

The published version of the KLB-1 phase diagram section (Fig 1, Jennings & Holland, JPet, 2015) vs raw output from Perple\_X 6.9.1 with the KLB-1\_JH.dat input file ([www.perplex.ethz.ch/perplex/examples/examples\\_JH\\_2015\\_klb-1\\_benchmark/](http://www.perplex.ethz.ch/perplex/examples/examples_JH_2015_klb-1_benchmark/) compiled by D. Bandyopadhyay) and all Perple\_X options set to **default** except:

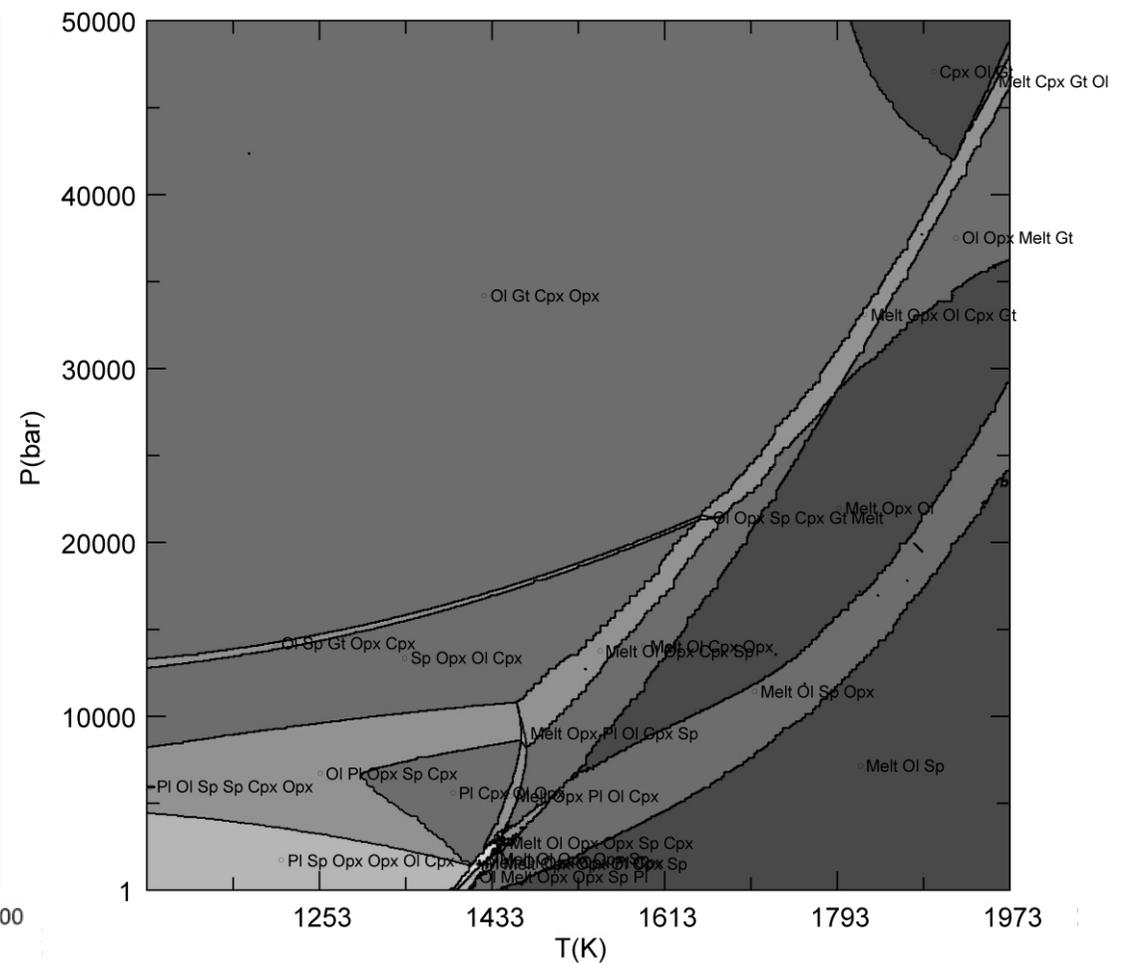
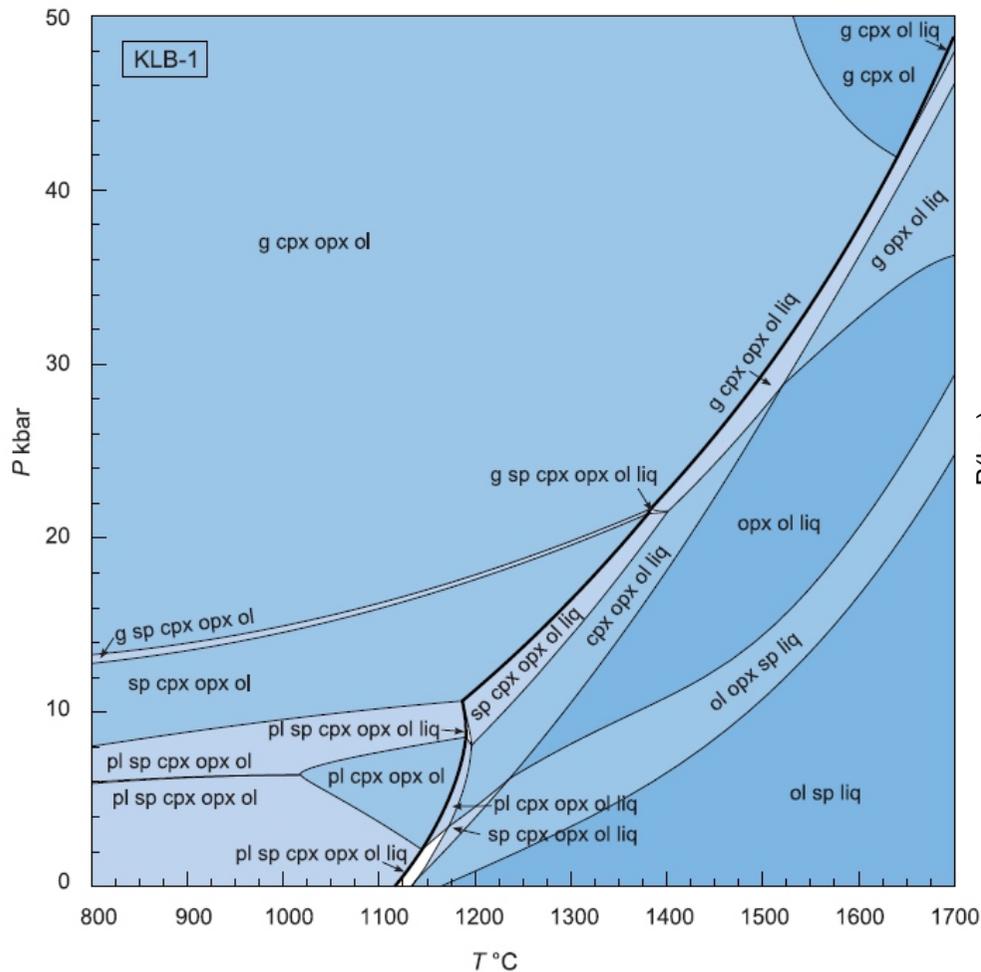
```

intermediate_savrpc T | default: [F]
intermediate_savdyn T | default: [F]
grid_levels          1 5 | default: [1 4]
x_nodes              10 60 | default: [10 40]
y_nodes              10 60 | default: [10 40]

