

Nagurney et al. Supplemental Material Part V

Part V: Comparison of Results with Thermocalc Datasets 5.5 and 6.2

Ds6.2 Calculations not Described in Main Text:

Rappold Complex Sample 35F03: In the ds6.2 calculation, garnet core isopleths intersect at 537 °C and 4.9 kbar, consistent with 12 °C and 0.5 kbar of overstepping (Supplemental Figure 8A). At P - T conditions greater than garnet-in in the TEC, $\Delta\mu_{\text{MnO}} < 0$ (Supplemental Material Figure 1C). $\Delta\mu_{\text{MgO}}$, $\Delta\mu_{\text{CaO}}$, $\Delta\mu_{\text{FeO}}$, and $\Delta\mu_{\text{Al}_2\text{O}_3}$ are initially zero, with $\Delta\mu_{\text{MgO}}$ becoming positive at 530 °C and 4.6 kbar, $\Delta\mu_{\text{FeO}}$ becoming negative at 532 °C and 4.7 kbar, $\Delta\mu_{\text{CaO}}$ becoming positive at 535 °C and 4.8 kbar, and $\Delta\mu_{\text{Al}_2\text{O}_3}$ being the final chemical potential to experience a difference between the TEC and MSC at 541 °C and 5.0 kbar (Supplemental Figure 8C).

In both ds5.5 and ds6.2 the general topologies of the pseudosections for this sample are very similar, with a few minor differences. Biotite is stable across the entire P - T range of interest in the ds6.2 diagram but is unstable at low temperature in ds5.5 (Figure 3A, Supplemental Figure 8A). In calculations with both datasets, biotite, chlorite, garnet, ilmenite, muscovite, plagioclase, and quartz are stable in the field where garnet core isopleths intersect (Figure 3A, Supplemental Figure 8A). The garnet stability field is slightly expanded in ds6.2 versus ds5.5, but the P - T where the garnet core isopleths intersect barely changes between the two calculations, so there is more reported overstep in the ds6.2 calculation. This is consistent with other studies (White et al. 2014; Waters 2019) which also showed a greater garnet stability field in ds6.2 versus ds5.5.

The ds5.5 calculation shows a difference in the chemical potential of all oxide components of interest between the TEC and MSC at all P - T conditions greater than garnet-

in in the TEC (Figure 3A). Deviation in $\Delta\mu_{\text{CaO}}$, $\Delta\mu_{\text{FeO}}$, and $\Delta\mu_{\text{Al}_2\text{O}_3}$ in the ds6.2 calculation are delayed to slightly higher P - T , though all chemical potentials experience a deviation at P - T conditions nearly coincident with those at which the garnet core isopleths intersect (Supplemental Figure 8C).

Eastern Vermont Sample TM549a: The intersection of garnet core isopleths in TM549a calculated with ds6.2 is at 550 °C and 6.3 kbar (Supplemental Figure 9A), which is consistent with 45 °C and 2.0 kbar of overstepping. At all P - T conditions above garnet-in, $\Delta\mu_{\text{MnO}}$ is negative (Supplemental Figure 9C). $\Delta\mu_{\text{MgO}}$ becomes positive and $\Delta\mu_{\text{CaO}}$ becomes negative ~ 10 °C above garnet-in, while $\Delta\mu_{\text{FeO}}$ becomes negative ~ 15 °C above garnet-in (Supplemental Figure 9A) and $\Delta\mu_{\text{Al}_2\text{O}_3}$ is zero until 531 °C and 5.4 kbar (Supplemental Figure 9C).

The general topologies of pseudosections calculated with ds5.5 and ds6.2 are nearly identical (Figure 4A & Supplemental Figure 9C). In both calculations, biotite, chlorite, garnet, muscovite, plagioclase, and quartz are stable in the field where the garnet core isopleths intersect (Figure 4A & Supplemental Figure 9C). A small staurolite stability field that is present in the ds6.2 calculation is absent in the ds5.5 calculation. The ds6.2 calculation implies a larger amount of overstep (45 °C versus 35 °C) than the ds5.5 calculation.

In both the ds5.5 and ds6.2 pseudosection calculations, $\Delta\mu_{\text{MgO}}$ is positive and $\Delta\mu_{\text{MnO}}$, $\Delta\mu_{\text{CaO}}$, and $\Delta\mu_{\text{FeO}}$ are negative at P - T conditions above garnet-in, but in the ds6.2 calculation there is a larger P - T interval where $\Delta\mu_{\text{MgO}}$, $\Delta\mu_{\text{CaO}}$, and $\Delta\mu_{\text{FeO}}$ equal zero (Figure 4C & Supplemental Figure 9C). Both calculations produce a P - T range in which $\Delta\mu_{\text{Al}_2\text{O}_3}$ is effectively zero directly above garnet-in, with a correlation between the P - T conditions at

which $\mu_{\text{Al}_2\text{O}_3}$ differs between the TEC and MSC and the intersection of garnet core isopleths, though that correlation is less explicit in ds6.2.

