JÜLICH
FORSCHUNGSZENTRUM

Measurement and numerical simulation of viscosities in slag-systems under gasification conditions

12. Juli 2011 | Thomas Nentwig, Michael Müller (IEK-2)

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- Introduction
- Build-up of a new high-temperature high-pressure viscosimeter
- A new viscosity model
- Comparison of the new model with literature and FactSage 6.2 calculations
- Comparison of FZJ measurements with the new model and FactSage 6.2 calculations
- Outlook

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Introduction

- Many different industrial and natural processes
- Viscosity is important to understand this processes
- General and good working model would help all scientists and engineers
- Important to have the possibility to measure viscosities
  - Build up of a high-temperature high-pressure viscosimeter
- Development of a new model for viscosity calculations
  - Possibility to compare calculations and measurements

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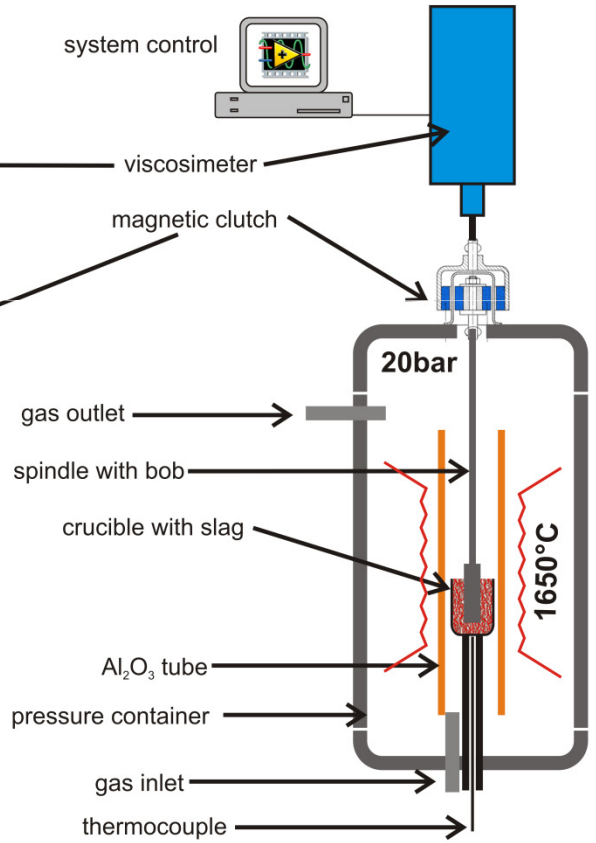
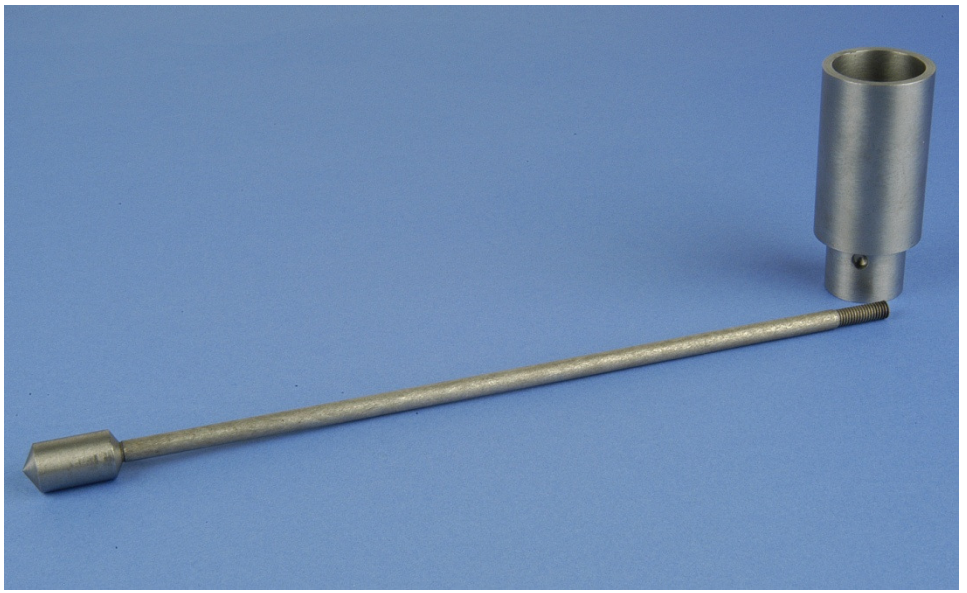
The high-temperature, high-pressure viscosimeter

- Rotational viscosimeter
- Temperature: up to 1650 °C
- Pressure: up to 20bar
- Measurements under Ar/4%H_2 or Ar
- System control with LabVIEW



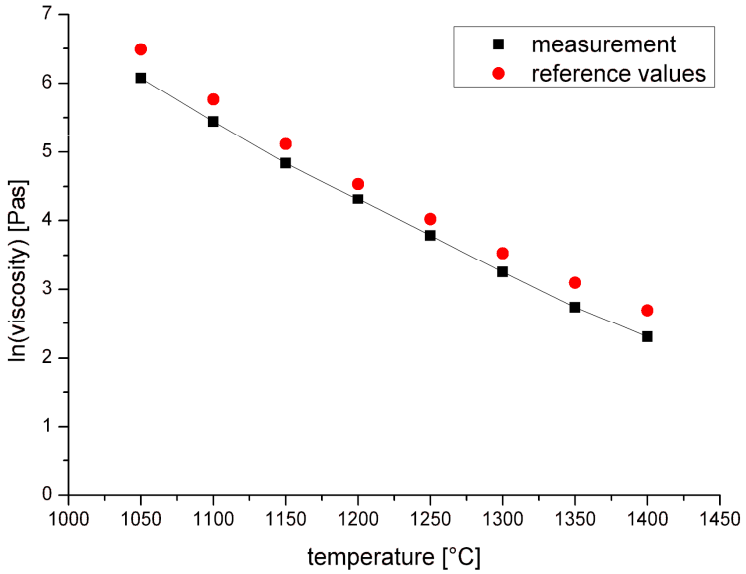
Spindle and crucible

- Molybdenum spindle/bob and crucible
- Melting point: 2623°C
- Diameter bob: 14 mm, diameter crucible: 29 mm
  - “Endless” gap (7.5 mm)
- Sample volume: 29cm³



Calibration and measurement error

- Calibration with standard glass G1
- Reference measurement with standard glass DGG1



