Holland et al. (2018) W144 benchmark attempt (May 13, 2019).

Configuration:

1) The input files for the Perple_X calculations presented here are at www.perplex.ethz.ch/perplex/examples/example_holland_et_al_2018_melt_model

2) The data used for this benchmark was copied in late April 2019, from www.esc.cam.ac.uk/research/research-groups/research-projects/tim-hollands-software-pages/thermocalc-1/mantle-melting-files. This data was modified after the 2018 publication was finalized and then again in March 2019. The data files actually used for the calculations in Holland et al. (2018) are not available and certainly not identical to the data used here and currently in THERMOCALC.

3) The above-mentioned data files indicate changes to the White et al. (2014) biotite model that are otherwise undocumented. Calculations with a biotite model that accounts for these changes (Bi(HGP)) lead to larger discrepancies than obtained with original White et al. (2014) model. Therefore, the calculations reported here were made with Bi(W).

Results (depicted on page 3 of this document):

1) The agreement between the dashed phase boundaries depicted for the W144 composition depicted in Figure 12 of Holland et al. (2018) and obtained with Perple_X is generally good and appears to confirm the Perple_X implementation of the melt(HGP) and Aqfl(HGP) (siliceous aqueous fluid) models.

2) Holland et al. (2018) indicate that their computed (at 6 - 12 kbar) solidus is coincident with that of White et al (2014). This implies that the solidus computed with Perple_X is discrepant by 5-10 K. This discrepancy appears insignificant given the uncertainty concerning the benchmark configuration.

3) Holland et al. (2018) describe modifications to the White et al. (2014) cordierite model (Crd(W)). The modified cordierite (Crd(HGP)) and biotite (Bi(HGP), see configuration note 2) models result in substantial displacements of the phase boundaries depicted by White et al. (2014). It seems probable that the Bi(HGP) model variant was used for the calculations depicted in Figures 10 and 11 of Holland et al. (2018), but not in the calculations mentioned re Figure 12.

Mitigation of Rough Phase Boundaries in the W144 Benchmark by Non-Linear Subdivision and Reach-Increments

The presence of a major element in minor amounts in one or more major phases is a common source of rough phase boundaries. The reason strong partitioning of an element causes computational instability is that a small change in the composition of the phase in which the element is enriched causes changes that may be at the limit of the compositional resolution in the other phases of the system. In the w144_suprasolidus_HGP_default calculation this problem is manifest by the supra-solidus phase boundaries involving cordierite, because the concentration of iron in cordierite is much higher than it is in the melt phase. This source of phase boundary roughness can be eliminated by two methods in Perple_X:

reach-increments - w144_suprasolidus_HGP_reach_increment - reach-increments widen the range over which the composition of a phase may change during adaptive optimization iteration. This method is robust and can be implemented by simply setting the global_reach_increment option in perplex_option.dat. The downside to using reach-increments is that they are computationally costly, even if they are applied only to specific solution models rather than globally (as done in the example).

nonlinear subdivision schemes - w144_suprasolidus_HGP_non_linear - non-linear subdivision schemes are recommended in solution models for any compositional variable whose maximum value is expected to be below the value specified by the initial_resolution option. The downside non-linear subdivisions is that it requires that if it is used injudiciously it can become computationally costly. For additional information refer to the discussion of nonlinear subdivisions in the commentary at the beginning of the 6.8.7 solution-model file.

In general, the solution models in the Perple_X solution-model file specify neither reach_increments or non-linear subdivision schemes because it is not possible to anticipate how a particular solution model will be used. For example the melt(HGP) model can be used for both ultramafic and felsic melts, in the former iron may be a major element, whereas in the latter iron is a minor or trace element.

