Holland et al. (2018) KLB-1 Benchmark Attempt (May 6, 2019)

UPDATE October, 2019: the “raw” result on page 2 was generated with the 6.8.8 version of Perple_X from khgp.dat, khgp_perplex_option.dat and the default 6.8.8 version of solution_model.dat. The other solution model files included with this benchmark will only run with 6.8.7 and must be replaced with the 6.8.8 version of solution_model.dat.

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) Holland et al. (2018) do not directly specify the bulk composition used. The composition used here was inferred by Debaditya Bandyopadhyay. It is unlikely that this is a major source of discrepancy in the benchmark.

3) Holland et al. (2018) do not specify which feldspar model is stable in the feldspar phase fields. The Fsp(C1) model was used in all results here. It is unlikely that this is a major source of discrepancy in the benchmark.

4) The data used here 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 had been modified in March 2019 and is not identical to that used for the calculations presented in Holland et al. (2018). It is unlikely that this is a major source of discrepancy in the benchmark.

There are three major sources of discrepancies between THERMOCALC and Perple_X:

Type I - Data transcription errors, discrepancies in problem configuration, and computational errors (usually in Perple_X).
Type II - Spurious solvi resulting from limited resolution in Perple_X.
Type III - Metastable phase relations computed in THERMOCALC.*

Results:

1) The agreement of the major phase boundaries (solidus, liquidus, and plagioclase-, garnet-, and spinel-lherzolite) boundaries suggests Type I errors are not important. Possible exceptions are the persistent discrepancy in the suprasolidus Opx-out phase boundary and the equally persistent stability fields for chromite at both low temperature and high pressure.

2) The Perple_X result indicates solvi in both pyroxene phases. Perple_X calculations made at high resolution demonstrate that the Cpx solvus is spurious (Type II error), but that the Opx solvus is legitimate; thus the Opx phase relations in the THERMOCALC result are metastable (Type III error*). Perple_X calculations made for simplified chemical models (following page), suggest that K, Ti, and Cr in the Opx model stabilize small amounts of a Ca-rich Opx phase. The amounts (< 1 vol%) of the Ca-poor Cpx phase and the Ca-rich Opx phase are relatively minor, but do have consequences (points 3 & 4 below). Whether these consequences are significant is a matter of metaphysical debate. Refer to page 4 of this document for discussion of a partially successful attempt to reproduce the metastable Holland et al. (2018) phase relations by restricting the range of compositions considered by Perple_X.

3) Calculations without Ti and K (page 3), which are responsible for stabilizing the Ca-rich Opx phase within the spinel- and garnet-lherzolite field, and calculations in which the range of Opx is restricted to eliminate the Ca-rich Opx phase (page 4), suggest that Type III error is responsible for widening the Sp-Grt transition in the THERMOCALC result. It is probable that similar effects are responsible for the low-P-T spinel field of the THERMOCALC result.

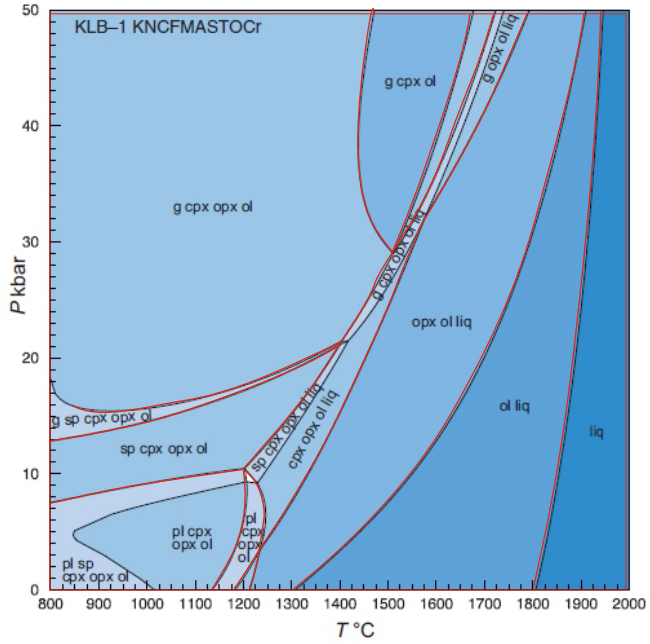
4) The high-P low-T and low-P high-T spinel fields in the Perple_X result are caused by the stability of ~1 vol% Cr-rich spinel. This is likely due to Type III error.

