

The published version of the KLB-1 phase diagram section (Fig 1., Holland et al., JPet, 2013) vs raw output from Perple_X 6.8.8 (computed with the klb-1_hhph.dat input file, compiled by Bob Myhill).

klb-1_hhph calculation: global_reach_increment = 1, initial_resolution = [1/16 1/24], x/y_nodes = [60 60], all other options default.

Computation time ~8 h.

A global_reach_increment of 1 was specified to reduce cosmetic flaws. Without global_reach_increment computation time is reduced by > 2 orders of magnitude (< 20 min). The reduction in initial_resolution from its default value (1/48) is necessary to prevent VERTEX from exhausting memory during the auto-refine stage of the calculation.

The absence of a stability field for the NAI phase in the Perple_X calculation is the only notable discrepancy. The absence of the NAI in the KLB-1 section is consistent with the MORB calculation (see morb_hhph_benchmark) which indicates the NAI phase is less stable in Perple_X than indicated in the original publication. This discrepancy is likely due to a change, or transcription error, in the NAI phase data. The similarity of phase boundaries irrespective of the presence of the NAI phase suggests that the NAI phase has no significant influence on bulk properties in the original calculation.

