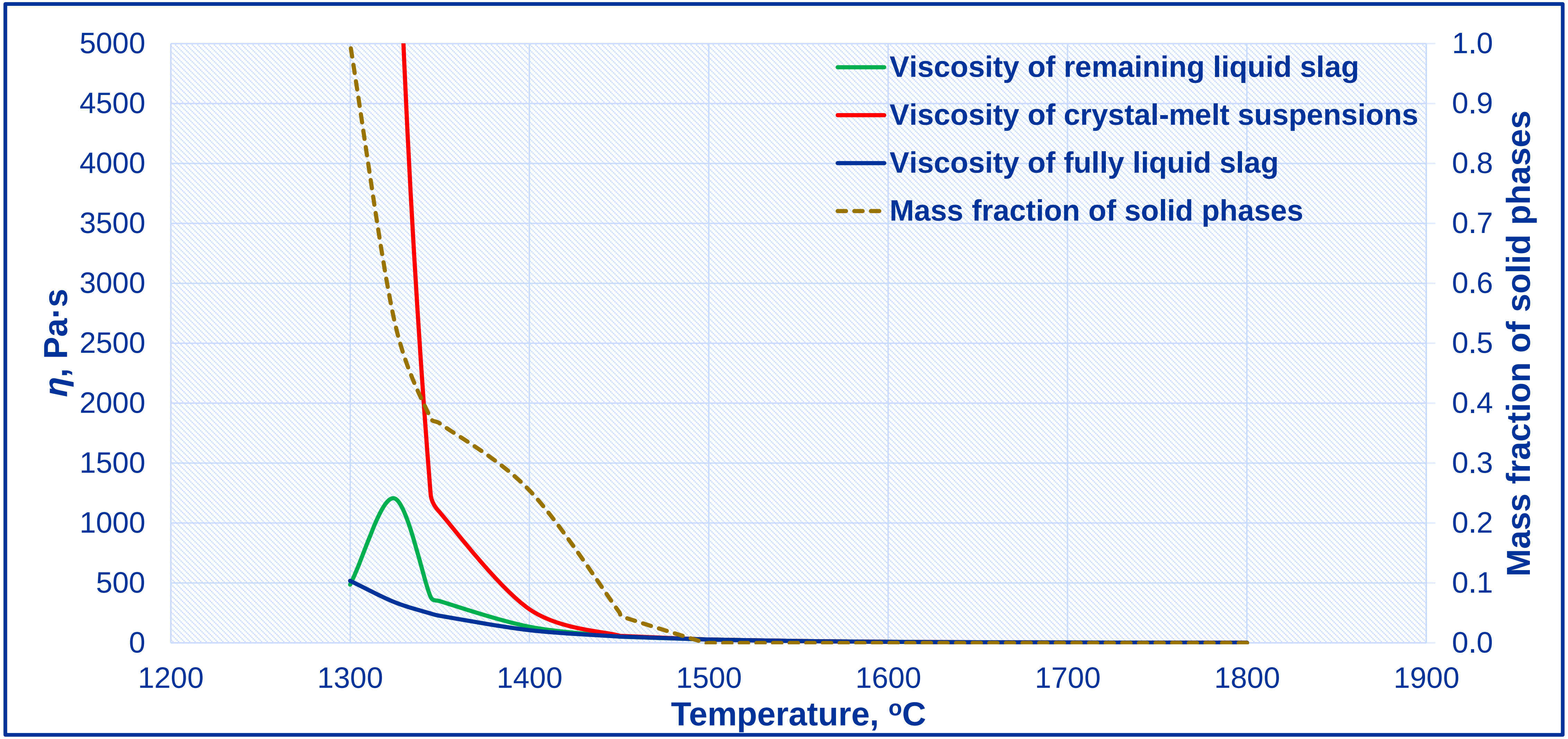
Slag composition, mole fraction			
SiO_2	Al_2O_3	CaO	MgO
0.60	0.20	0.15	0.05



