

Notes on HeFESTo

The purpose of HeFESTo is to determine self-consistently the equilibrium phase assemblage and physical properties of multi-component mantle systems. Much of the foundation is given in *Stixrude & Lithgow-Bertelloni* (2005,2011). Some applications are discussed in *Xu et al.* (2008) and *Stixrude & Lithgow-Bertelloni* (2012). When using HeFESTo, please cite *Stixrude & Lithgow-Bertelloni* (2005) or *Stixrude & Lithgow-Bertelloni* (2011), depending on the application, and, if separate, the paper specifying the parameter set used. *Stixrude & Lithgow-Bertelloni* (2021) specifies the latest published parameter set.

Briefly the code computes for a given pressure, temperature, and bulk composition, i) the stable phase assemblage, including the abundances and compositions of the phases coexisting in equilibrium ii) the physical properties of those phases iii) the physical properties of the multi-phase assemblage and iv) scaling of physical properties to seismological time scales. More details on capabilities are given in the specification of the input file below. Items marked (*) are capabilities that are still unpublished.

The input file is called:

control – specifies the bulk composition, range of conditions to be explored, and the set of mantle phases and species (end-members) to be included in the minimization.

There are many output files, including:

fort.56 – Physical properties of the assemblage

fort.66 – Relative amounts of phases

fort.99 – Relative amounts of species

Further details on the structure of these files are given below.

References

- Stixrude, L. and C. Lithgow-Bertelloni, Thermodynamics of mantle minerals: 1. Physical properties, *Geophysical Journal International*, 162, 610-632, doi: 10.1111/j.1365-246X.2005.02642.x , 2005.
- Stixrude, L. and C. Lithgow-Bertelloni, Thermodynamics of mantle minerals II, Phase equilibria, *Geophysical Journal International*, 184, 1180-1213, 2011.
- Stixrude, L. and C. Lithgow-Bertelloni, Geophysics of chemical heterogeneity in the mantle, *Annual Reviews of Earth and Planetary Sciences*, 40, 569-595, doi: 10.1146/annurev.earth.36.031207.124244, 2012.
- Stixrude, L. and C. Lithgow-Bertelloni, Thermal expansivity, heat capacity, and bulk modulus of the mantle, *Geophysical Journal International*, 228, 1119-1149, 2022.
- Xu, W., C. Lithgow-Bertelloni, L. Stixrude, and J. Ritsema, The effect of bulk composition and temperature on mantle seismic structure, *Earth and Planetary Science Letters*, 275, 70-79 doi:10.1016/j.epsl.2008.08.012, 2008.

Structure of control file.

- Line 1.

First pressure (or density) (P1), last pressure (or density) (P2), number of pressure intervals (nP), first temperature (or entropy) (T1), last temperature (or entropy) (T2), number of temperature intervals (nT), ensemble flag (iensem), super-adiabatic temperature (superad), frozen temperature (tfreeze).

Possible choices for the ensemble flag:

0: NPT ensemble. This is the standard

-1: read in a temperature profile from a file that must be called "ad.in" and which must contain columns: Pressure, Unused, Temperature. In this case, T1 and T2, are ignored and nT=0.

-2: NPS ensemble*. In this case, T1 and T2 are entropies in units of J/g/K.

-3: Hugoniot*. The code computes the Hugoniot, with the unshocked state given by the equilibrium assemblage at P1, T1. T2 is ignored and nT=0.

-4: NVT ensemble*. In this case P1 and P2 are volumes in units of cm³/g.

-5: NVS ensemble*. In this case T1 and T2 are entropies in units of J/g/K and P1 and P2 are volumes in units of cm³/g.

-6: Frozen equilibria*. The equilibria computed at P1 and T1 are unchanged for the remainder of the pressure, temperature calculations.

- Line 2.

Number of components, c. Further entries are not used.

- Line 3.

Specifies that all components are oxides. Should not be changed.

- Lines 4 to 4+c-1.

Name of component, first amount of component, last amount of component, number of intervals. Note that the number of intervals should be the same for all components.

Name of component is specified by the chemical symbol of the cation.

Amounts are specified in mole fraction of the oxide on a single cation basis (e.g. SiO₂, AlO_{1.5})

- Line 4+c

Level of theory (normally only for testing): ityp, ivtyp, ittyp, iltyp

Entries should be:

1,1,1,2 (for parameter set inv251010 and earlier)

1,1,1,1 (for later parameter sets)

ityp .eq. 1: Volume dependence of VDOS: full theory quadratic in theta

ityp .eq. 2: Volume dependence of VDOS: Full theory linear in theta

ityp .eq. 3: Volume dependence of VDOS: q=constant

ivtyp .eq. 1: Volume dependence of G: Full expansion

ivtyp .eq. 2: Volume dependence of G: Truncated expansion

ityp .eq. 1: Temperature dependence of G: Full theory

ityp .eq. 2: Temperature dependence of G: eta prop. V

ityp .eq. 3: Temperature dependence of G: eta constant

ityp .eq. 4: Temperature dependence of G: eta prop. Gq

iltyp .eq. 1: New Landau theory, post SLB11*

iltyp .eq. 2: Landau theory as in SLB11

- Line 4+c+1

Absolute path to the directory containing the parameter files

- Line 4+c+2

Number of end-member species

- Remaining lines

These specify the phases to be included; a code to indicate whether they are present (1) or not (0) in the initial guess; and the names of the end-member species to be included for that phase. Note that the initial guess must span the bulk composition. Names of phases and species must match the names of the corresponding parameter files.

Structure of fort.56

Pressure (GPa), Depth (km), Temperature (K), Density (g/cm^3), Bulk sound Velocity (km/s), Shear wave velocity (VS) (km/s), Longitudinal wave velocity (VP) (km/s), VS modified by attenuation (km/s), VP modified by attenuation (km/s), Enthalpy (kJ/g), Entropy (J/g/K), thermal expansivity (10^{-5} K^{-1}), isobaric heat capacity (J/g/K), isothermal bulk modulus (GPa), Shear attenuation (QS), Longitudinal attenuation (QP), Quenched density (g/cm^3), most abundant phase.

Note. The thermal expansivity, isobaric heat capacity, and isothermal bulk modulus include metamorphic contributions*. The wave velocities do not include metamorphic contributions.