Software for Calculating Viscosities of Molten Oxides

Dmitry Saulov and Klaus Hack

GTT Technologies

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Outline

- Motivation
- Urbain-type viscosity models
- Software capabilities up to date
- Further Development

Motivation

Behaviour of mineral matter is an important issue in coal utilisation processes

Slag viscosity is of particular importance for high temperature entrained flow gasifiers

Coal blending and fluxing are commonly used to maximise resource utilisation

The software is aimed

- to predict phase equilibrium for coal mineral matter at operational conditions
- to predict slag viscosity
- to assist in development of coal blending and fluxing strategies

Urbain Formalism

Urbain viscosity equation

$$\eta = AT\exp\left(\frac{1000B}{T}\right)$$

"Compensation Law" (Theoretically derived)

$$-\ln A = mB + n$$

"Family" of liquids	*m*	*n*
Network oxides (SiO_2, GeO_2)	0.154	13.24
Ionic liquids (Slags)	**0.2981**	**11.15**
Liquid metals	0.2188	12.612
Liquid salts	0.7232	12.405
H-bounded liquids (H_2O, methanol, etc.)	2.4296	11.396

Kalmanovich & Frank

SiO_2-Al_2O_3-CaO-MgO

$$\eta = AT\exp\left(\frac{1000B}{T}\right)$$

$$\ln A = -(0.2812B + 11.8279)$$

$$B = B_0 + B_1 X_{SiO_2} + B_2 X_{SiO_2}^2 + B_3 X_{SiO_2}^3$$

$$B_0 = 13.8 + 39.9355\alpha - 44.049\alpha^2$$
$$B_1 = 30.481 - 117.1505\alpha + 129.9978\alpha^2$$
$$B_2 = -40.9429 + 234.0486\alpha - 300.04\alpha^2$$
$$B_3 = 60.7619 - 153.9276\alpha + 211.1616\alpha^2$$

$$\alpha = \frac{X_{CaO} + X_{MgO} + X_{FeO} + X_{Na_2O} + X_{K_2O} + 2X_{TiO_2}}{X_{CaO} + X_{MgO} + X_{FeO} + X_{Na_2O} + X_{K_2O} + 2X_{TiO_2} + X_{Al_2O_3}}$$

Kondratiev & Jak

GTT-Technologies

SiO_2-Al_2O_3-CaO- 'FeO'

$$\eta = AT\exp\left(\frac{1000B}{T}\right)$$

Separate *B*-values for different modifiers

Compositional dependence of the parameter *m* in "Compensation Law" $m = m_A X_A + m_C X_C + m_F X_F + m_S X_S$

n	m_A	m_C	m_F	m_S
9.322	0.370	0.587	0.665	0.212

$$B_i = b_i^0 + b_i^1\alpha + b_i^2\alpha^2, \text{ where } \alpha = \frac{X_{Mod}}{X_{Mod} + X_{Amf}}$$

Kondratiev & Jak

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SiO_2-Al_2O_3-CaO-'FeO'

$$B = \sum_{i=0}^{3} b_i^0 X_S^i + \sum_{i=0}^{3}\sum_{j=1}^{2}\left(b_i^{C,j} \frac{X_C}{X_C + X_F} + b_i^{F,j} \frac{X_F}{X_C + X_F} \right)\left(\frac{X_C + X_F}{X_C + X_F + X_A} \right)^j X_S^i$$

	j/i	**0**	**1**	**2**	**3**
b_i^0	0	13.31	36.98	-177.70	190.03
$b_i^{C,j}$	1	5.50	96.20	117.94	-219.56
	2	-4.68	-81.60	-109.80	196.00
$b_i^{F,j}$	1	34.30	-143.64	368.94	-254.85
	2	-45.63	129.96	-210.28	121.20

Comparison of the Models

$$\Delta = \frac{1}{N}\sum_{n=1}^{N}\left|\frac{(\eta_n)_{\text{calc}} - (\eta_n)_{\text{exp}}}{(\eta_n)_{\text{exp}}}\right|$$