For comparison, computation times for the three examples reproduced here are:

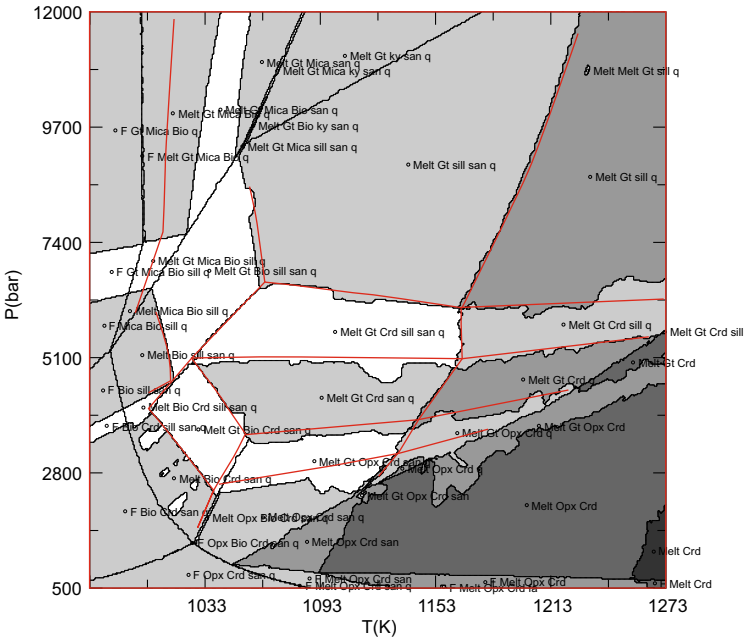
w144_suprasolidus_HGP_default - 12 h.
w144_suprasolidus_HGP_non_linear - < 2 minutes.
w144_suprasolidus_HGP_reach_increment - < 2 minutes.

Both non-linear subdivision and reach-increments result in comparable, and significant, improvements to the result obtained using the default computational options; and the non-linear subdivision method accomplishes the improvements at drastically lower cost.

Red phase boundaries correspond to those depicted by dashed curves in Figure 12 of Holland et al. (2018), i.e., the phase boundaries actually computed with the new melt model.

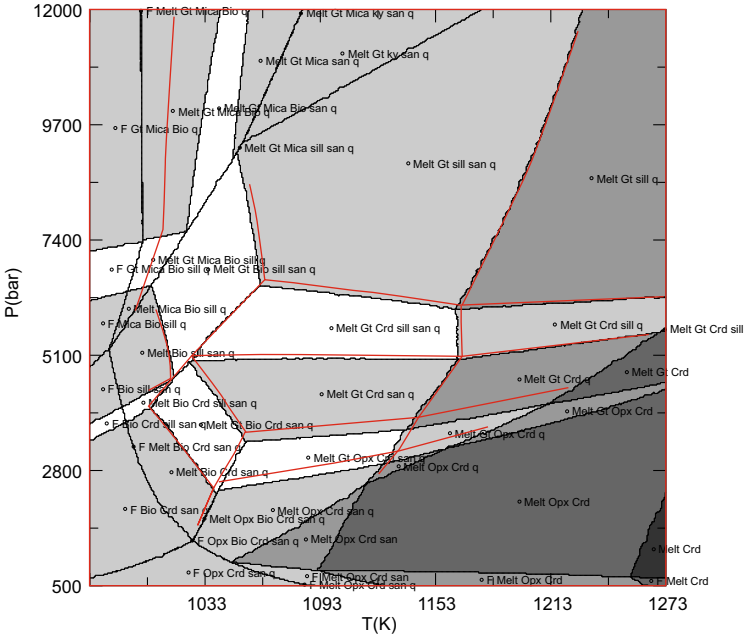
w144_suprasolidus_HGP_default

- melt(GHP) specifies linear subdivision
- no reach-increments
- computation time < 2 min.



w144_suprasolidus_HGP_non_linear

- melt(GHP) specifies nonlinear subdivision for fo, fa, sil and wo species
- no reach-increments
- computation time < 2 min.



w144_suprasolidus_HGP_reach_increment

- melt(GHP) specifies linear subdivision
- global_reach_increment = 4
- computation time ~15 hour.