Conclusion:

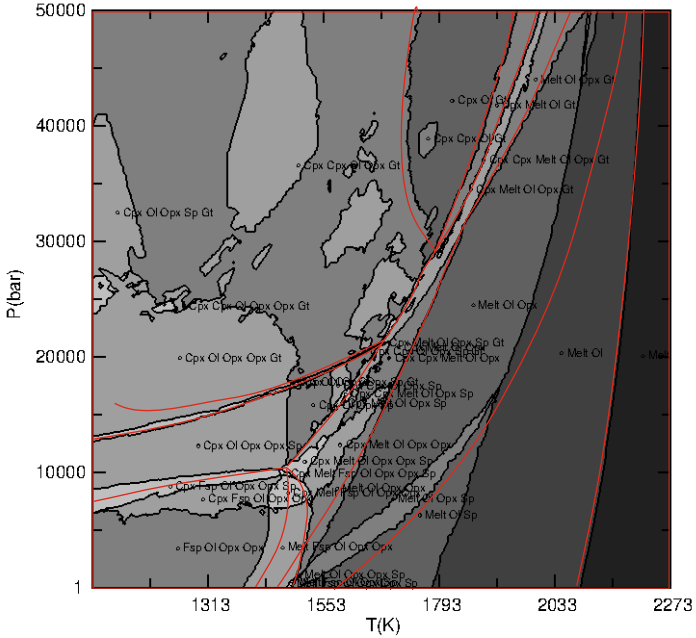
The KLB-1 section depicts phase relations that are metastable in the context of the Holland et al. (2018) thermodynamic model. The Opx model is the likely cause of this metastability, but the Cpx model also appears to be problematic. Attempts to reproduce the metastable phase relations by restricting the range of possible Opx compositions fail because the restrictions stabilize a second Cpx phase.

*The term “Type III Error” is used to mean that the reported phase relations are not predicted by Gibbs energy minimization from the thermodynamic model, this does not necessarily mean that the results are empirically incorrect. For example, the prediction of a Ca-rich Opx phase in the Perple_X result is thermodynamically correct, but empirically incorrect; likewise the stability of spinel within the plagioclase-lherzolite field in the Holland et al. (2018) result may be empirically correct, but is most likely thermodynamically incorrect.

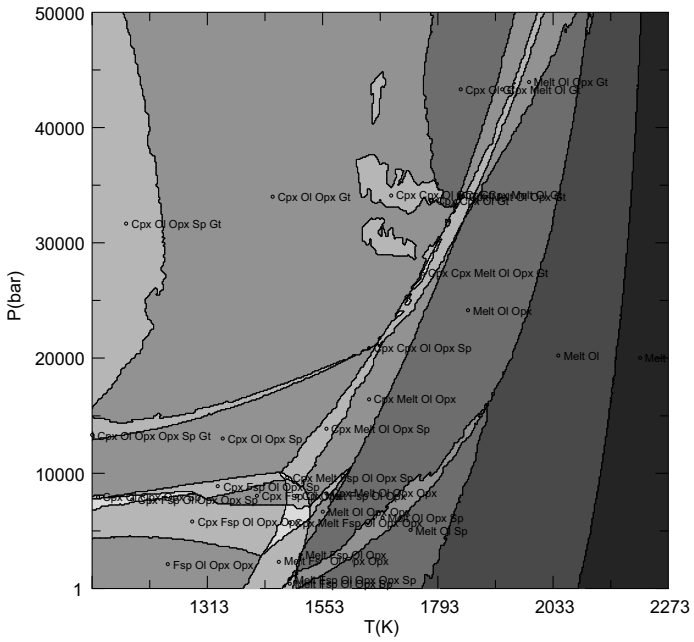
THERMOCALC, Holland, Green, and Powell (2018)