System	Kalmanovich & Frank	Kondratiev & Jak
SiO_2	99.9	19.1
Al_2O_3-SiO_2	41.5	30.1
CaO-SiO_2	24.3	10.9
'FeO'-SiO_2	717.6	8.1
Al_2O_3-CaO-SiO_2	24.6	31.2
CaO-'FeO'-SiO_2	594.4	9.9
Al_2O_3-CaO-'FeO'-SiO_2	169.6	29.2

Roscoe's Equation

$$\eta_R = \eta_L (1 - R V_S)^{-n}$$

model parameters

First approximation:
rigid spheres of various sizes
→ R=1; n= 2.5

Applicability range: $0 < V_s < 0.3$

New Interactive Software: ViscCalc

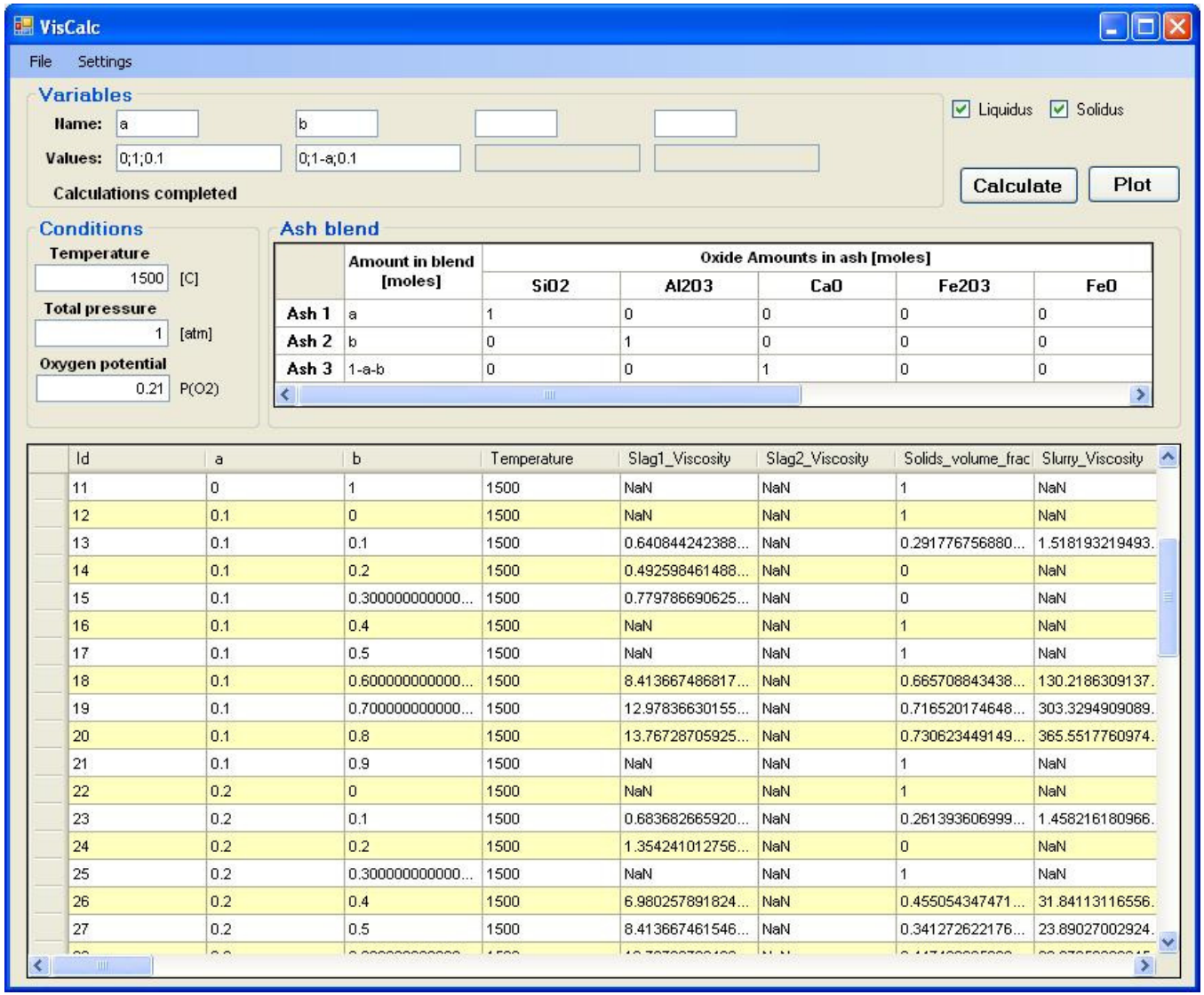
Based on the theoretical background outlined above a new interactive software has been developed.