- Maximum Error: $\pm$ 8% for $\ln(\eta) > 3.5$

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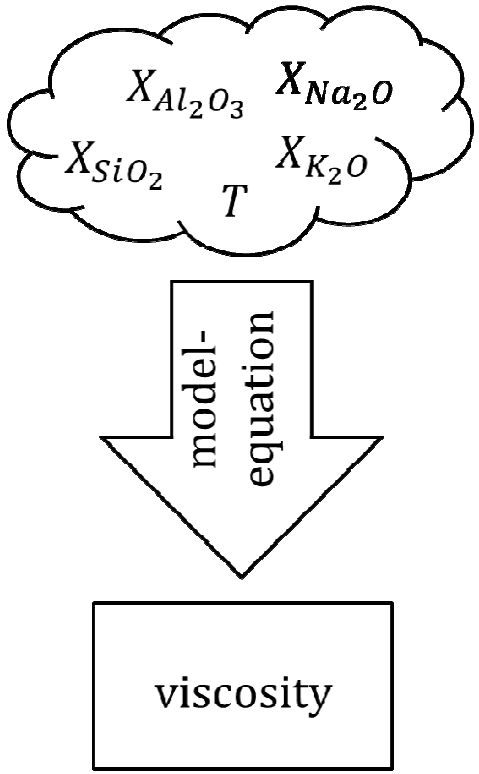
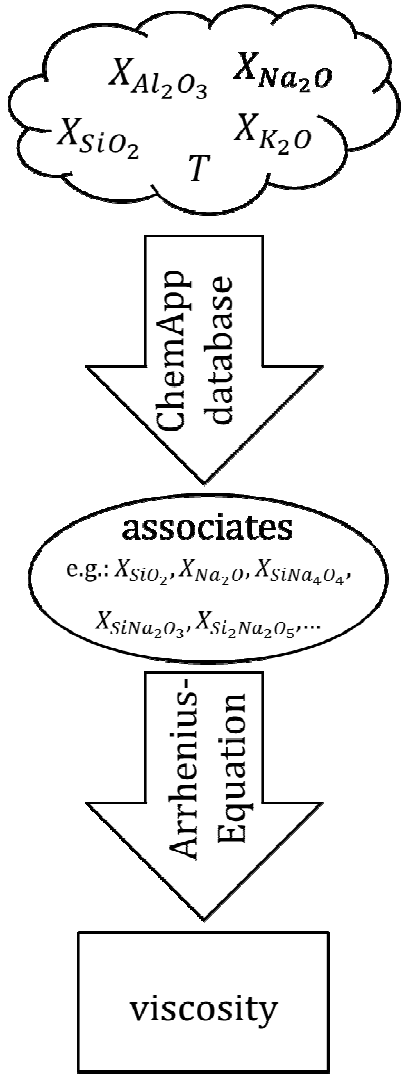
Classical slag models (Shaw, Urbain,…)

- Input: temperature, composition
- Calculation of viscosity by special equation
- Problem: most work only with special composition and/or temperature range
- Enhancement with new components can be complicate (parameters in the model-equation are not useable for different components)



Idea

- Input: temperature, composition
- Inner slag structure is important
- Assumption: liquid slag = associates
- FactSage compatible database (developed by Forschungszentrum Jülich and GTT)
- ChemApp → distribution of associates
- Arrhenius-Equation
- Calculation of viscosity
- Easy enhancement (parameters are the same for different composition)



Development of the new model

- System: SiO_2-Al_2O_3-Na_2O-K_2O
- 20 different associates
- Arrhenius: $\ln(\eta) = \sum_{i=1}^{20} X_i \cdot \left[\ln(\eta_{0,i}) + \frac{1000 \cdot \theta_i}{T}\right]$
- 40 parameters
- Literature research with SciGlass
- Calculation of the parameters with Excel SOLVER