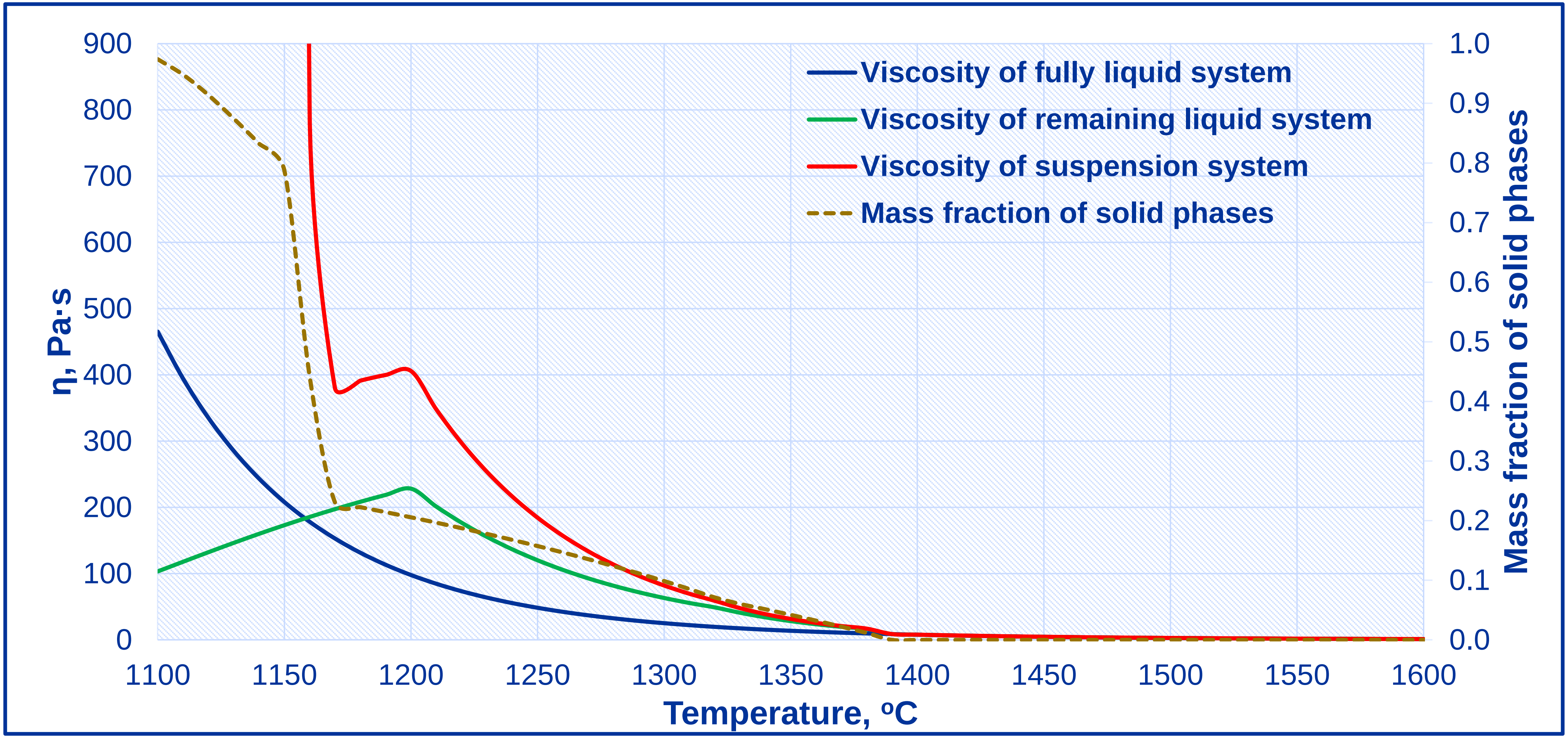
One-dimensional phase mapping

Temperature, °C	Composition of the remaining liquid slag, mole fraction				Mass fraction of solid phases
	SiO_2	Al_2O_3	CaO	MgO	
1600	0.600	0.200	0.150	0.050	0
1550	0.600	0.200	0.150	0.050	0
1500	0.600	0.200	0.150	0.050	0
1498.29	0.600	0.200	0.150	0.050	0
1451.19	0.608	0.185	0.155	0.052	0.045
1450	0.608	0.184	0.155	0.052	0.052
1400	0.637	0.162	0.135	0.065	0.255
1350	0.660	0.145	0.119	0.076	0.366
1344.86	0.662	0.144	0.118	0.077	0.375
1324.43	0.702	0.133	0.110	0.055	0.541
1300	0.673	0.115	0.129	0.083	1.000