It makes use of the viscosity models as described and integrates these with thermodynamic equilibrium calculations.

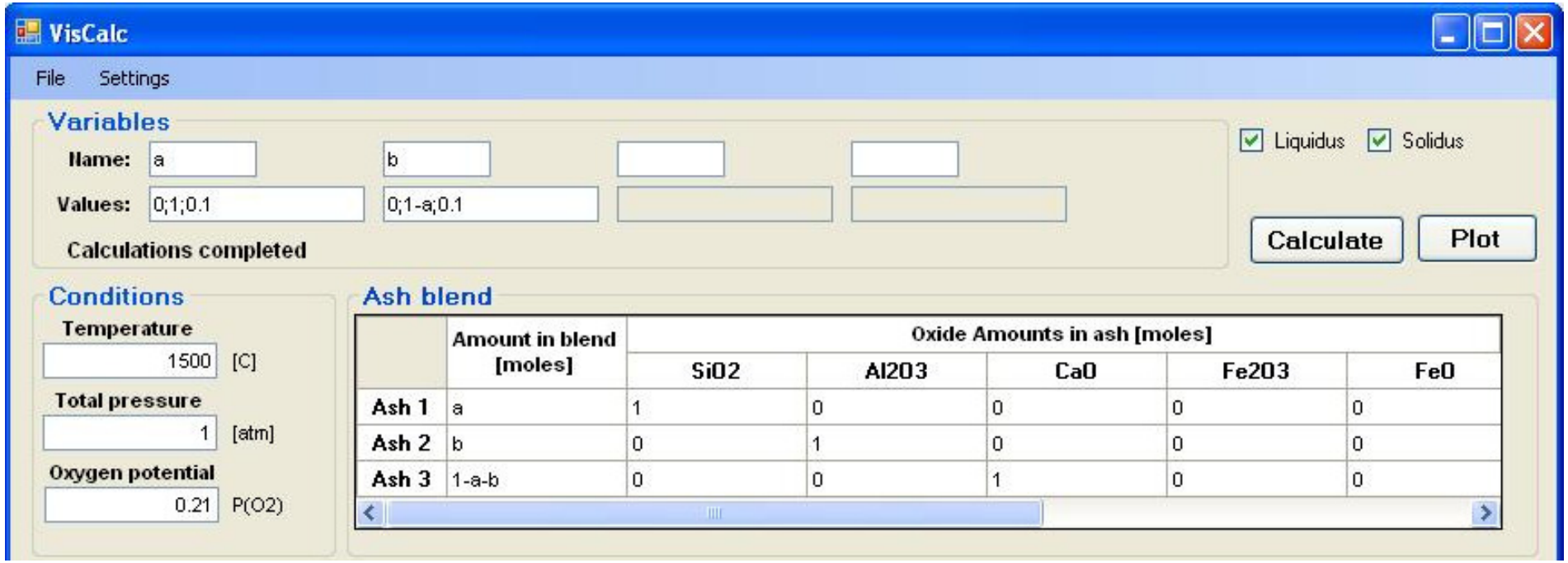
The equilibrium calculations are performed using GTT‘s own **Programmer‘s Library**