```

Computation time ~24 minutes. When all options are set to **default** the result on the following page is obtained in ~4 minutes.

The discrepant low pressure, 2-Opx phase field in the Perple\_X result is thermodynamically correct as demonstrated by comparing the Gibbs energies computed with 6.9.0, which reproduces the published phase relations, and 6.9.1. Although thermodynamically correct, the 2-Opx phase field is petrologically implausible and caused by model calibration errors such as those recently corrected for the Holland et al. (JPet, 2018) models (Dec 5, 2020; Perple\_X update file).



Raw output from Perple\_X 6.9.1 with the KLB-1\_JH.dat input file and all Perple\_X options set to **default**

Computation time ~4 minutes.

The output shows two types of phase boundary roughness: roughness caused by Perple\_X's gridding strategy (e.g., the regions circled in cyan) and roughness caused by low optimization precision (e.g., the flaws circled in red). Roughness caused by the gridding strategy is step-like and occurs on the scale of the grid spacing (the `x/y_nodes` options) and its overtones (the `grid_levels` option), this type of roughness is minimized by specifying high auto-refine stage values for the `x/y_nodes` options. Roughness caused by low optimization precision is less regular than that caused by gridding and typically occurs on a larger scale. In the 6.9.1 version of Perple\_X, the easiest way to increase precision is to increase the number of compositions retained during optimization by setting `intermediate_savrpc` and `intermediate_savdyn` to T. If setting these options does not eliminate the problem then modifying `optimization_precision` (the absolute precision in energy/mole during successive LP optimization) and `replicate_threshold` (compositions separated from a refinement point composition by a Euclidean distance less than `replicate_threshold` are discarded) may help.