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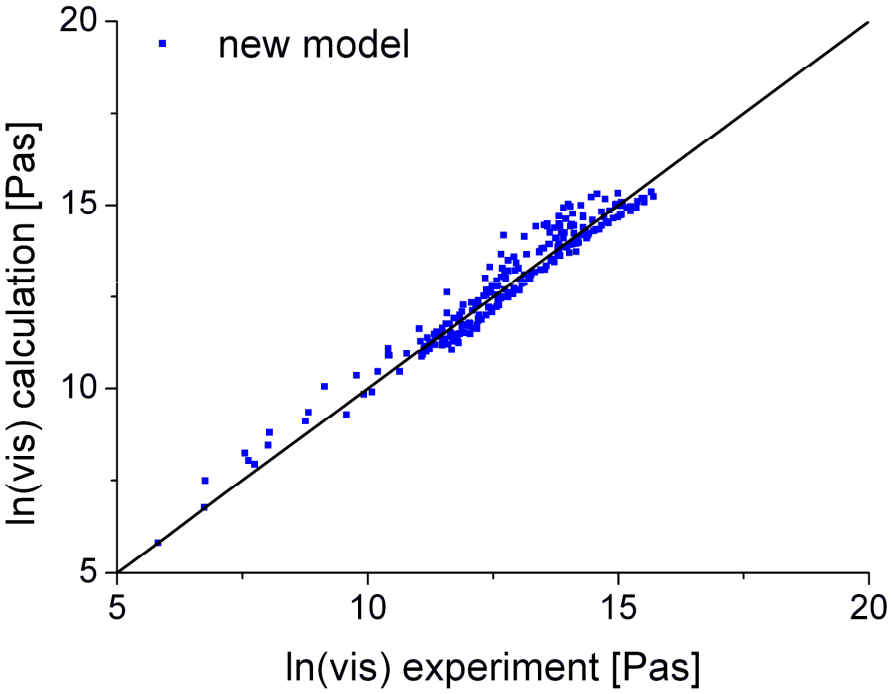
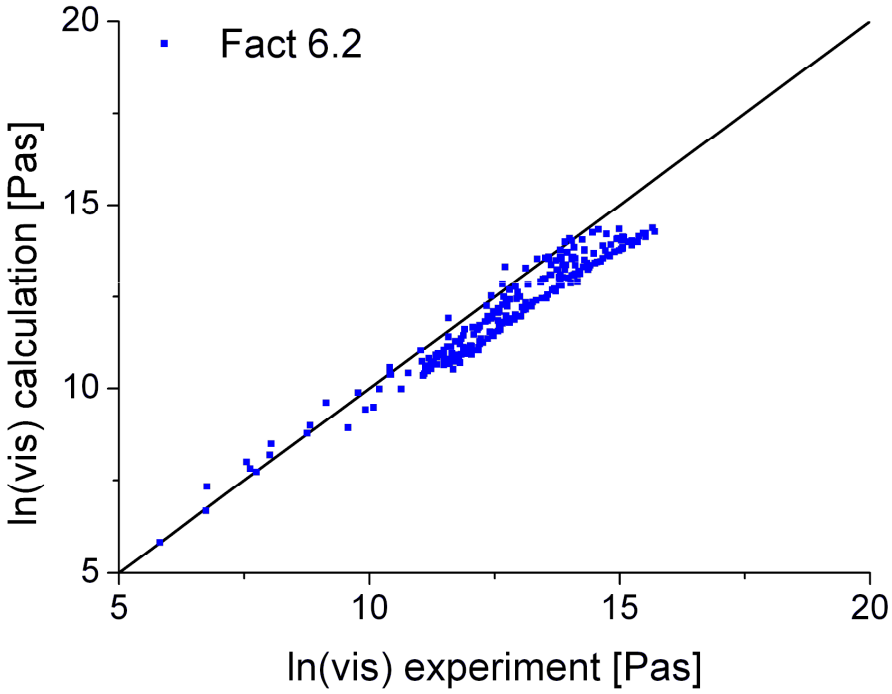
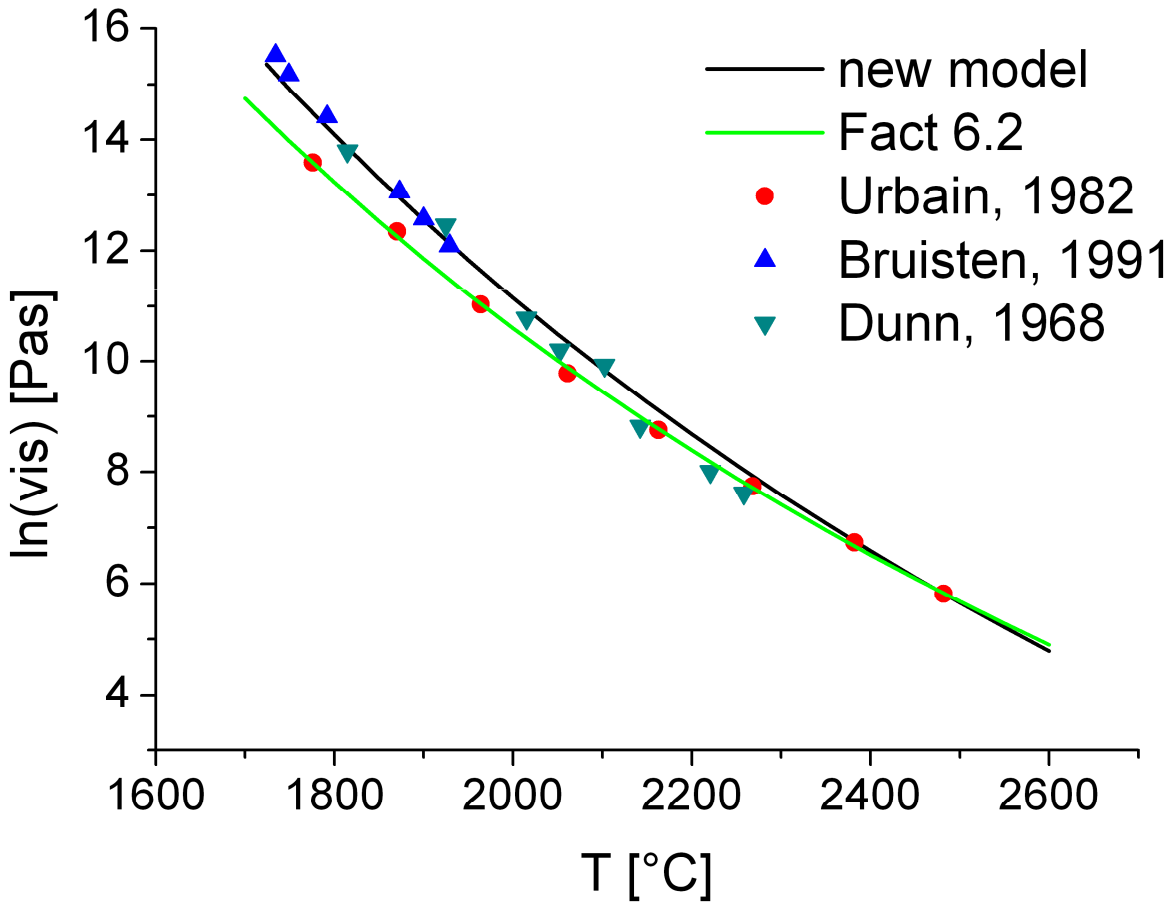
SiO_2

