i-Melt: machine learning model of lava properties

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Motivation

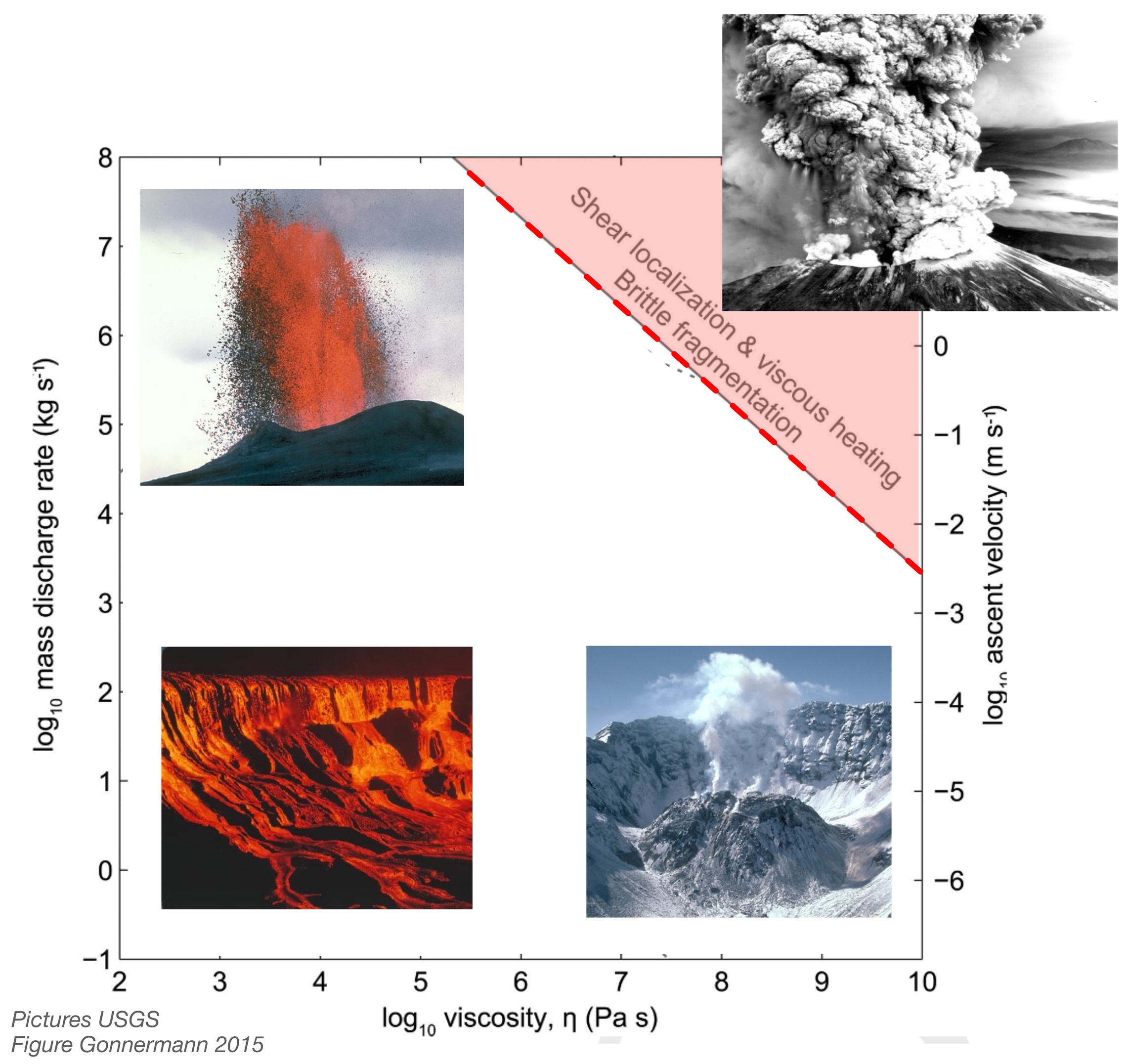

Figure 1. Volcanic eruption styles as a function of the mass discharge rate in the conduit of a volcano and of the lava viscosity. Original figure from Gonnermann, 2015; pictures from USGS.

Viscosity plays a key role in controlling the effusive/explosive dynamics of volcanic eruptions (figure 1). It is a complex function that depends on many parameters, including temperature and melt chemical composition (figure 2). Most models for viscosity predictions are currently empirical, and bring no insights about viscous flow processes.

