Supplementary file for: Andrews, J.A., Kristjánsdóttir, G.B., Eberl, D.D. & Jennings, A.E. 2013. A quantitative x-ray diffraction inventory of volcaniclastic inputs into the marine sediment archives off Iceland: a contribution to Volcanoes in the Arctic System. Correspondence: John T. Andrews, Institute of Arctic and Alpine Research and Department of Geological Sciences, University of Colorado, P.O. Box 450, Boulder, CO 80309, USA. E-mail: andrewsj@colorado.edu.

Supplementary File 1

Differentiation between volcanic glasses and other amorphous silica materials

By their very nature, amorphous material, such as biogenic silica and volcanic glass, cannot be resolved with great accuracy and precision by quantitative x-ray diffraction (qXRD) as, in contrast to minerals such as quartz, calcite and kaolinite, amorphous materials do not have a unique, sharply defined x-ray diffraction (XRD) pattern (see Fig. 2). Important questions in the use of qXRD are: (1) can it differentiate between tephras of different compositions; and (2) can the XRD patterns distinguish between volcanic glass/tephra and other relatively amorphous silica-rich materials, such as diatoms, opal, chert and obsidian? Chert has similar XRD peaks to quartz but they are smaller in amplitude. The RockJock v6 standards indicate a 2-theta peak in opal at 21.55°, which is distinct from the 20.88° 2-theta peak in quartz and chert.

To investigate this facet of our study we prepared 10 samples for analysis (Supplementary Table S2), with the letter G standing for the glass component. The samples included two samples from Hekla-4, a rhyolitic tephra and three separate units of the basaltic Saksunarvatn tephra (Jóhannsdóttir 2007). Jennings prepared a sample of nearly pure diatoms that were taken from core MD99-2317, East Greenland. We also included three samples of Icelandic basalt, and a sample of quartz that had been ground in the McCrone mill for 40 min (Supplementary Table S2). The inclusion of the basalt samples was to ascertain whether glacially erosion of the basalt could contribute to the offshore volcaniclastic glass component, and the addition of the quartz was to evaluate whether finely ground quartz could be mistaken for glass and/or diatoms.

The XRD intensity patterns were then pasted into RockJock v6 so that we could ascertain the effect of including or excluding different amorphous materials (Supplementary Table S2). The agreement between the observed and predicted patterns is illustrated by both the degree of fit (DOF) and the total wt% of the selected composition, which should ideally be close to 100 %. The list of selected minerals is shown in full in part (a) of Supplementary Table S2, but in the other tables only the various amorphous materials are listed, and the other minerals are summed as either non-clay minerals or clay minerals.

In the first test we only included the White River glass, diatoms and chert. The tephra samples and the basalts have a mixture of feldspars including the felsic anorthclase feldspar and various plagioclase feldspars. Pryoxene is especially abundant in the three basalt samples. The basalts had low total amorphous materials compared with the other samples, of which the diatom sample had the highest levels. The pure ground quartz had a high wt% (37.6%) classified as chert. The five tephra samples had estimated White River glass contents of between 15 and 31%, but also have large wt% of diatoms (ca. 10-16%), which is understandable given their XRD pattern (Fig. 2).

Test B (Supplementary Table S2b) involved adding opal and obsidian to the expected mineral suite. The resulting totals of amorphous materials did not differ substantially from Test A, and the main difference was that obsidian captured a significant fraction of what had been classified as White River glass in Test A. The comparison of tests A and B on their total amorphous silica components have an r2 = 0.99.

In the third experiment, C (Supplementary Table S2c), all three volcanic glass standards were included. The basalt samples still recorded low values and the ground quartz still had a high wt% classified as chert. The five tephra samples had their highest wt%s associated with the Hekla glass standard and total glass wt%s varying between 36 and 52%. The diatom sample has a large wt% (49.7%) assessed as Hekla glass. The r2 value for the fit between the amorphous sums in A versus C is still highly significant.

In Test D (Supplementary Table S2d) we added the standards for the White River, Hekla-4 and Saksunarvatn tephras as well as the three glass standards and the other amorphous silicates. The correlation between the total amorphous material's wt% in A versus D is now r2 = 0.84 with the major change being an increase in the wt% of Saksunarvatn tephra being associated with the three basalt samples. In general, the addition of the Saksunarvatn tephra explains the increase in the total amorphous wt%s.

Conclusion

These five tests, in which we incrementally increased the number of “glass-like” materials, shows that this does not result in major changes in the sums of these components. We conclude from this that our assessment of the volcaniclastic fraction of sediments on the Iceland shelf (Fig. 5) is reasonable.

Reference

Jóhannsdóttir G.E. 2007. *Mid-Holocene to late glacial tephrochronology in west Iceland as revealed in three lacustrine environments.* MSc thesis, Institute of Earth Sciences, University of Iceland.