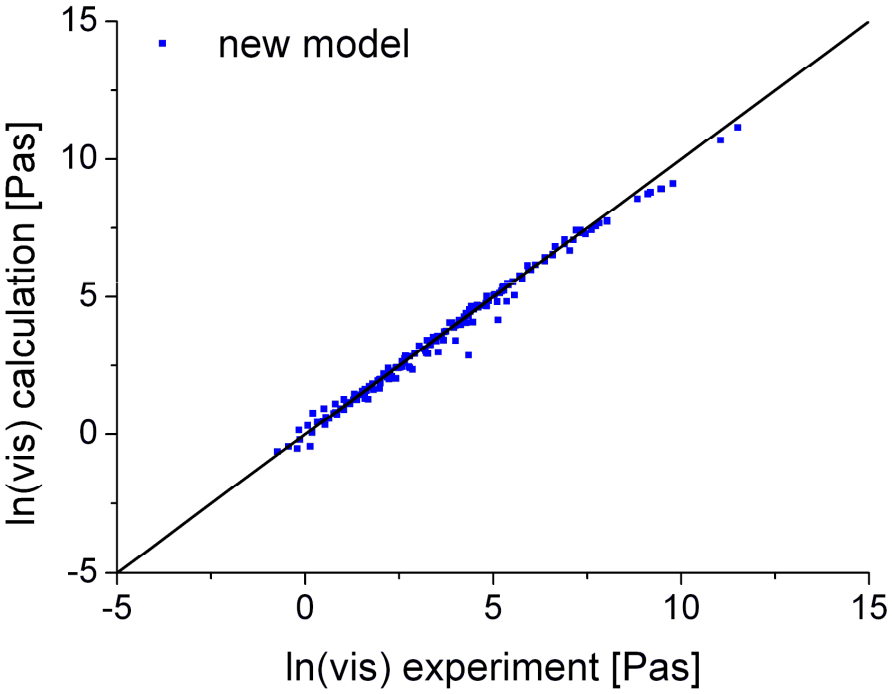




SiO_2



SiO_2-K_2O


new model
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ln(vis) experiment [Pas]
15
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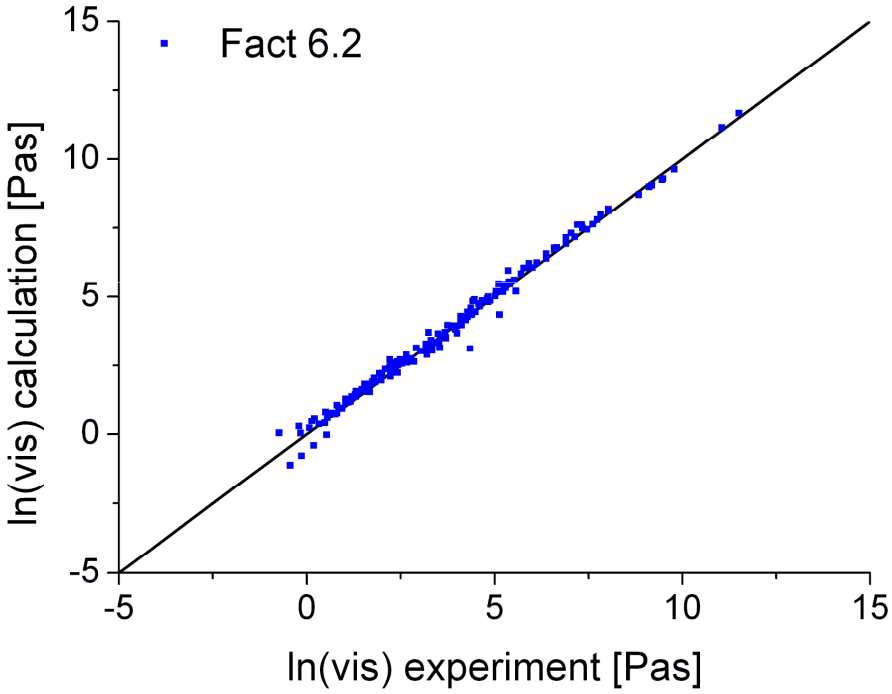
-5
-5
0
5
10
15