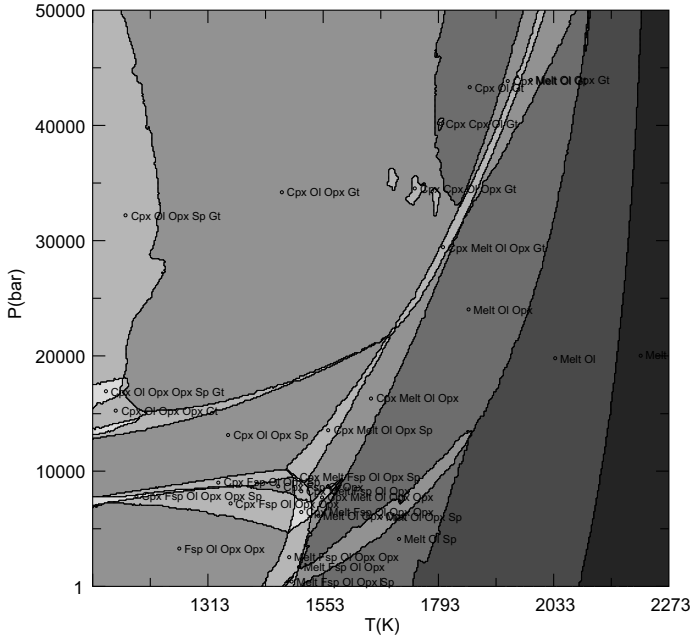
Perple_X, raw result, problem definition file KHGP.dat



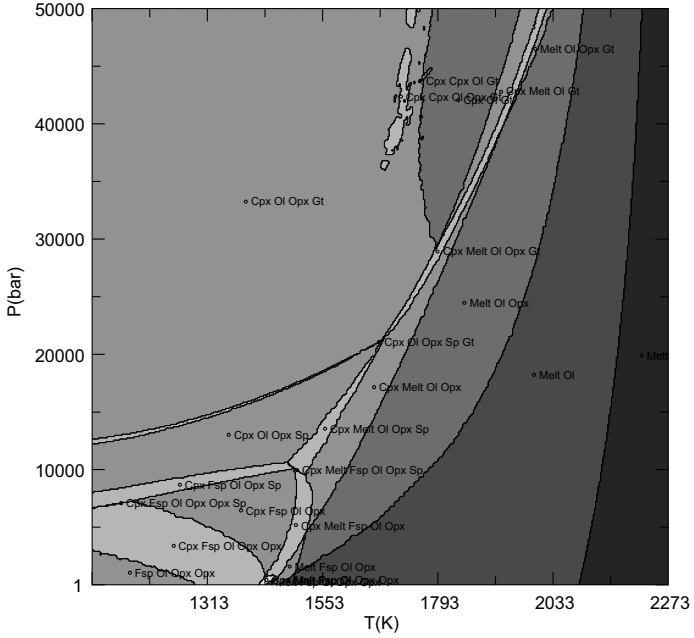
KLB-1 without Ti (problem definition file knoti.dat)



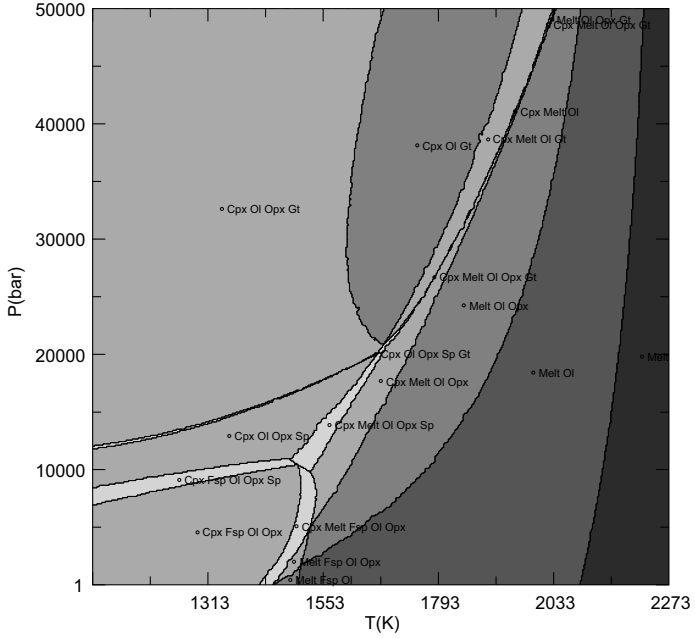
KLB-1 without Ti, K (problem definition file knotik.dat)



