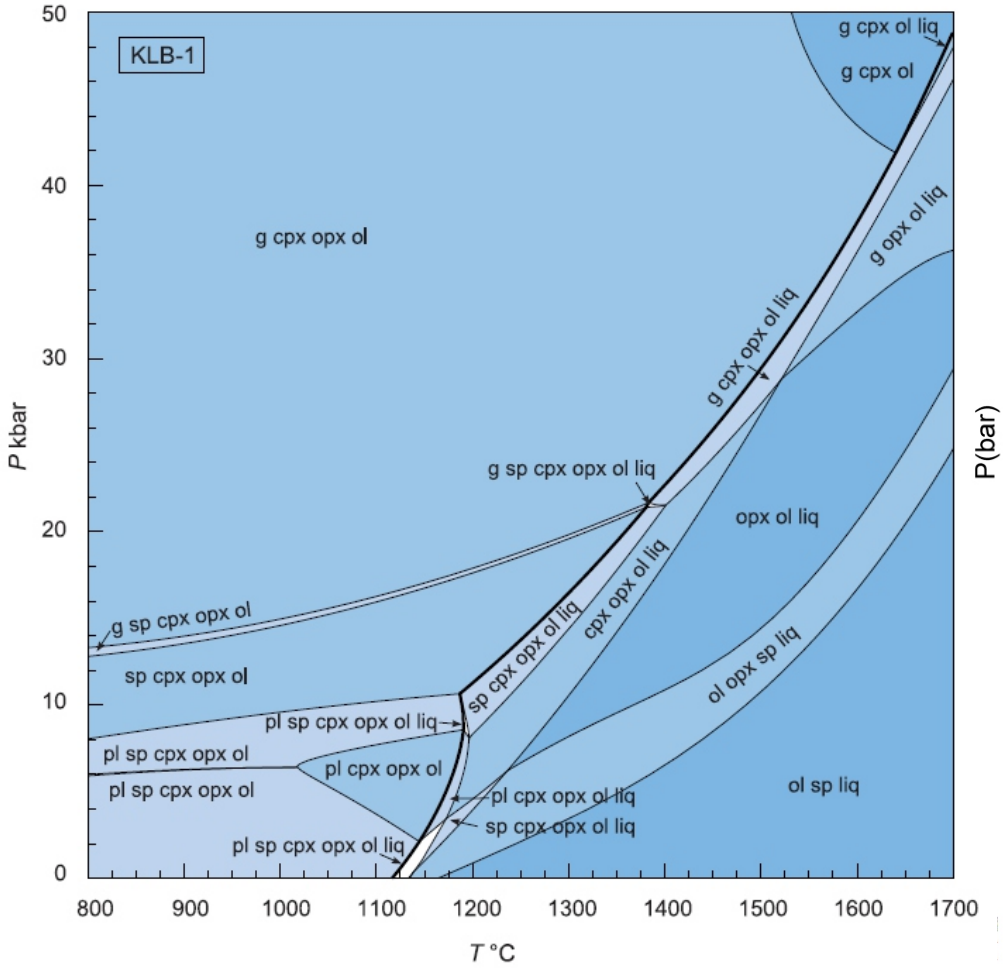
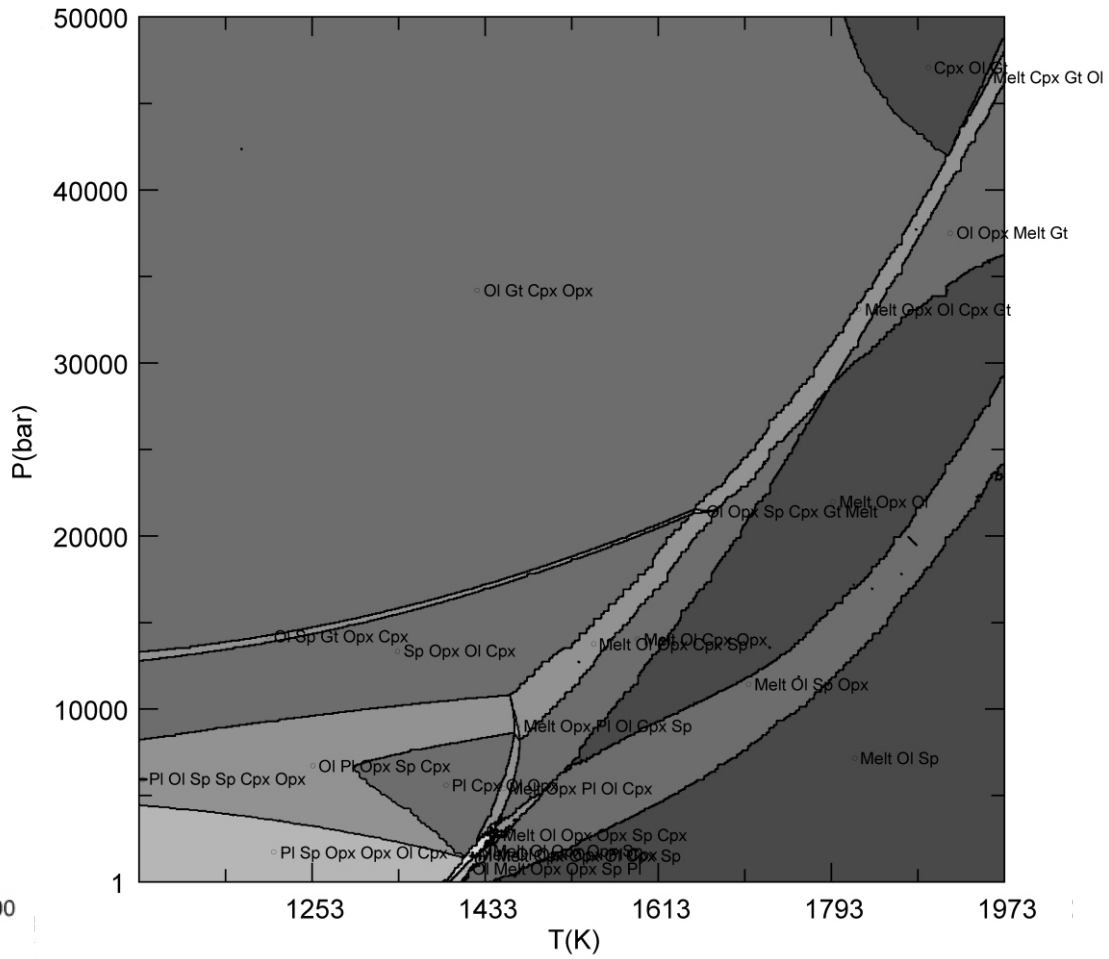
The published version of the KLB-1 phase diagram section (Fig 1, Jennings & Holland, JPet, 2015) vs raw output from Perple_X 6.9.1 with KLB-1_JH.dat (at www.perplex.ethz.ch/perplex/examples) and all Perple_X options set to **default** except:

```
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 computed from 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.