Fact 6.2
ln(vis) calculation [Pas]
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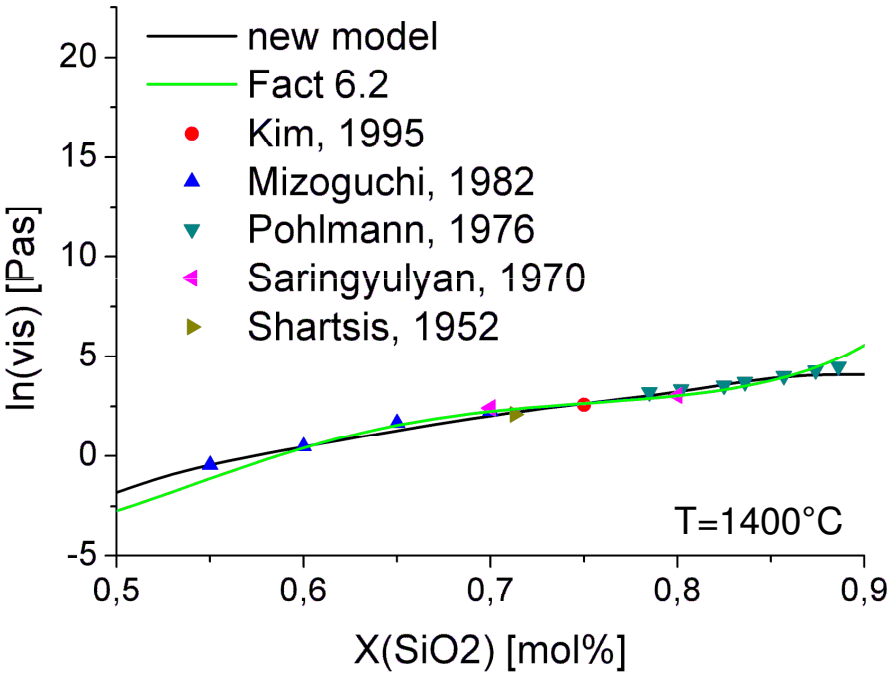
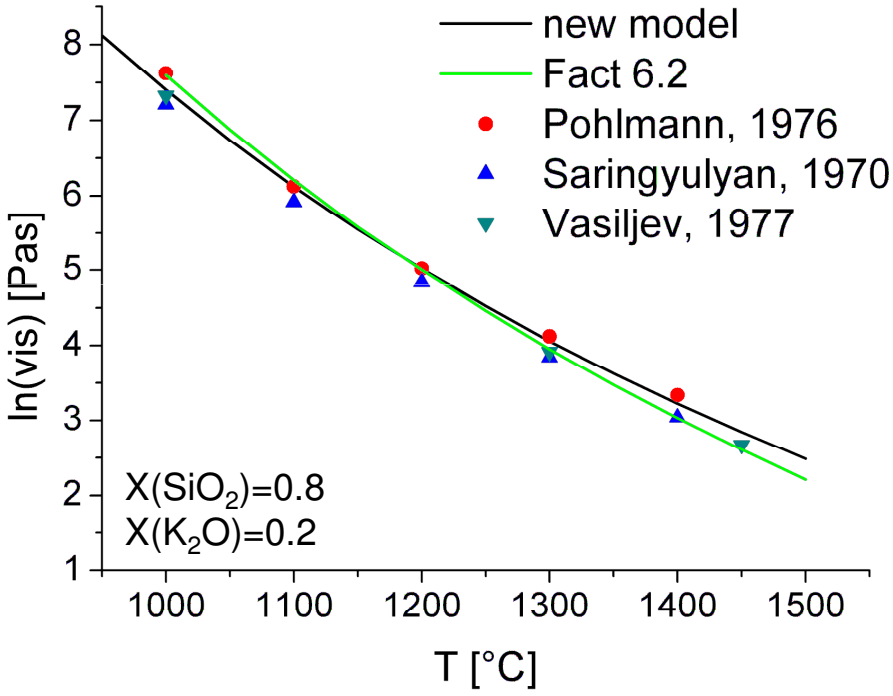
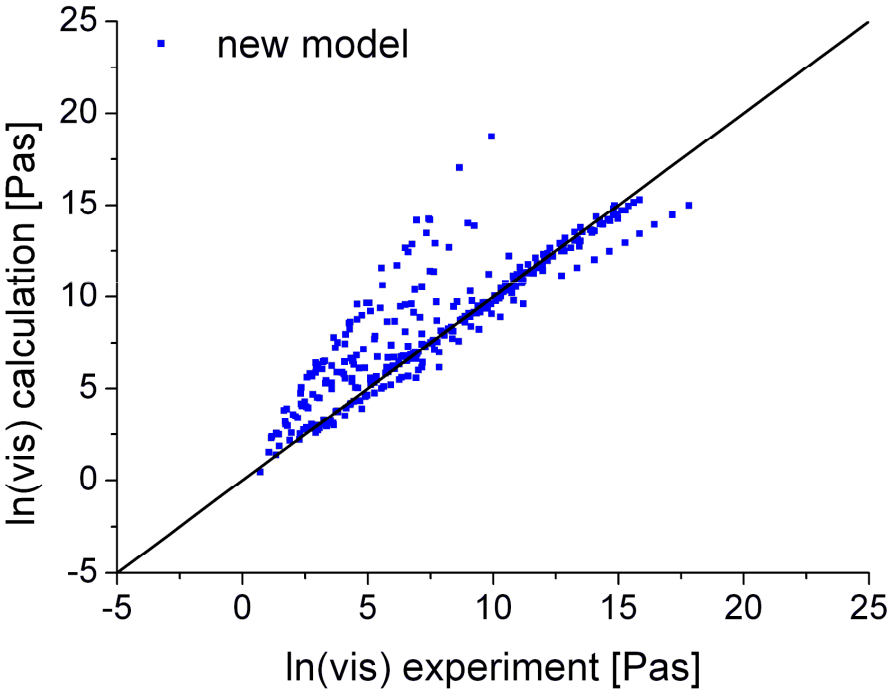
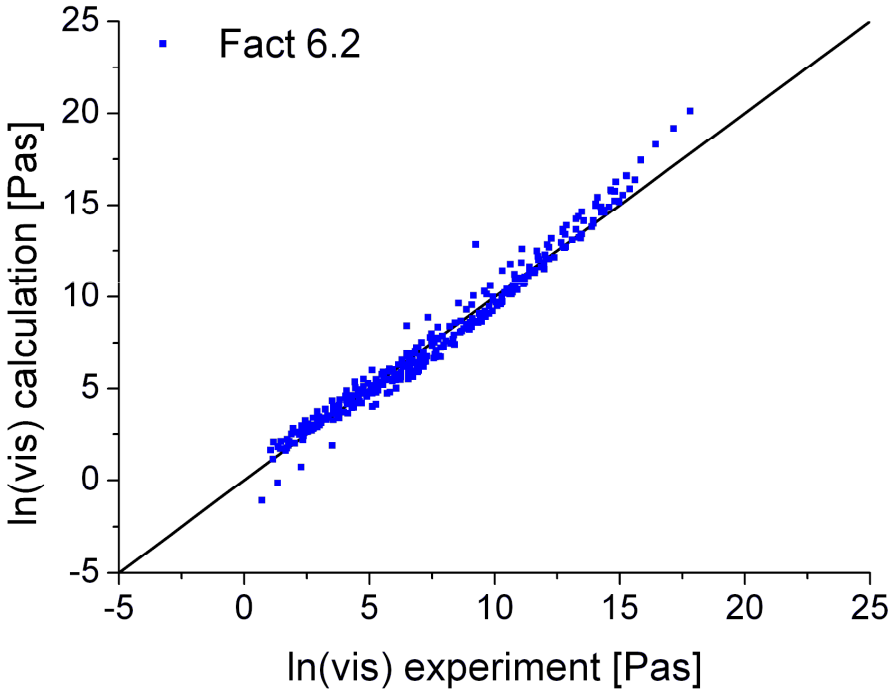
SiO_2-K_2O





