A Model for Silicate Melt Viscosity

[http://www.eos.ubc.ca/~krussell/]

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A) Temperature dependence:

T-dependence of viscosity (η) is modelled by the VFT equation - *A, B* & *C* are adjustable parameters.

$$\log \eta = A + \frac{B}{T(K) - C} \qquad (1)$$

B) Compositional Dependence [A, B & C]:

A is a constant independent of composition. Compositional effects are ascribed to ***B*** and ***C*** by linear combinations of oxide components (mol%) and several multiplicative oxide cross-terms:

$$B = \sum_{i=1}^{7}[b_i M_i] + \sum_{j=1}^{3}[b_{1j}(M1_{1j} \cdot M2_{1j})] \qquad (2)$$

$$C = \sum_{i=1}^{6}[c_i N_i] + [c_{11}(N1_{11} \cdot N2_{11})] \qquad (3)$$

where *M*'s and *N*'s are combinations of mol. % oxides reported in Table 1 for ***B*** and ***C***, respectively.

C) Model Coefficients

Table 1. Coefficients for calculation of VFT parameters B and C [A=-4.55 (±0.21)[a]] from melt compositions expressed as mole % oxides.

	Oxides	**Values**		**Oxides**	**Values**
b_1	SiO_2+TiO_2	159.6 (7)	c_1	SiO_2	2.75 (0.4)
b_2	Al_2O_3	-173.3 (22)	c_2	TA[c]	15.7 (1.6)
b_3	FeO(T)+MnO+P_2O_5	72.1 (14)	c_3	FM[d]	8.3 (0.5)
b_4	MgO	75.7 (13)	c_4	CaO	10.2 (0.7)
b_5	CaO	-39.0 (9)	c_5	NK[e]	-12.3 (1.3)
b_6	Na_2O + V[b]	-84.1 (13)	c_6	ln(1+V)	-99.5 (4)
b_7	V + ln(1+H_2O)	141.5 (19)	c_{11}	(Al_2O_3+FM+CaO	0.30 (0.04)
b_{11}	(SiO_2 +TiO_2)*(FM)	-2.43 (0.3)		- P_2O_5)*(NK+V)	
b_{12}	(SiO_2+TA+P_2O_5)*(NK+H_2O)	-0.91 (0.3)			
b_{13}	(Al_2O_3)*(NK)	17.6 (1.8)			

[a]Numbers in brackets are 95% c.l.
[b] V = Sum of H_2O+F_2O_{-1};
[c] TA=Sum of TiO_2+Al_2O_3;
[d] FM=Sum of FeO(T)+MnO+MgO;
[e] NK= Sum of Na_2O + K_2O

D) Explicit Formulae

$$B = \begin{bmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \\ b_5 \\ b_6 \\ b_7 \end{bmatrix} \cdot \begin{bmatrix} SiO_2 + TiO_2 \\ Al_2O_3 \\ FeO + MnO + P_2O_5 \\ MgO \\ CaO \\ Na_2O + V \\ V + \ln(1 + H_2O) \end{bmatrix} + \begin{bmatrix} b_{11} \\ b_{12} \\ b_{13} \end{bmatrix} \cdot \begin{bmatrix} (SiO_2 + TiO_2) * (FM) \\ (SiO_2 + TA + P_2O_5) * (NK + H_2O) \\ (Al_2O_3) * (NK) \end{bmatrix}$$

$$C = \begin{bmatrix} c1 \\ c2 \\ c3 \\ c4 \\ c5 \\ c6 \end{bmatrix} \cdot \begin{bmatrix} SiO_2 \\ TA \\ FM \\ CaO \\ NK \\ \ln(1 + V) \end{bmatrix} + \left[c_{11}\right] \cdot \left[(Al_2O_3 + FM + CaO - P_2O_5) * (NK + V)\right]$$

E) Example Calculation:

Table 2. Sample calculation of viscosity (Pa s) using model coefficients (Table 1).

Sample[1]	Wt%	$Wt\%_N$	Mol%	B-Terms	Values	C-Terms	Values
SiO_2	62.40	61.23	62.38	b_1	10018.8	c_1	171.5
TiO_2	0.55	0.54	0.41	b_2	-2043.2	c_2	191.8
Al_2O_3	20.01	19.63	11.79	b_3	6.69	c_3	40.27
FeO(T)	0.03	0.03	0.03	b_4	363.2	c_4	99.2
MnO	0.02	0.02	0.02	b_5	-379.1	c_5	-49.21
MgO	3.22	3.16	4.80	b_6	-858.7	c_6	-204.5
CaO	9.08	8.91	9.73	b_7	1253.4	c_{11}	85.3
Na_2O	3.52	3.45	3.41	b_{11}	-738.7		
K_2O	0.93	0.91	0.59	b_{12}	-733.8	**A (constant)[2]**	**-4.55**
P_2O_5	0.12	0.12	0.05	b_{13}	831.6	**B (computed)[2]**	**7720**
H_2O	2.00	2.00	6.80			**C (computed)[2]**	**334**

[1] Iron-free andesite melt with 2.00 wt.% H_2O.

[2] Log η = A + B/(T(K) - C); predicted value for this melt at 1273 K is 3.67 Pa s.