ChemApp™

Main Window


VisCalc
File
Settings
Variables
Name:
a
b
Values:
0;1;0.1
0;1-a;0.1
Calculations completed
Liquidus
Solidus
Calculate
Plot
Conditions
Temperature
1500
[C]
Total pressure
1
[atm]
Oxygen potential
0.21
P(O2)
Ash blend
Amount in blend [moles]
Oxide Amounts in ash [moles]
SiO2
Al2O3
CaO
Fe2O3
FeO
Ash 1
a
1
0
0
0
0
Ash 2
b
0
1
0
0
0
Ash 3
1-a-b
0
0
1
0
0
Id
a
b
Temperature
Slag1_Viscosity
Slag2_Viscosity
Solids_volume_frac
Slurry_Viscosity
11
0
1
1500
NaN
NaN
1
NaN
12
0.1
0
1500
NaN
NaN
1
NaN
13
0.1
0.1
1500
0.640844242388...
NaN
0.291776756880...
1.518193219493.
14
0.1
0.2
1500
0.492598461488...
NaN
0
NaN
15
0.1
0.300000000000...
1500
0.779786690625...
NaN
0
NaN
16
0.1
0.4
1500
NaN
NaN
1
NaN
17
0.1
0.5
1500
NaN
NaN
1
NaN
18
0.1
0.600000000000...
1500
8.413667486817...
NaN
0.665708843438...
130.2186309137.
19
0.1
0.700000000000...
1500
12.97836630155...
NaN
0.716520174648...
303.3294909089.
20
0.1
0.8
1500
13.76728705925...
NaN
0.730623449149...
365.5517760974.
21
0.1
0.9
1500
NaN
NaN
1
NaN
22
0.2
0
1500
NaN
NaN
1
NaN
23
0.2
0.1
1500
0.683682665920...
NaN
0.261393606999...
1.458216180966.
24
0.2
0.2
1500
1.354241012756...
NaN
0
NaN
25
0.2
0.300000000000...
1500
NaN
NaN
1
NaN
26
0.2
0.4
1500
6.980257891824...
NaN
0.455054347471...
31.84113116556.
27
0.2
0.5
1500
8.413667461546...
NaN
0.341272622176...
23.89027002924.

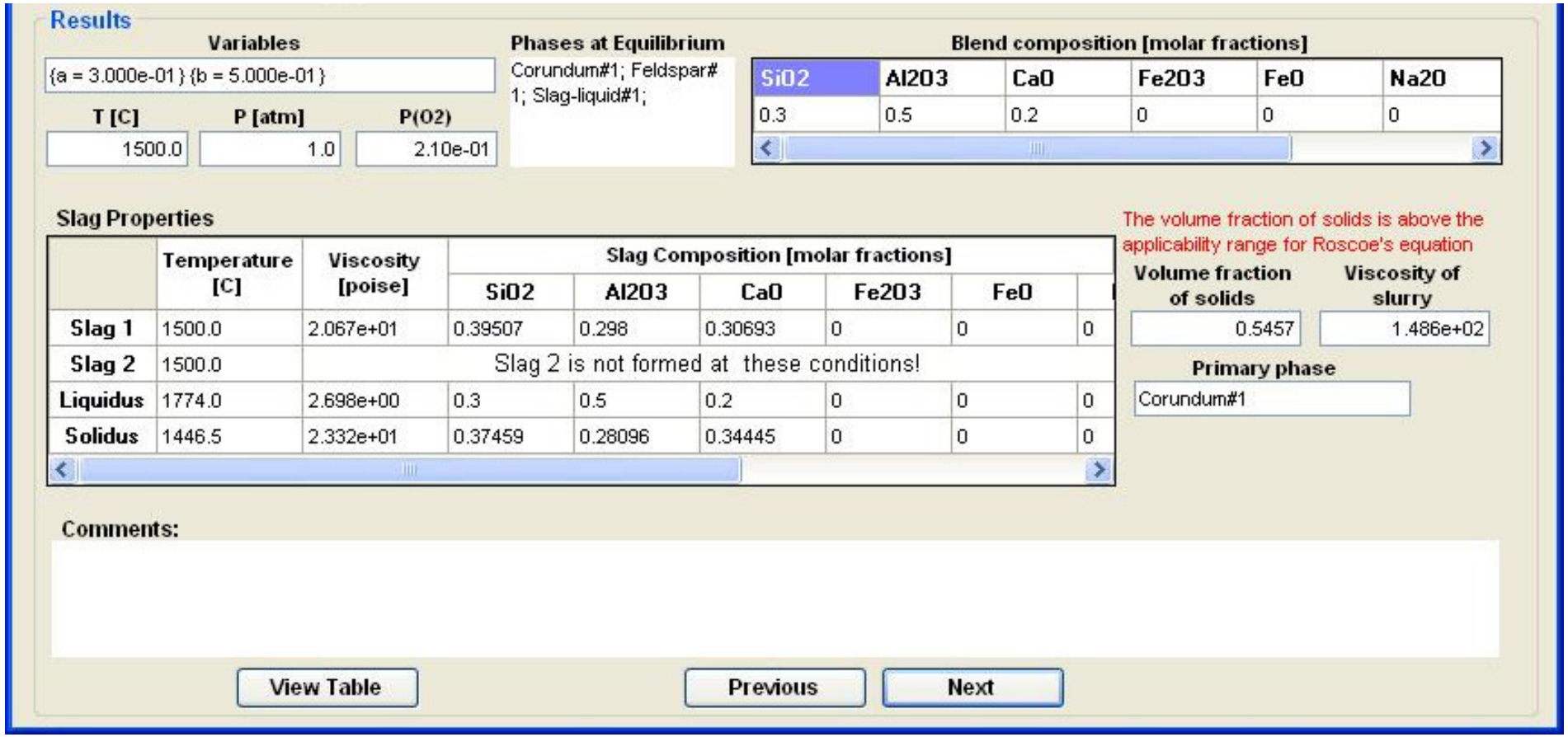
Main Window (Input)



