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SolEx: A Model for COHSCI Fluid Solubilities and Exsolved Gases in Basalts

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We assume that the behaviour of the fluid phase is controlled by the volumetrically dominant volatile species, H2O and CO2. Sulphur, in the form of SO2 and H2S, and HCl partition between the melt and fluid phases. Measurements were made on basalts from Stromboli, Italy and Masaya, Nicaragua to determine these partition coefficients as a function of pressure for SO2 and Cl (Lesne et al., subj, J Pet), and results from Hekkla, Iceland (Moune et al., 2009, Cont Min Pet 157 p691) constrain H2S behaviour. The model of Churakov and Gottschalk (2003, GCA 67 p2415) is applied to calculate fugacity coefficients and equilibrium coefficients for the reaction Xmelt –> Xfluid are thereby deduced.

In the forward model, total volatile inventories and melt composition are specified by the user. The parameterisation of Dixon (1997, Am Min 82 p368) is used to predict the partitioning of CO2 and H2O between vapour and melt phases. H2S dominates at oxidation states of Δ NNO < -0.5 whereas SO2 is dominant at Δ NNO > +0.5 (Jugo et al., 2010, GCA 74 p5926). We simplify this by assuming a step-change such that all S is reduced below and oxidised above Δ NNO = 0. An iterative procedure is employed to predict the partitioning of S and Cl components between fluid and melt phases. Melt and gas compositions and gas volume fraction are thereby modelled over pressures from 5 – 4000 bar. This approach satisfactorily reproduces independent literature data on S and Cl behaviour in basalt.

SolEx is a user-friendly software package available for OS X and Windows, facilitating modelling of closed- and open-system COHSCl degassing from basalts. A C++ library is also available upon request, for the incorporation of SolEx into other fluid-mechanical or thermodynamic models of magmatic processes.