

DATABASE SYSTEM TO MANAGE NERNST DISTRIBUTION COEFFICIENTS AND ITS APPLICATION FOR PETROGENETIC MODELING

VERMA, S.P., TORRES-ALVARADO, I.S., GUEVARA, M. and GONZÁLEZ-CASTILLO, O.Y. Centro de Investigación en Energía, UNAM, Apdo. Postal 34, 62580 Temixco, Morelos, Mexico.

The study of the behavior of trace elements during geological processes has become an important part of modern geology, due to the fact that trace element distribution in a system can be described using mathematical expressions. Quantitative models are now developed for systems controlled by crystal-melt or crystal-fluid equilibria (use of Nernst distribution coefficient, K_d). Experiments have shown that K_d can vary largely with temperature, pressure, melt composition, and oxygen fugacity. Therefore, mineral/melt partition or distribution coefficients should be very carefully selected during petrogenetic modeling, in order to assure physico-chemical conditions similar to the magmatic system being modeled. This demands extensive compilations of K_d values. A software package is presented, which stores and manages distribution coefficients for petrological purposes. The system uses an efficient code written in C language for personal computers, and due to its modular structure, it is suitable to become part of a general petrological software system. It takes advantage of commercial database systems for compilation purposes and calculates elemental as well as bulk distribution coefficients automatically from an extensive database. Although this system has already been used successfully to model petrogenetic processes in volcanic rocks, it can be modified easily to compute any other kind of petrological models using trace elements.