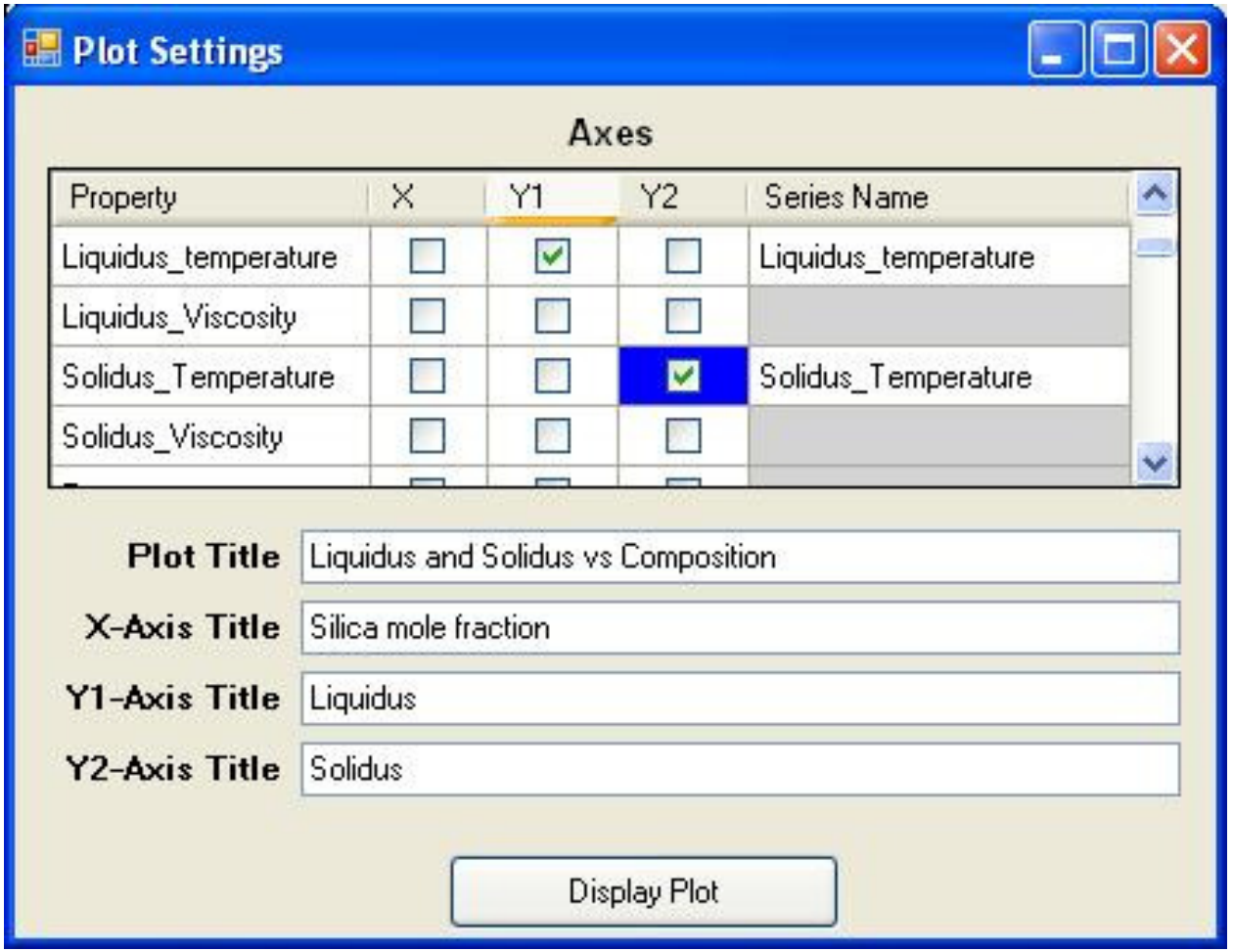
Main Window (Table)