Viscosity estimation for suspensions



Viscosity estimation for suspensions



Viscosity estimation for suspensions

Thermodynamic database

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Mass fraction of crystals

↓

Density data of crystals → Volume fraction of crystals ← Density model of melts

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Einstein-Roscoe model

↓

$$\eta_s = \eta_l \cdot \eta_r$$

Viscosity estimation for suspensions

Slag composition, mole fraction			
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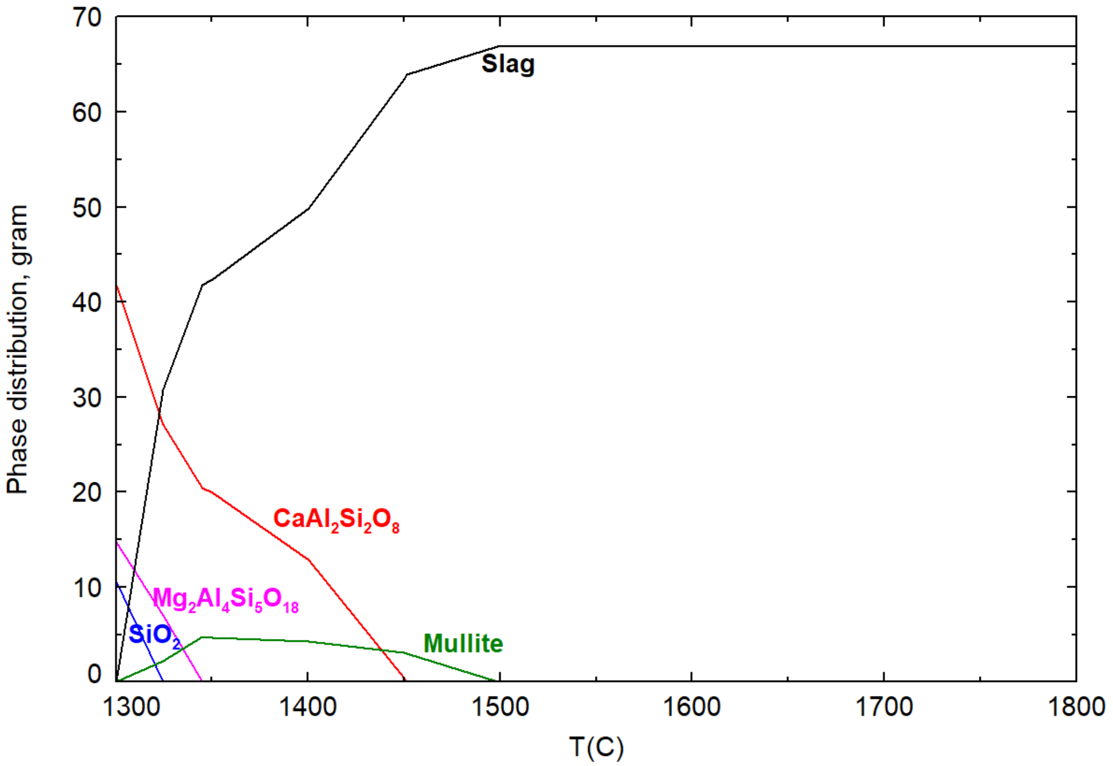

Crystalline	Temperature, ºC	Density, g/cm^3
Mullite	25	3.05 (average)
$CaAl_2Si_2O_8$	25	2.75
$Mg_2Al_4Si_5O_{18}$	25	2.51
SiO_2	25	2.65

✚

Density model for slag:

