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Appropriate mixing models to estimate thermal properties of clastic and chemical/biochemical rocks

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In order to estimate thermal properties of a wide variety of clastic and chemical/biochemical sedimentary rocks, accurate determinations of mineral composition and porosity were carried out on core samples. Then we applied mixing law models combining values of thermal properties of rock-forming minerals and pore fluid. All models are based on different ways of averaging the thermal conductivity of the components with respect to their volume fractions. The bulk heat capacity was calculated as the weighted average of the heat capacity of the mineral grains and the fluid filling the pores. On the contrary, estimating the bulk thermal conductivity required the choice of a mixing model that well describes the rock structure and the geometrical relationship between minerals and voids. Based on parallel and series arrangements of the minerals with respect to the direction of heat flow, the harmonic and arithmetic mean models are applicable to anisotropic rocks. These models give the upper and lower limits of the matrix thermal conductivity. A model that describes the thermal conductivity of the isotropic rock is the geometric mean, where several components of known conductivity are randomly orientated and distributed. A more complex model by Hashin and Shtrikman was chosen for the determination of the conductivity of macroscopically homogeneous and isotropic multi-component rocks. One of the major problems is the allowance for the presence of fluid in the pores. So the Brailsford and Major model was employed to predict the thermal conductivity of a system containing two solid phases immersed in a continuous fluid. Additional parameters were introduced into a mixing law in order to incorporate the rock structure. Rocks, containing crack-like fluid-filled inclusions, were treated as macroscopically homogeneous, but the determination of their bulk conductivity required consideration of micro-structural details. For this purpose, the model by Zimmerman was used. This approach assumes spheroids that are randomly distributed in a homogeneous mixture where the shape of pore is defined by the aspect ratio of the spheroids.

Laboratory thermal conductivity and heat capacity measurements were used for validating the results of the mixing models. Measurements were carried out parallel and perpendicular to the core axis, which always coincides with the vertical. The heat capacity measurements allowed the weighted average approach and the absolute difference between the computed and measured is lower than 5%. The Hashin and Shtrikman's model provided accurate estimations of the matrix thermal conductivity of homogeneous isotropic samples. Spherical pores seem to be consistent with laboratory results and Zimmerman's model thermal conductivity is larger by 3.5%. For selected lithologies, photomicrograph analysis allowed us to distinguish flat fractures or oblate porosity from a simple spherical shape and to include a proper aspect ratio in the model. If a proper aspect ratio is chosen, deviations between computed and measured thermal conductivity can significantly decrease. An anisotropy effect depending from compaction is important in the case of rocks rich in sheet silicates. Due to rotation of these minerals, the vertical conductivity decreases with increasing depth of burial and compaction.

Finally, a technique that combines the effects of mineral composition, anisotropy, temperature and pressure was developed for the estimation of the thermal properties at different depth. New compaction curves for the investigated lithotypes and relationships between vertical thermal conductivity of sheet silicates and depth or porosity were found.