Id	a	b	Temperature	Slag1_Viscosity	Slag2_Viscosity	Solids_volume_frac	Slurry_Viscosity
11	0	1	1500	NaN	NaN	1	NaN
12	0.1	0	1500	NaN	NaN	1	NaN
13	0.1	0.1	1500	0.640844242388...	NaN	0.291776756880...	1.518193219493.
14	0.1	0.2	1500	0.492598461488...	NaN	0	NaN
15	0.1	0.300000000000...	1500	0.779786690625...	NaN	0	NaN
16	0.1	0.4	1500	NaN	NaN	1	NaN
17	0.1	0.5	1500	NaN	NaN	1	NaN
18	0.1	0.600000000000...	1500	8.413667486817...	NaN	0.665708843438...	130.2186309137.
19	0.1	0.700000000000...	1500	12.97836630155...	NaN	0.716520174648...	303.3294909089.
20	0.1	0.8	1500	13.76728705925...	NaN	0.730623449149...	365.5517760974.
21	0.1	0.9	1500	NaN	NaN	1	NaN
22	0.2	0	1500	NaN	NaN	1	NaN
23	0.2	0.1	1500	0.683682665920...	NaN	0.261393606999...	1.458216180966.
24	0.2	0.2	1500	1.354241012756...	NaN	0	NaN
25	0.2	0.300000000000...	1500	NaN	NaN	1	NaN
26	0.2	0.4	1500	6.980257891824...	NaN	0.455054347471...	31.84113116556.
27	0.2	0.5	1500	8.413667461546...	NaN	0.341272622176...	23.89027002924.

