Modeling of the solubility of a two-component $H_2O + CO_2$ fluid in silicate liquids

PAOLO PAPALE*

CNR-GNV, Centro di Studio per la Geologia Strutturale e Dinamica dell'Appennino, Via S. Maria 53, 56126 Pisa, Italy

ABSTRACT

The solubility of a two-component, $H_2O + CO_2$ fluid in silicate liquids was modeled by assuming mechanical, thermal, and chemical equilibrium between the fluid and liquid phases. The liquid phase was treated as a 12-component (10 major oxides + H₂O + CO₂) mixture, and its thermodynamic properties were calculated on the basis of a regular and non-isometric mixing equation for the excess Gibbs free energy. The mole fractions of the exsolved and dissolved water and carbon dioxide were calculated on the basis of two chemical equilibrium and two mass-balance equations expressing the conservation of the exsolved and total mass of volatiles. The model was then calibrated by processing nearly 1000 experimental H₂O and CO₂ solubility determinations from the literature in natural and synthetic silicate liquids covering a wide range of pressure-temperature-composition conditions. The results show that the present model predicts with reasonable accuracy the solubility of water and carbon dioxide in silicate liquids over the entire range of fluid phase compositions and for pressures from atmospheric to several hundreds of megapascals and temperatures from about 1000 to 1900 K. The predicted isobaric-isothermal sections of the $H_2O + CO_2$ saturation surface show a transition from essentially Henrian to strongly non-Henrian behavior as the pressure is increased from tens to hundreds of megapascals, consistent with the majority of experimental results made at low, medium, and high pressure. The presence of a very small amount of CO₂ in the system significantly increases the volatile saturation pressure, suggesting that in most cases the multicomponent nature of the fluid phase cannot be neglected when modeling volcanic processes such as magma chamber and conduit ascent dynamics. The predicted closed- and open-system saturation conditions differ significantly. Under open-system conditions, the dissolved H₂O content increases and the dissolved CO₂ content decreases compared with the closed-system conditions. This results in a more efficient H₂O enrichment of the fluid phase with decreasing pressure under open-system conditions. The present model can be used to investigate the behavior of volatiles in the volcanic environment provided that the basic assumption of equilibrium is satisfied.