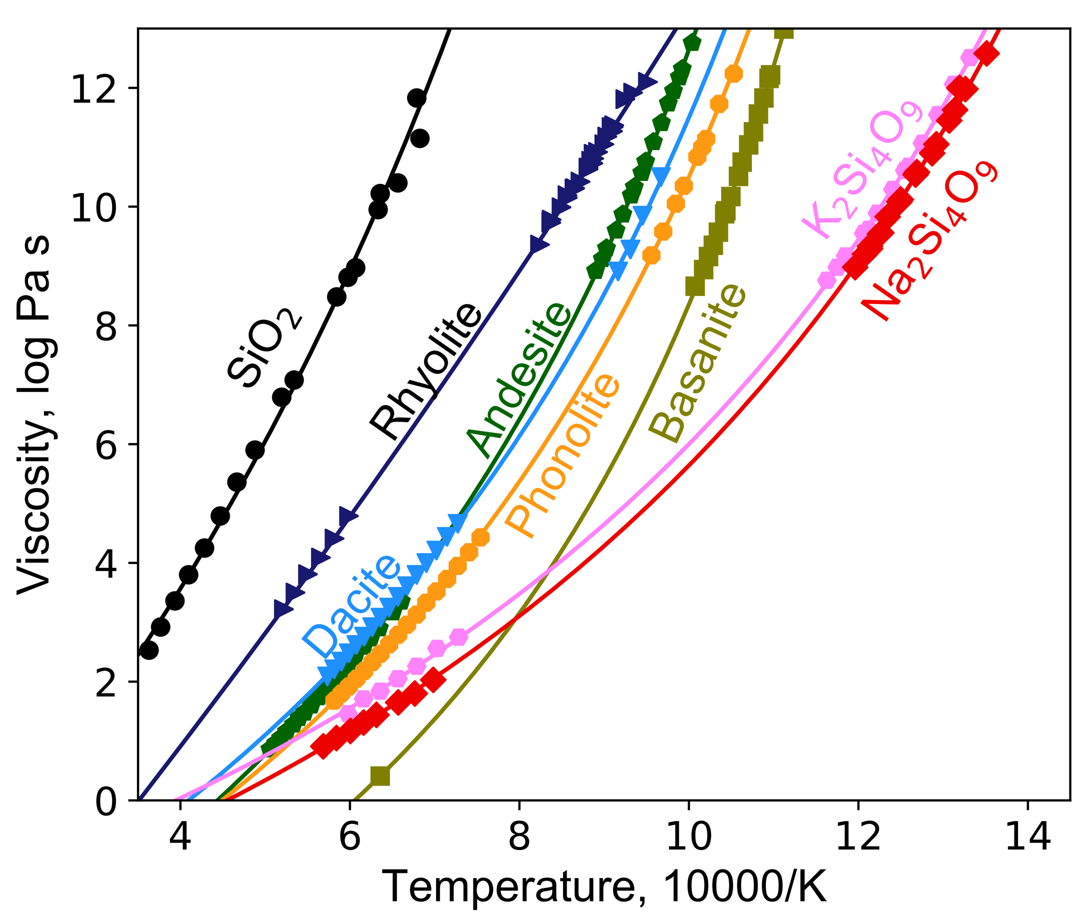

Figure 2. Viscosity of a few reference lavas and melts. [1]

i-Melt

i-Melt is a Physics-guided neural network model. It combines a feed-forward neural network with several physical equations for predictions of viscosity. It further predicts the properties of glasses quenched from the melts, such as density and optical refractive indexes that are important for the glass-making industry. This model is thus multi-task (figure 3). The model takes the chemical composition of the melt as its input, and returns predictions for numerous structural and physical properties. At the moment, i-Melt has been developed for a simple system, Na_2O-K_2O-Al_2O_3-SiO_2 (figure 3, [2]).