SiO_2-Al_2O_3-Na_2O





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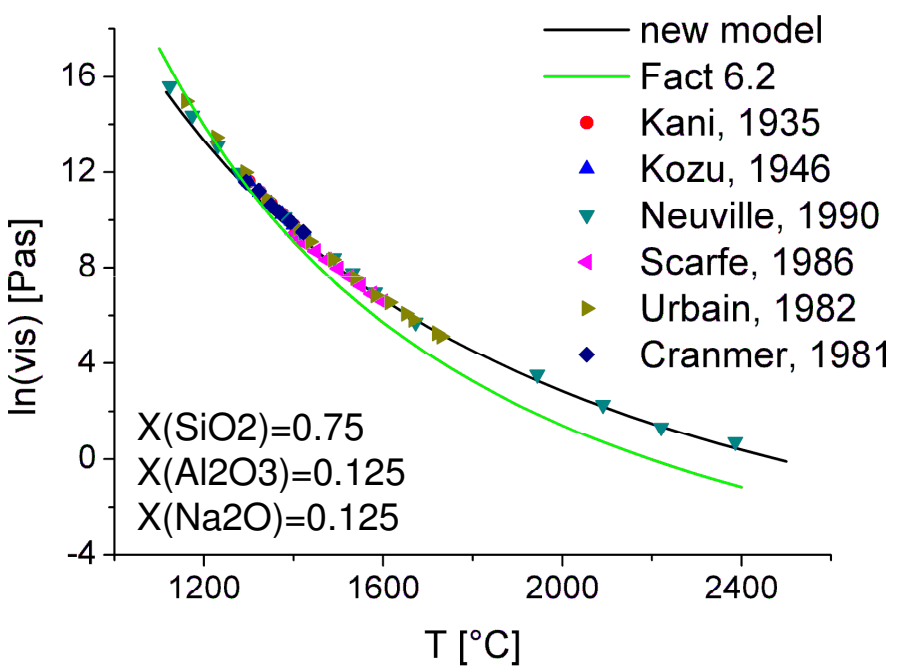
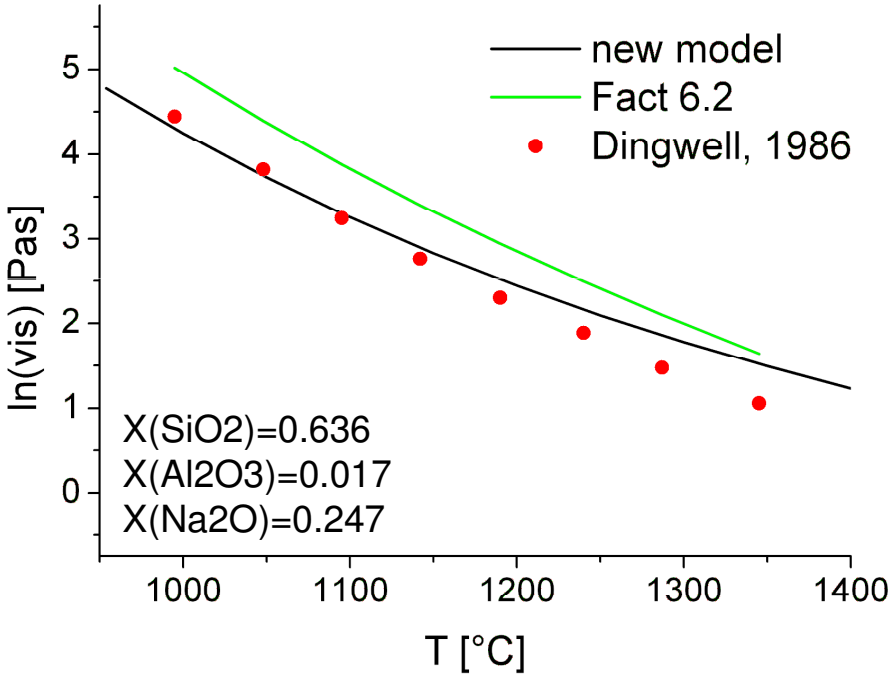
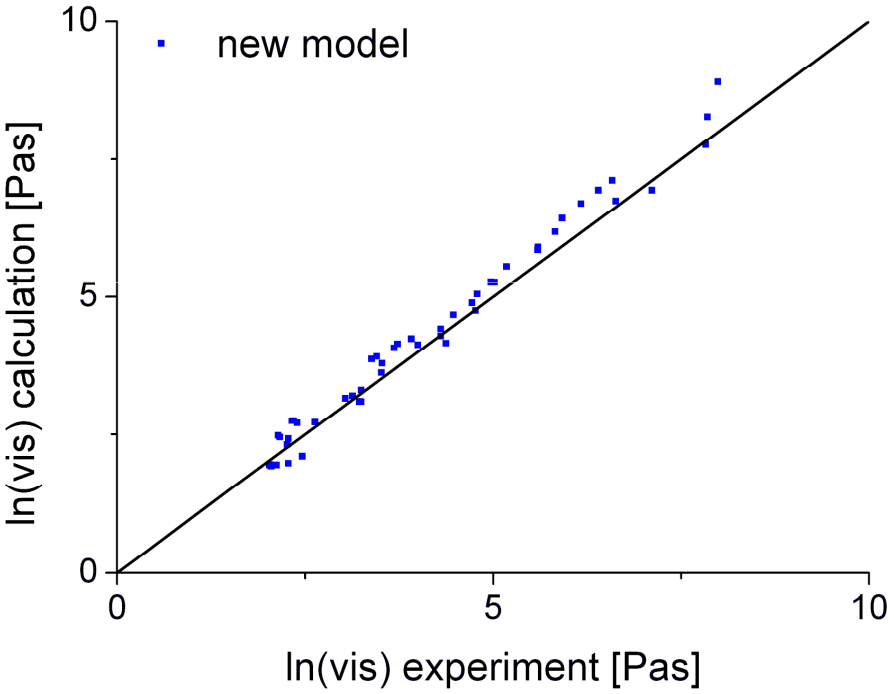
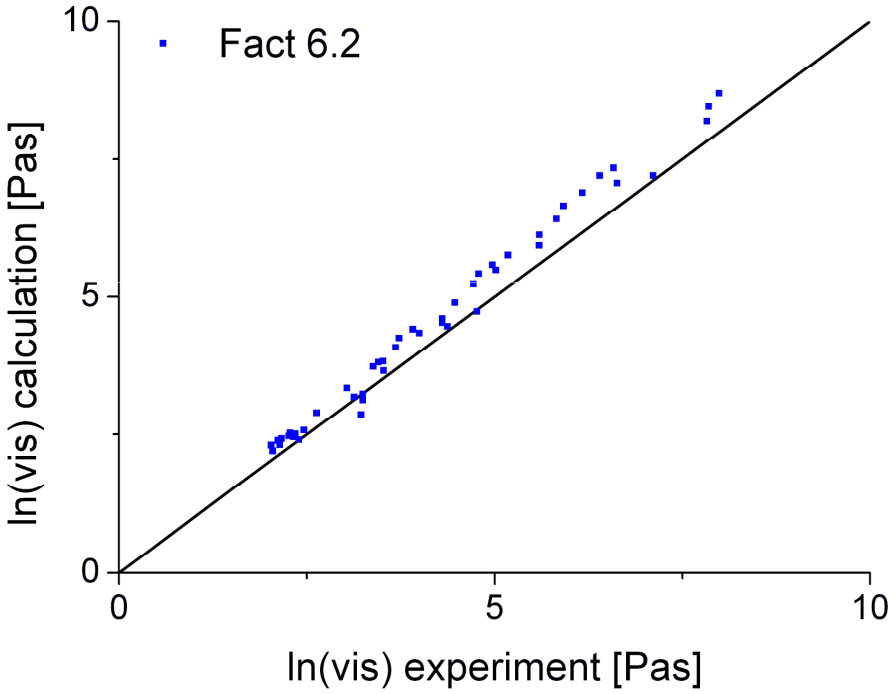


