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Testing the results of pseudosection modelling of the metamorphism of mafic rocks using THERMOCALC

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The investigation of metamorphism using mafic rocks is classic since the early 1940s, when Eskola defined the metamorphic facies. Since then, several approaches to investigate their mineralogy and P-T conditions of metamorphism were developed. Recent advances in thermodynamic datasets and activity-composition models for pyroxene and amphibole allowed the calculation of pseudosections for mafic rocks, however, not much work was done to compare pseudosection output with rocks from where a parallel P-T calculation is available or to confront it with experimental results or even to evaluate different outputs calculated with different sets of thermodynamic datasets and accompanying activity-composition models. An evaluation of modeling using different datasets and the comparison between pseudosections and experimental results or parallel P-T estimates were made for six mafic compositions. Among the diagrams obtained, there are cases where the pseudosection-based P-T estimate differs from the independent estimate and cases where the observed assemblage is not calculated to be stable anywhere in the diagrams. In the first case, the differences are up to 1.0 kbar, or 100 °C. In the second case, there are two main inconsistencies. The first is an underestimation of the stability field of garnet, which is calculated to be stable just at pressures higher than at least 11 kbar. This is likely due to the absence of manganese in the model systems available. The second main inconsistence is an overestimation of the stability field of diopside for compositions relatively unsaturated in SiO_2. In these cases diopside is calculated to be stable in temperatures as low as 425 °C, in disagreement not only with data specific to the analyzed samples, but with what is observed in mafic rocks in nature. Diopside's calculated stability at low temperatures seems to be related to the activity-composition models available for chlorite, actinolite and hornblende, which should allow these minerals to become poorer in SiO_2 at low temperatures. Regarding the different thermodynamic datasets and sets of activity-composition models, diagrams calculated for the same composition are similar in topology, but different when it comes to size and position of the fields. When discrepancies stemming from choice of thermodynamic dataset and set of activity-composition models are summed to variation caused by XFe3+ estimate and to uncertainties inherent in the calculations, P estimates for the same composition can differ as much as 5.5 kbar. Pseudosections calculated using the most recent set of activity composition models produce better results. We conclude that the thermodynamic datasets and activity-composition models available for mafic rocks are still in need of improvement, and that more work towards evaluating thermobarometric methods is needed.