General Comparison of Phase Stability in ds5.5 versus ds6.2:

In general, pseudosections calculated here in ds5.5 and ds6.2 are very similar, but there are a few key differences. The stability ranges of muscovite, chlorite, andalusite, sillimanite, and feldspar for all examples are typically the same in each dataset. The extent of garnet stability is also similar between the ds5.5 and ds6.2 calculations for samples 24-99 (Sikkim), AV26A (Pomfret Dome), and TM549A (Eastern Vermont). However, for sample 35F03 (Rappold Complex) the garnet stability field is slightly expanded in ds6.2 and for sample 93-CW-4 (Nelson Aureole), the stability field of garnet in the ds6.2 calculation is considerably more extensive than in ds5.5. For an average pelitic rock, (White et al. 2014) calculated a slightly expanded stability field of garnet in ds6.2 compared to ds5.5. However, for a pelitic rock that reached mid to upper amphibolite facies from the High Himalaya, (Waters 2019) found an extreme difference in the stability field of garnet, with ds6.2 calculating garnet to be stable over a far wider P - T range than ds5.5, consistent with the Nelson Aureole example here.

The stability of biotite tends to be consistent between the two thermodynamic datasets except in the case of sample 24-99 (Sikkim). In the ds5.5 calculation, biotite is stable above ~ 550 °C, first appearing at temperatures above garnet-in at most pressures. However, in ds6.2, biotite is calculated to be stable across the entire P - T range of the pseudosection. Neither White et al. (2014) nor Waters (2019) show any difference in the stability range of biotite between ds5.5 and ds6.2 in their calculations. It is currently unclear

to us the cause of the differences in the stability of biotite in ds5.5 and ds6.2 in the Sikkim example.

For samples 24-99 (Sikkim), 35F03 (Rappold Complex), and 93-CW-4 (Nelson Aureole), the stability fields of staurolite are almost identical between calculations with each dataset. For sample AV26A (Pomfret Dome), the stability field of staurolite is larger in ds5.5. For sample TM549A (Eastern Vermont), staurolite is not calculated to be stable in the ds5.5 pseudosection, but is present in the ds6.2 pseudosection. White et al. (2014) calculate a slightly expanded staurolite stability field in their ds6.2 pseudosection compared to their ds5.5 pseudosection.

There are some differences in the stability field of paragonite between ds5.5 and ds6.2 for sample 24-99 (Sikkim), and paragonite is not stable in either calculation for sample 35F03 (Rappold Complex). For sample AV26A (Pomfret Dome) paragonite is not present our ds5.5 pseudosections, but is stable at high pressures and low temperatures in the ds6.2 calculation. For sample 93-CW-4 (Nelson Aureole) and sample TM549A (Eastern Vermont), the paragonite stability field is expanded in ds6.2 compared to ds5.5. These results are consistent with White et al. (2014) who also showed an expanded field for paragonite at high pressures and low temperatures in their calculations for an average pelite.

Comparison of Chemical Potential Calculations:

There are many similarities of the $\Delta\mu_{\text{component}}$ calculations between ds5.5 and ds6.2, with a few key differences. In all calculations with both datasets, $\Delta\mu_{\text{MnO}}$ is negative immediately up temperature of garnet-in. $\Delta\mu_{\text{MgO}}$ is positive at P - T conditions above garnet-in, though this is delayed by several degrees in the Nelson Aureole and Pomfret Dome examples with

ds5.5 and in the Rappold Complex and Eastern Vermont examples in ds6.2. However, these differences in $\Delta\mu_{\text{MgO}}$ are minor. Trends in $\Delta\mu_{\text{CaO}}$, are nearly identical for ds5.5 and ds6.2, though the P - T condition at which $\Delta\mu_{\text{CaO}}$ deviates from zero can be slightly different in calculations with ds5.5 and ds6.2. In both ds5.5 and ds6.2, for the examples where garnet is apparently overstepped (Eastern Vermont, Pomfret Dome, Nelson Aureole), $\Delta\mu_{\text{FeO}}$ is zero immediately above garnet-in, becoming negative at higher P - T . For each sample the P - T at which $\Delta\mu_{\text{FeO}} \neq 0$ is slightly different between the ds5.5 and ds6.2 calculations. In 4/5 ds5.5 calculations and 5/5 of the ds6.2 calculations, $\Delta\mu_{\text{Al}_2\text{O}_3}$ is the final component to experience a deviation between the TEC and MSC. Since the trends are very similar between the ds5.5 and ds6.2 calculations, this shows that these trends are present in pseudosection calculations regardless of the choice of thermodynamic dataset.

References

- Waters, D.J. (2019) Metamorphic constraints on the tectonic evolution of the High Himalaya in Nepal: the art of the possible. Geological Society, London, Special Publications, 483, 325–375.
- White, R.W., Powell, R., Holland, T.J.B., Johnson, T.E., and Green, E.C.R. (2014) New mineral activity-composition relations for thermodynamic calculations in metapelitic systems. Journal of Metamorphic Geology, 32, 261–286.