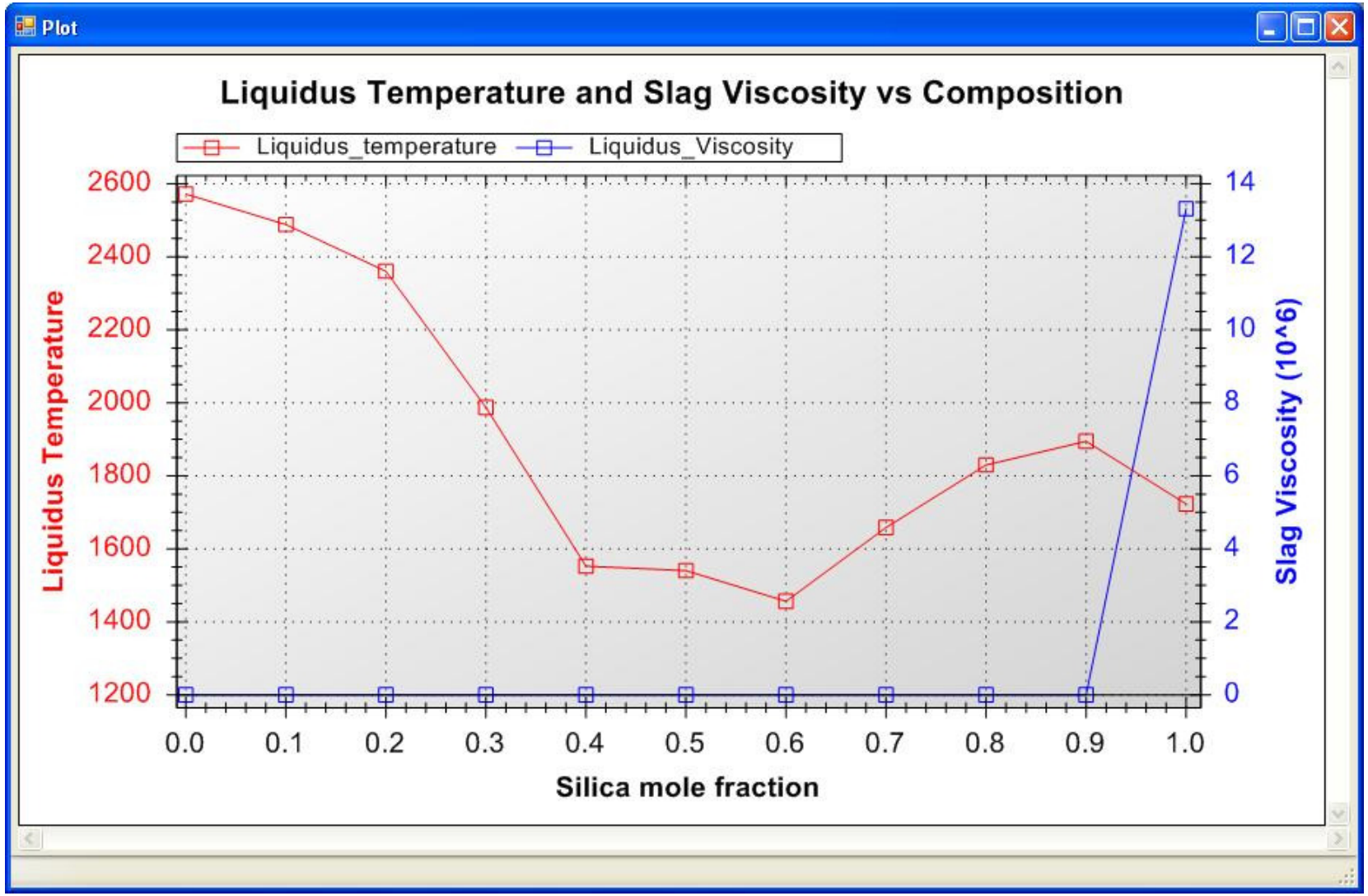
Main Window (Row)



Axes Selection



Plotting


Plot
Liquidus Temperature and Slag Viscosity vs Composition
Liquidus_temperature
Liquidus_Viscosity
Liquidus Temperature
Slag Viscosity (10^6)
Silica mole fraction
2600
2400
2200
2000
1800
1600
1400
1200
14
12
10
8
6
4
2
0
0.0
0.1
0.2
0.3
0.4
0.5
0.6
0.7
0.8
0.9
1.0

Demonstration

Further Development

- New viscosity models (Avramov)
- Plotting capabilities (Ternary diagrams)
- Bulk calculations (Imported tables)
- ?

Avramov vs Arrhenius

Avramov $\eta = \dfrac{\eta_0}{\sum X_i \exp(-E_i/RT)}$ average jump frequency

Concentrations of SU Constant Activation energies of SU

Arrhenius $\eta = \eta_0 \exp\left(\sum X_i E_i / RT\right)$ average activation energy

Avramov vs Arrhenius

The system Na_2O-SiO_2, 1200°C