1. Bottinga et al. (1982)
2. Mills and Rhine (1989)
3. Ghiorso and Kress (2004)

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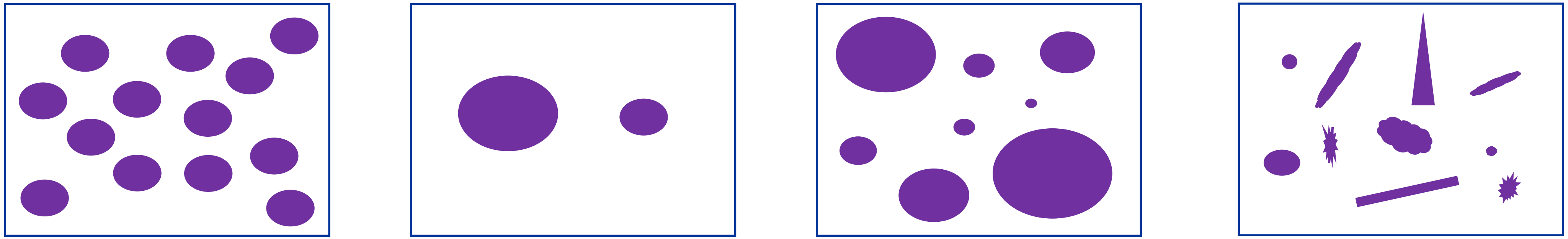
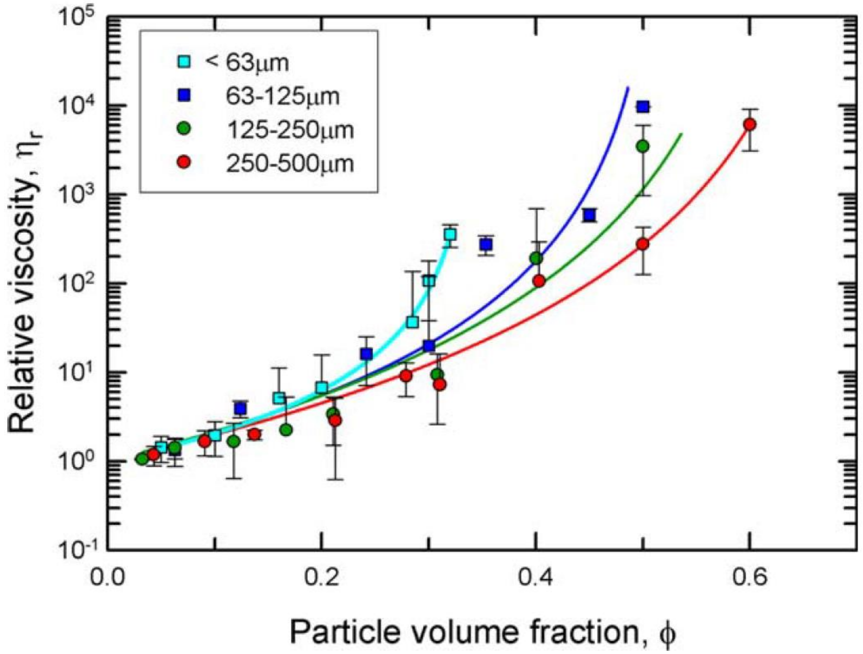
Volume fraction of each crystalline phase