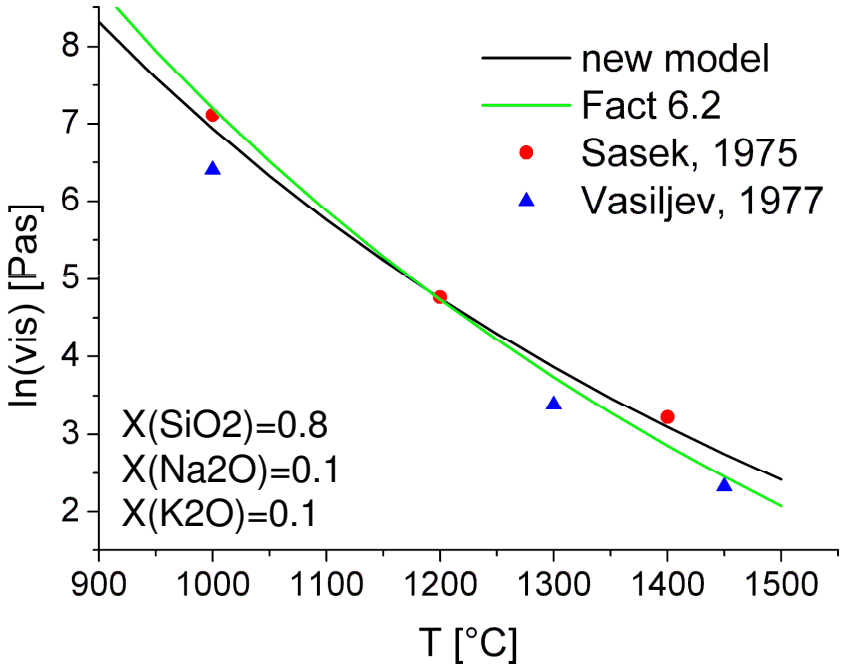


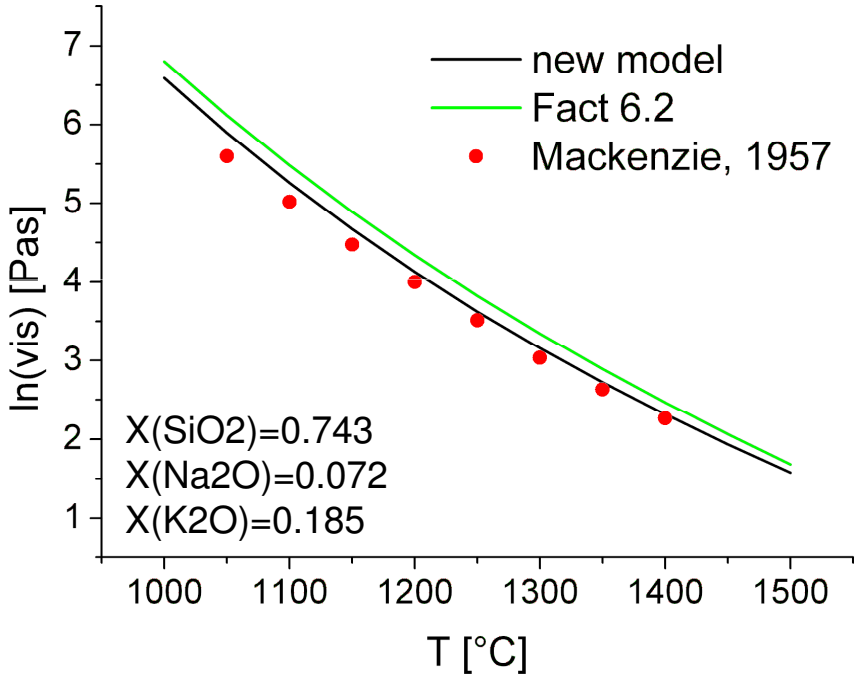
SiO_2-Na_2O-K_2O



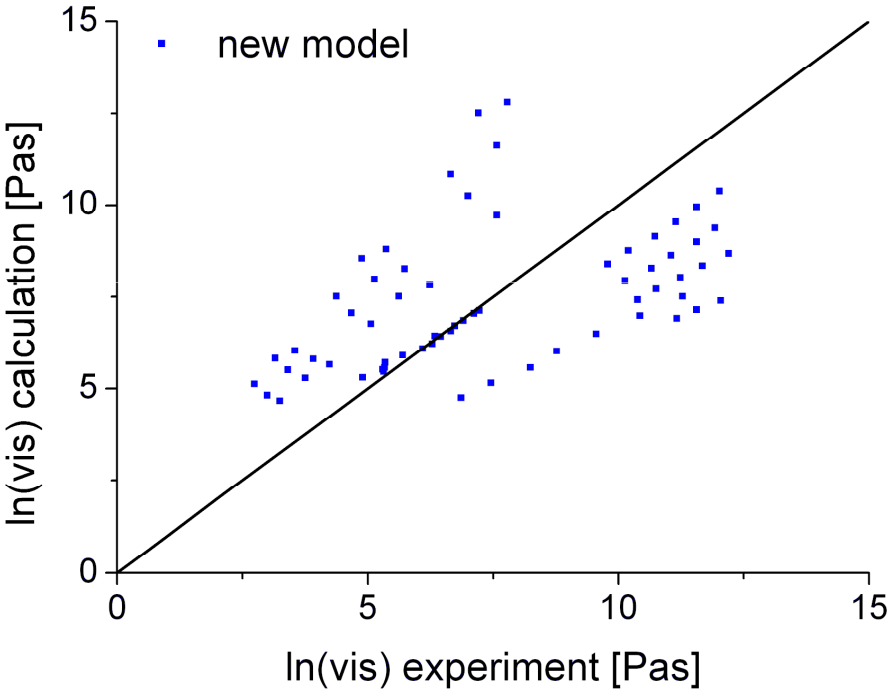


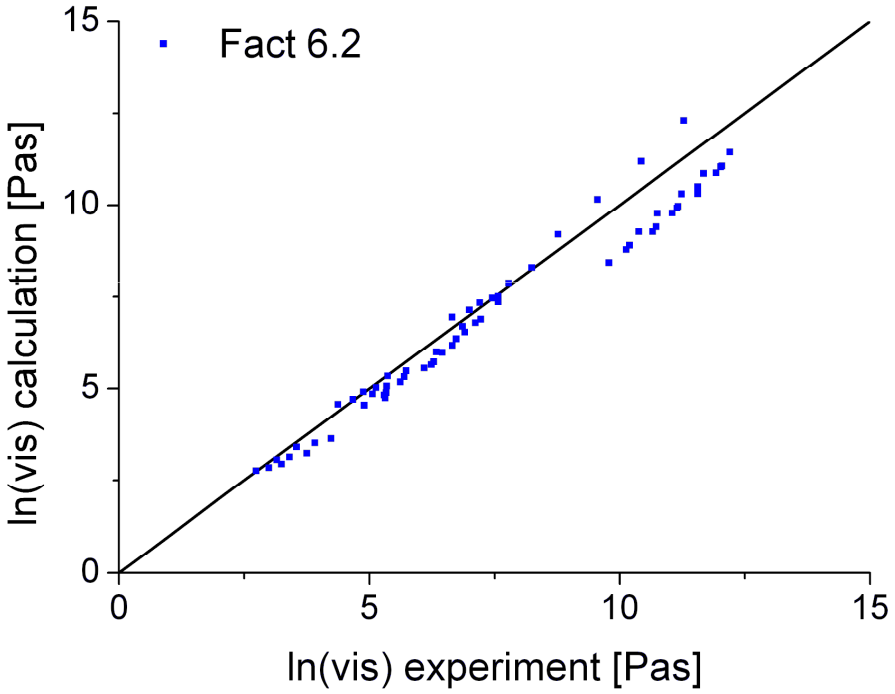
SiO_2-Na_2O-K_2O





SiO_2-Al_2O_3-Na_2O-K_2O





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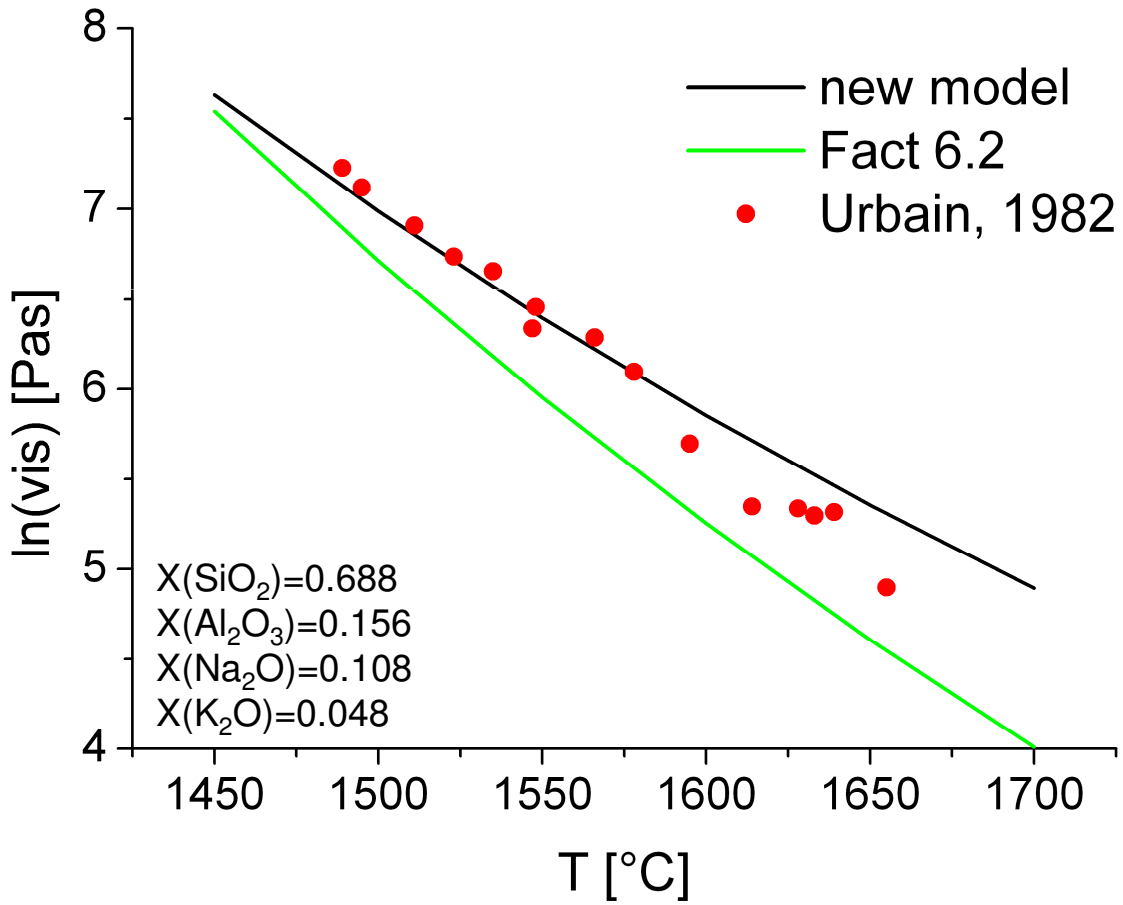

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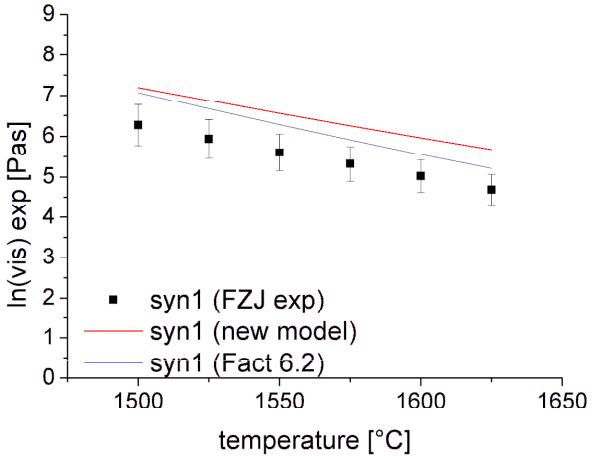
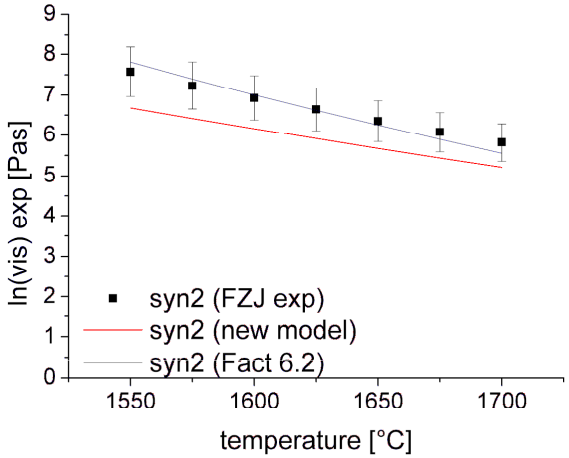
Preparation and compositions of the samples

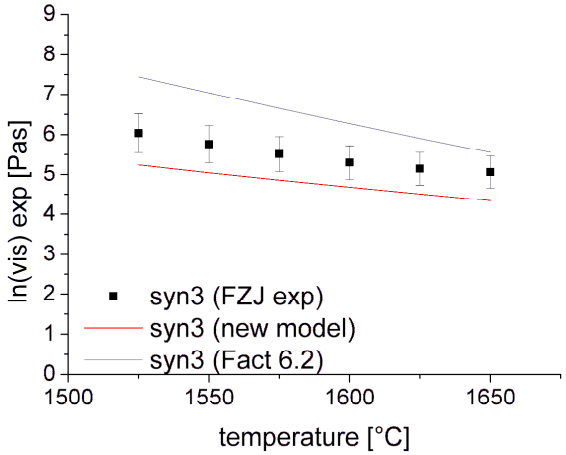
- Raw materials: SiO_2, Al_2O_3, $NaAlO_2$, K_4SiO_4
- Mixing for a few hours for homogenizing
- Heating up in a platinum crucible with 5 K/min to 1600 °C
- Hold at 1600 °C for 5 hours under air
- 3 different synthetic slags

mol%	SiO_2	Al_2O_3	Na_2O	K_2O
syn1	73.8	16.6	9.5	0.1
syn2	81.8	8.6	7.2	2.6
syn3	73.8	16.3	2.6	7.4

Comparison of experiment and calculation







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Outlook

- Optimization of the parameters in the SiO_2-Al_2O_3-Na_2O-K_2O system
- Optimization of the parameters in the SiO_2-Al_2O_3-CaO-MgO system (Master Thesis)
- Consolidation to a complete set of parameters for the SiO_2-Al_2O_3-CaO-MgO-Na_2O-K_2O system
- Adoption of new components (FeO/Fe_2O_3, TiO_2,…)
- Viscosity measurements for obtaining new data in unknown composition regions and validation of the model

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Thank you very much for your attention.