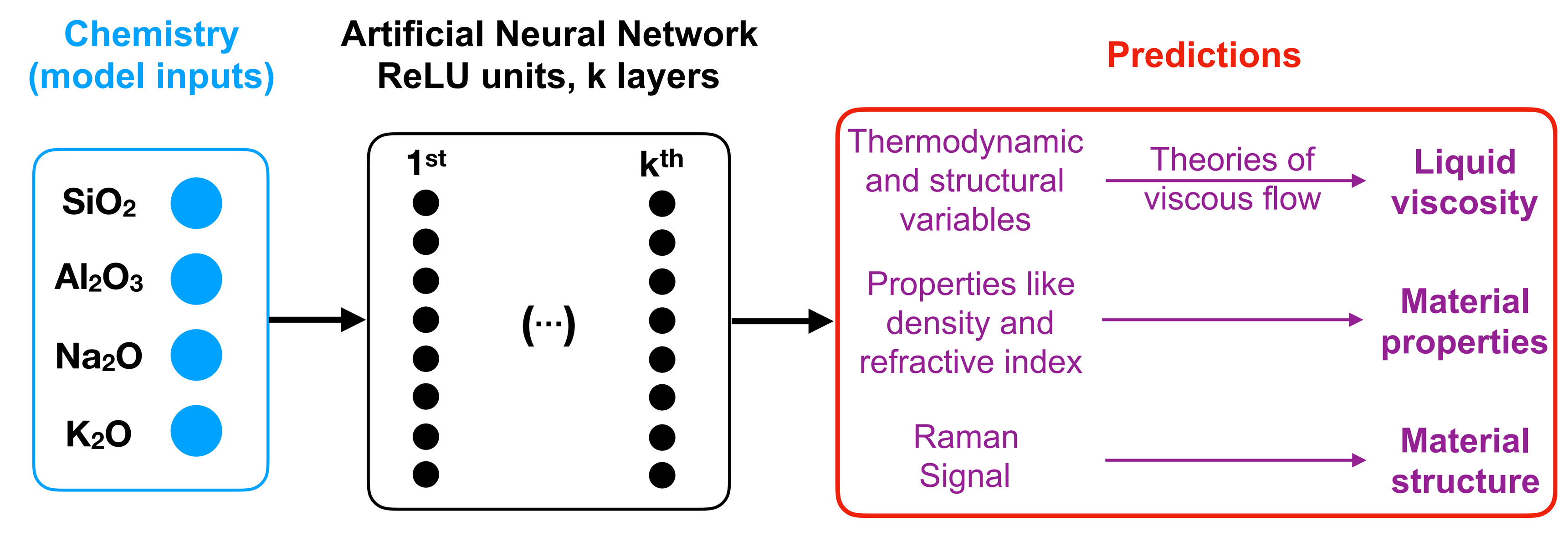

Figure 3. Scheme of i-Melt. Le Losq et al., GCA, in review.

The DiiP master internship project

The initial code was written by Charles Le Losq, with help from Andrew Valentine. Several key issues were identified:

- **CaO and MgO:** important elements in lavas that need to be included in the model; data need to be compiled.
- **Transfer learning:** Could re-using networks trained for the Na_2O-K_2O-Al_2O_3-SiO_2 quaternary system help improve convergence and limit over-fitting?
- **Code improvement:** various code improvements can be done and require some work.

We received a grant from the DiiP, University of Paris, to fund Barbara Baldoni, master student at IPGP, to work on solving these issues.

Progress

At the time of generating this poster, several points have been addressed, enabling significant improvements to i-Melt:

- **Data compilation for CaO-MgO-Na_2O-K_2O-Al_2O_3-SiO_2 melts.** Viscosity, density, Raman spectra and optical refractive index of glasses and melts have been compiled. This represents 758 compositions for viscosity (each one with different temperatures, representing a total of 5954 data points), 585 compositions for density, 122 for Raman spectra, and 642 for optical refractive index.
- **Code improvement** k-fold batch training, network shape selection, and transfer learning are now possible. Other bug fix and code improvements were also made.

Hyper-parameter selection

Hyper-parameter selection is critical and a difficult task. The data set is rather small, so over-fitting is a constant problem. Several strategies were deployed to avoid this: *dropout, early stopping, L2 norm, and bagging of final selected models*. In addition to the number of layers and of hidden units per layers, this amounts to many hyper-parameters. In addition to **random search**, we are now exploring **Bayesian optimization** for hyper-parameter selection.

Predicting the rheology of lavas

Using the new model for CaO-MgO-Na_2O-K_2O-Al_2O_3-SiO_2 melts, we can study systematic variations in melt properties with the magmatic differentiation through crystal fractionation (Bowen series).

Figure 4 shows how, as silica concentration goes up when a basalt crystallizes, the viscosity at 1100°C and the density of the quenched melt vary. We observe an important increase of the viscosity as the melt evolves from a basalt to a rhyolite in the chamber. Reaching a mol fraction of silica around 0.68, viscosity goes above 10^5 Pa·s. Beyond such values, brittle fragmentation — the source of explosive eruptions — becomes possible [3]. Its probability of occurrence will increase further as silica concentration continues to increase. In parallel, we observe a large decrease in quenched melt density. This implies a large increase in magma buoyancy, which will further increase the "eruptability" of the magma.