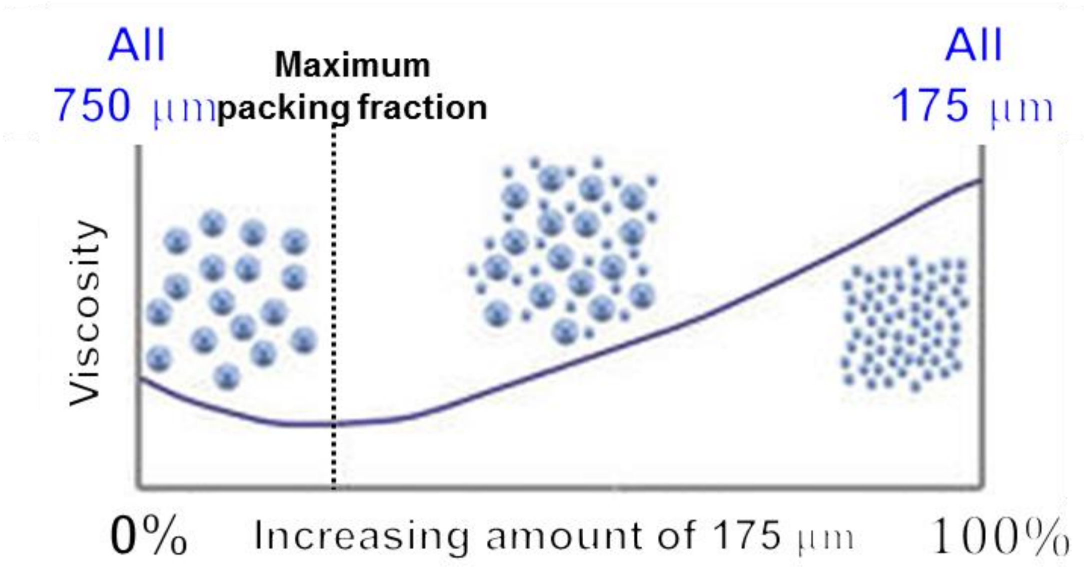
Viscosity estimation for suspensions



Volume fraction | Particle size | Size distribution | Particle shape

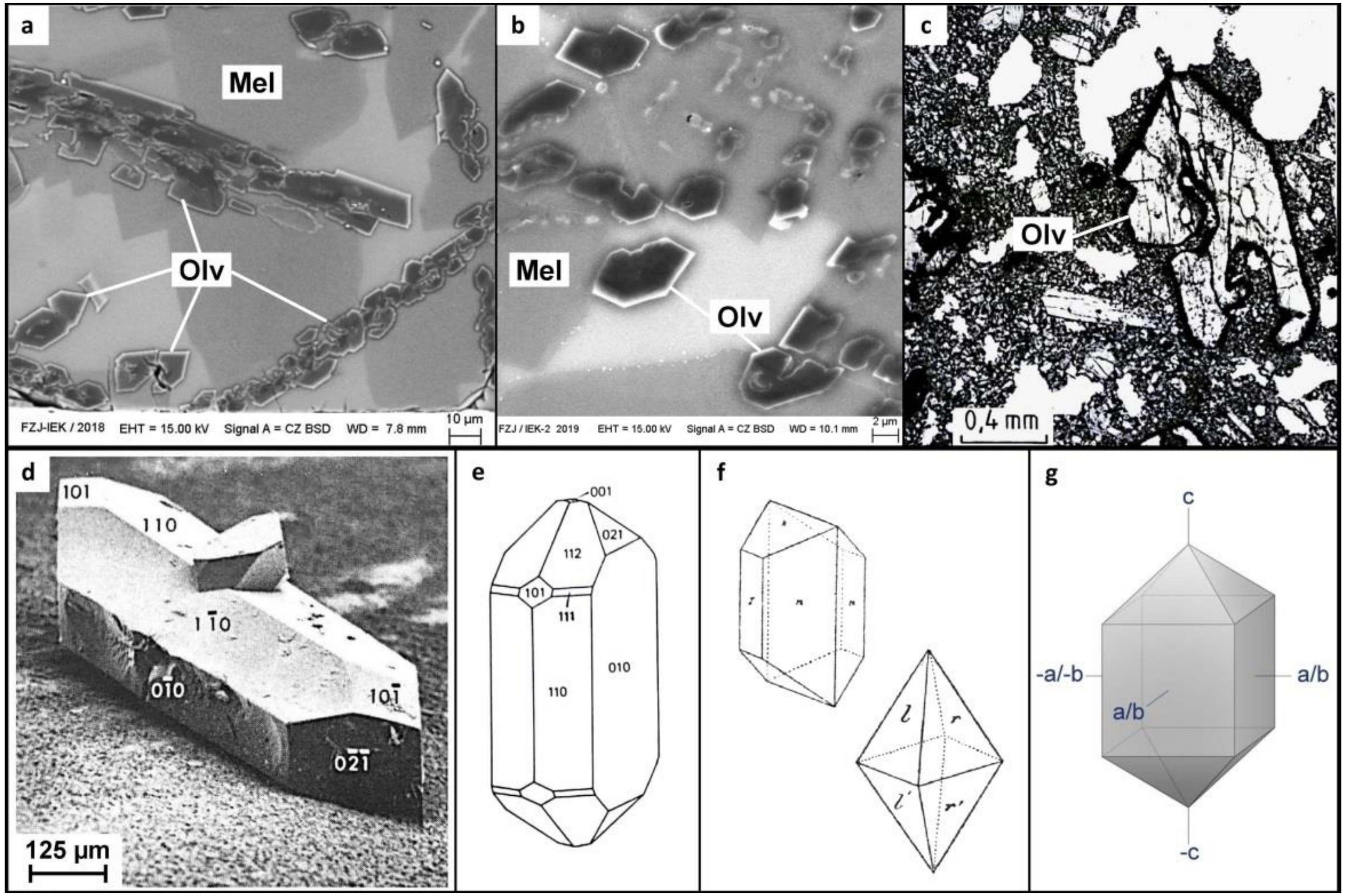


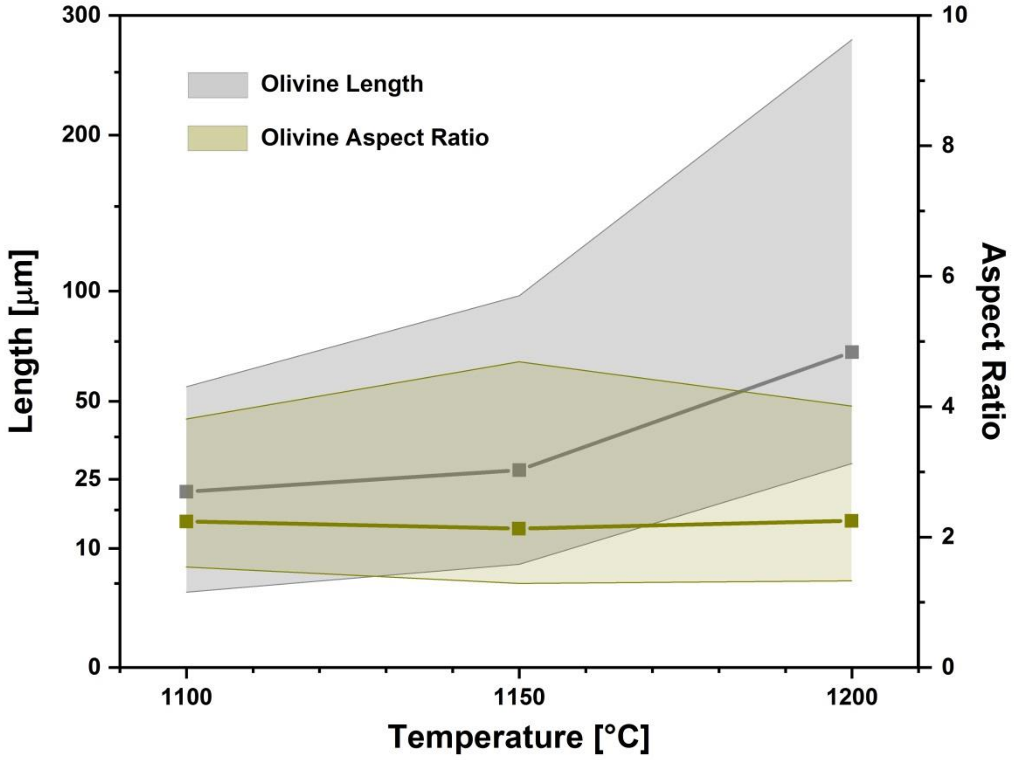
Source: Gaudio et al., Geochemistry, Geophysics, Geosystems, 14, (2013) 2661-2669.



Source: Fletcher et al., Malvern Instruments Ltd , Malvern, Worcestershire, UK.

Viscosity estimation for suspensions





Source: J. P. Schupsky et al., Fuel Process. Technol. 201 (2020) 106345.

Outlook

- **Working on the modified Einstein-Roscoe model**:

$$\boldsymbol{\eta_r = (1 - \sum_i \alpha_i \cdot V_i)^{-2.5}}$$

where: $\boldsymbol{\alpha_i}$ is the weighting factor to determining the contribution of the crystalline phase *i* to the relative viscosity; $\boldsymbol{V_i}$ is the volume fraction of the crystalline phase *i*. The summation term $\boldsymbol{\sum_i \alpha_i \cdot V_i}$ refers to the effective volume fraction.

- **Assessing the model parameters using the viscosity data in combination with the crystal morphology**

Thank you for your attention!

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