**Determining diffusivities, prefactors and ages using FTIR data and a diffusion model**

The time evolution of the concentration of molecular water in a uniform slab of thickness may be described using a diffusion equation

Equation S1

where is time, is the position across the thickness of the slab and is the local diffusivity for molecular water which depends on the concentration. In this work, the shards of rhyolite glass are assumed to be surrounded on both sides by water; the concentration at the walls is fixed to the solubility of water in the glass. The initial concentration of molecular water is set to be throughout the shard. To find the concentration at some time , we solve the above numerically using a finite difference method to find derivative terms and an explicit Euler scheme to propagate over time.

Two different treatments of diffusivity are presented for comparison. Firstly, we consider a constant diffusivity which does not vary with local concentration, . Secondly, we use the concentration dependent expression of Zhang and Behrens (2000),

Equation S2

where is a constant prefactor, is the diffusivity in micrometres squared per second, is the pressure in megapascals, is the temperature in kelvin, and is the mole fraction of total water on a single oxygen basis. To find , we use an effective molecular weight of 32.2094982 for this rhyolite composition and assume a fixed concentration of hydroxyl groups due to minimal interconversion below the glass transition temperature, as explained in the text.

Given a measured thickness and a known diffusivity for molecular water , it is possible to find and an average hydration  at any time . Conversely, given an age and a measured average hydration , it becomes possible to determine the diffusivity or prefactor for the concentration dependent diffusivity in Equation S2. For simplicity, we initially consider the case of a constant diffusivity . This may be re-cast as a root-finding problem, where we may define a function

and find the value of where . Since a larger will always lead to greater hydration at a given age, the function varies monotonically and will change sign either side of the solution. Thus, we are able to apply an iterative bisection scheme to find the root: initial limits for , termed and , are chosen such that and ; the value of is determined, where ; if , then the solution lies between and , while if , the solution lies between and ; the process is repeated using the new limits until the desired convergence is reached.

Note that the same process may be applied to find a prefactor (Equation S2), or the age of a shard given a pre-determined diffusivity or prefactor. The latter is proposed as a way to date shards using measured thicknesses and hydrations.

When upper and lower estimates for the diffusivity span many orders of magnitude, bisection may require more than a dozen iterations to reach a desired accuracy. Since each iteration requires solution of the diffusion equation, it is desirable to have a fast implementation of the solver. In this work, MATLAB code kindly provided by Michael Hudak (Hudak and Bindemann 2020; Hudak et al 2021) was modified and translated into Fortran, pre-compiled using the Intel oneAPI compiler (ifort) and used to find given a thickness, temperature, pressure, boundary concentration, and a definition of diffusivity. The root-finding itself was implemented using GNU Octave. Code for the solver and bisection scheme may be provided on request.