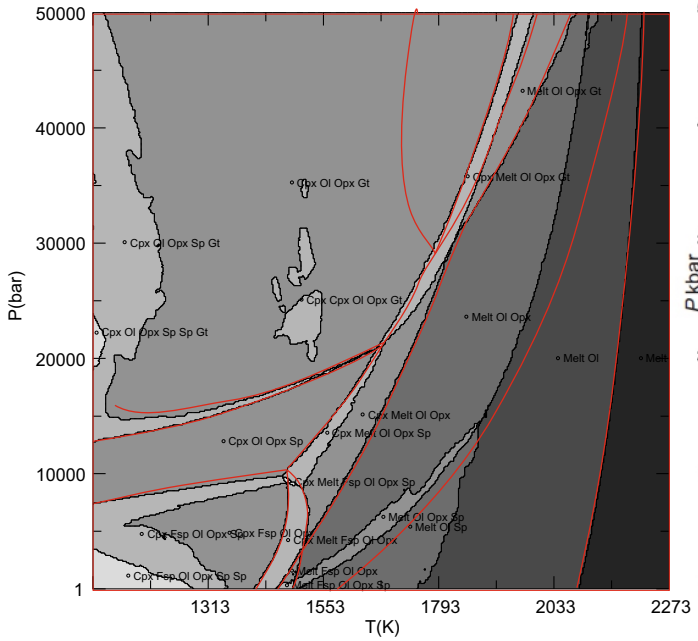
KLB-1 without Ti, K, Cr (problem definition file knotikcr.dat)



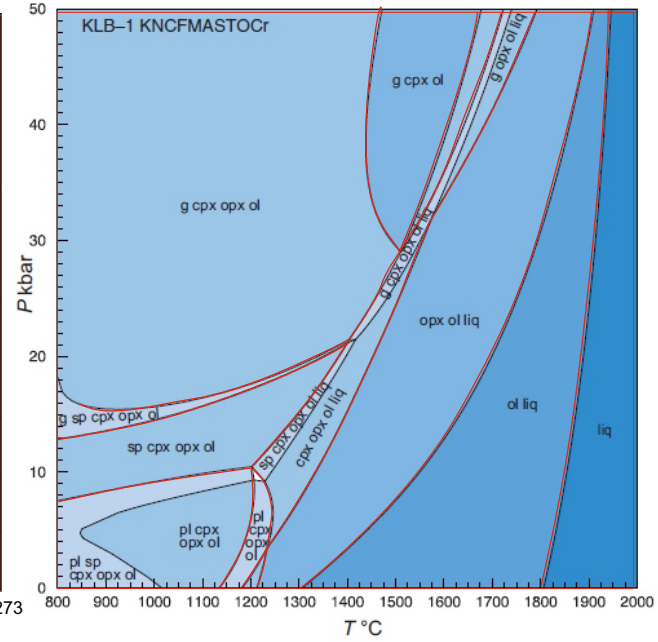
KLB-1 without Ti, K, Cr, excess O(problem definition file knotikcro.dat)



KLB-1: KHGP_hard_limits_II.dat



THERMOCALC, Holland, Green, and Powell (2018)



Although it is dubious practice, it is possible to force Perple_X to compute metastable phase relations by restricting the compositional range of a solution by setting the hard_limits option to “on”. It is bad practice, because in general the metastable phase relations obtained are dependent on the restrictions. In other words, it is necessary to know the phase relations that are to be predicted, before they are predicted. Two such calculations are depicted here:

khgp_hard_limits_II - (Ca+Na)/(Ca+Na+Mg+Fe2) (X(2,1) in the solution model) on the M2 site of Opx(HGP) is restricted to the range 0-0.3 and (K+Na+Ca)/(K+Na+Ca+Fe2+Mg) on the M2 site of Cpx(HGP) is restricted to the range 0.5-1. This calculation reproduces the plagioclase-lherzolite phase relations of the THERMOCALC result, lending some support to the conjecture that the absence of the chromite fields in the Holland et al. (2018) section is an oversight. The patchy 2-Cpx field is clearly resolution-dependent and almost certainly spurious. Likewise, the absence of the Grt+Cpx+Ol field at high pressure is clearly a consequence of the restriction in the range of Cpx composition.

khgp_hard_limits_III - to recover the Grt+Cpx+Ol field, this calculation was made with the same restriction on Opx as in kghp_hard_limits_II, but no restriction on the M2 site Cpx composition. Although this calculation does recover the Grt+Cpx+Ol it is clearly marred by, at least partially, spurious Cpx two-phase fields in which a dominant Ca-rich Cpx coexists with a minor Ca-poor Cpx. The pervasive occurence of 2-Cpx fields at low pressure and temperature suggests that they are entirely a numerical artifact (i.e., resolution dependent), this is consistent with the low-pressure RE-46 benchmark in which 2-Cpx fields are widespread and show no indication of resolution dependence.

KLB-1: KHGP_hard_limits_III.dat