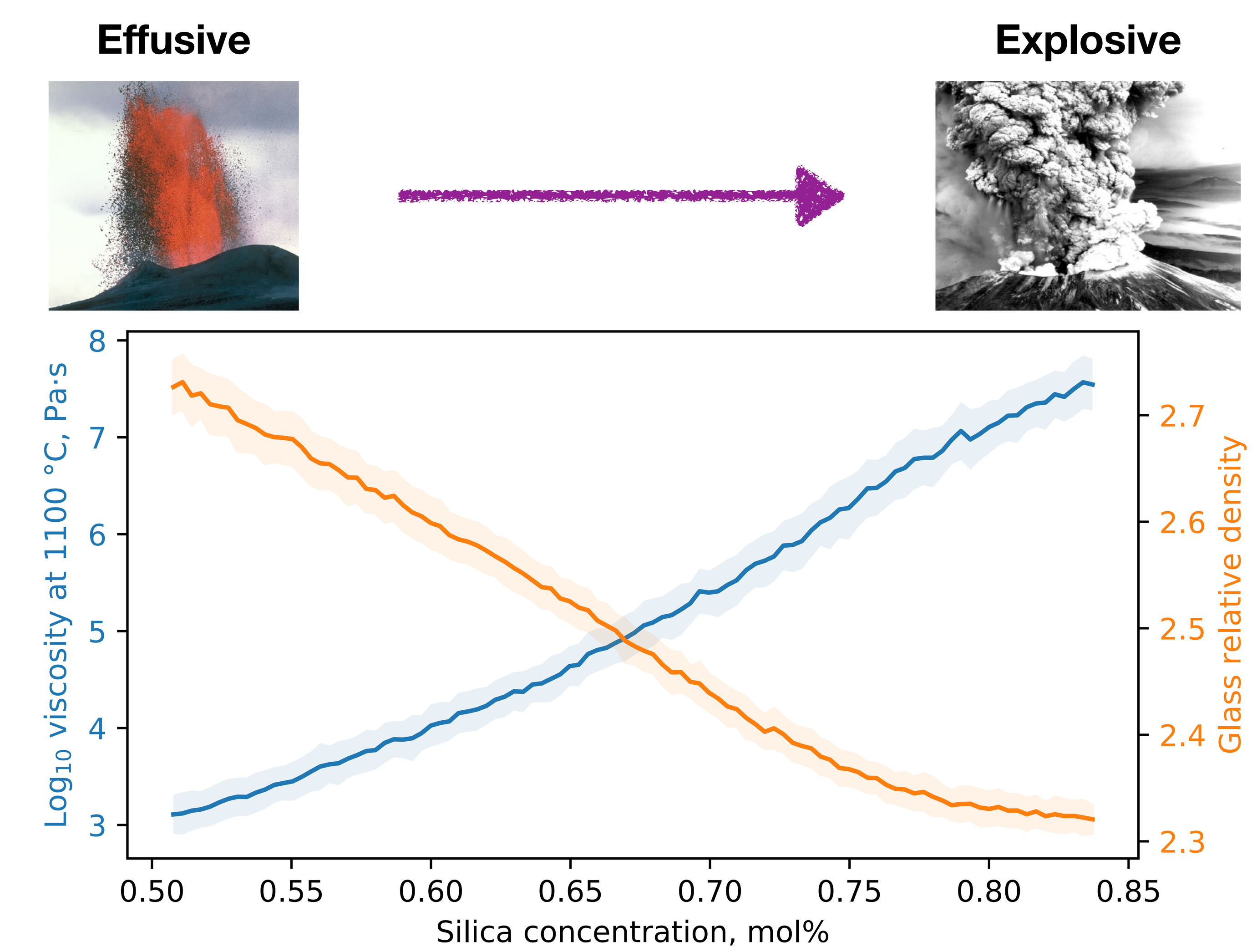

Figure 4. Variations of the temperature at a viscosity of 12 log Pa·s for melts along a calca-alkaline magmatic evolution trend, ranging from a simplified MORB basalt to a rhyolite.

References

[1] C. Le Losq and D. R. Neuville. Molecular structure, configurational entropy and viscosity of silicate melts: Link through the adam and gibbs theory of viscous flow. *Journal of Non-Crystalline Solids*, 463:175–188, May 2017.

[2] C. Le Losq, A. Valentine, B. O. Mysen, and D. R. Neuville. Structure and properties of aluminosilicate glasses and melts: insights from a deep learning model. *Geochimica et Cosmochimica Acta*, in revision.

[3] Paolo Papale. Strain-induced magma fragmentation in explosive eruptions. *Nature*, 397(6718):425–428, Feb 1999.

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