Interaction between lamprophiric and riolitic magmas in the Neoproterozoic Sergipano Belt, NE Brazil

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The Neoproterozoic Sergipano Belt occurs on the northeastern margin of São Francisco Craton and in south of and Pernambuco-Alagoas Domains. At the north area of Sergipe State a voluminous granitic rocks intrude a turbiditic Neoproterozoic sequence (Macururé Domain), which due to the action of a low to medium grade regional metamorphism, result in garnet-schists, meta-pelitic e meta-graywacke. In the core, these granitic plutons show magmatic foliation and, at some places, also a tectonic foliation, however in the border with metamorphic country rocks the contacts are abrupt, frequently showing dykes and an increasing of the metamorphic regional grade. The plutons are constituted by muscovite-granite on borders which gradually or suddenly become biotite-granites, hornblende-granites, hornblende-granodiorite, and sometimes, to monzonites, suggesting a magmatic zoning. These granites are medium to coarse rocks, with allotriomorphic, and occasionally porfiritic textures. The magmatic flux foliation is give by the hornblende, biotite or feldspar mineral alignment. Mafic-ultramafic rocks occur as micro-granular enclaves, with a variety of sizes, with or without a border of biotite or amphibole, and as well sin-plutonic dykes. The main enclaves mineralogy is composed by hornblende, biotite, opaque minerals, diopside, alkali-feldspar and plagioclase. The accessory minerals comprise apatite, allanite, carbonate and occasionally zircon. These rocks are correlated to lamprophyres and mafic-monzonites. The presence of these enclaves are indicative of felsic-mafic magmas co-existence and mixing. The geochemical data show that the granites have a shoshonitic to high-K calc-alkaline signature, and the enclaves are ultrapotassic. In the Harker's diagrams the alignment from mafic-ultramafic enclaves to granites from different massifs area straight. Yb and Ta contents suggest a volcanic arc signature. The field and geochemical data point out that some of the granitic rocks from Sergipano Belt are products of the interaction between mafic-ultramafic lamprophiric magmas and riolitic magmas of crustal nature. *Acknowledgements: We thanks the financial funds from FAPITEC and CNPq to the development of this project.*

Simulating iron(III) oxyhydroxide precipitation kinetics using a polymer-based modelling approach

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Conceptual Framework

The precipitation/dissolution behaviour of iron(III) oxyhydroxides (FeOx) is relatively well understood empirically at a macromolecular scale, but poorly described at the mechanistic level. Previously we have used a polymer-based kinetic modelling approach to describe these processes at the molecular scale (i.e. via mechanistic steps), and shown through a steady-state analysis of the resulting differential equations that this approach is consistent with the thermodynamic notion of a solubility limit.[1] Here I extend this approach to numerically simulate temporal evolution of FeOx precipitation and ageing, and compare simulation results with experimentally observed trends.

Modelling Approach

FeOx precipitation is described by sequential addition of monomeric Fe species (denoted by Fe') to other Fe' molecules and existing FeOx polymers, with kinetics controlled by the rate of water loss from Fe' molecules. FeOx dissolution is described by the sequential loss of Fe' from FeOx polymers, and FeOx ageing is described by internal reorganisation of the bonding structure in polymers. Model simulations with several thousand reactions of this type were run using Kintecus.[2]

Results and Conclusion

The polymer-based approach enabled simulation of key aspects of FeOx precipitation and ageing behaviour, including decreasing apparent reactivity and increasing particle size over time (Figure 1).

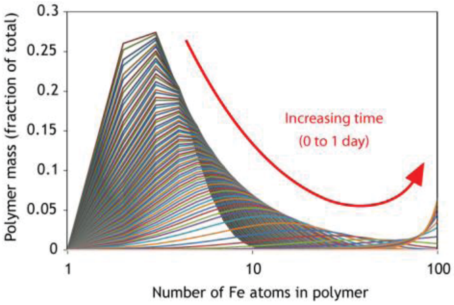

Figure 1: Evolution of FeOx particle size distribution over time at pH 8, as predicted by the polymer-based kinetic modelling approach.

The model was able to simulate the effect of pH on FeOx formation and dissolution kinetics, and successfully reproduced several other experimentally observed phenomena. The polymer-based kinetic modelling approach therefore appears useful to interpret and explain diverse experimental observations in the context of fundamental aquatic chemical reactions.

[1] Rose & Waite (2007) *Geochim. Cosmochim. Acta* **71**, 5605-5619
[2] Ianni (2012) *Kintecus v4.50*, www.kintecus.com