HyMaTZ: Hydrous Mantle Transition Zone

MANUAL (version 2.1, 09.06.2017)

A graphical Python program for calculating seismic velocities in the mantle transition zone as a function of water content

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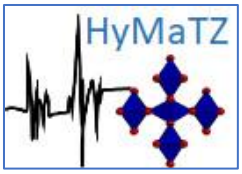
Overview

HyMaTZ is a program that calculates and displays seismic velocities in the transition zone of the Earth's mantle. After choosing a compositional model to work with (e.g. pyrolite, harzburgite, mixtures or layers), the user can examine the influence of water by applying experimental or theoretical constraints on how water influences the elastic moduli of Mg_2SiO_4 polymorphs. The user can also specify a user-preferred water content versus depth profile using a percentage of the maximum storage capacity, or as a customized profile. The output of HyMaTZ (V_p, V_s, *dlnV/dP*, etc. versus depth) are shown and can be compared with the corresponding outputs from global or regional seismic models. HyMaTZ contains the thermodynamic datasets for a number of compositional models as readable data files already calculated using Perple_X [*Connolly*, 2005] with the formalism and database of *Stixrude and Lithgow-Bertelloni* [2011]. Alternatively, the user can also use a user-preferred thermodynamic dataset. A disclaimer must be made here that in the present software version, water is not included as a chemical component in the calculation of the thermodynamic phase diagrams; its effect is only on the thermoelastic properties of the hydrous Mg_2SiO_4 polymorphs. HyMaTZ is meant as a direct visualization tool for understanding the change in the physics due to water incorporation in the nominally anhydrous minerals, but all the data/output can also be exported for producing customized graphs by the user.

Installation

HyMaTZ is a Python script with the following dependencies:
Python version 2.7 or 3.5 :: PyQt4 or PyQt5 :: matplotlib :: numpy :: scipy :: zipfile

The program is downloaded in .zip format to be extracted onto the user's computer. To launch the program, run Main.py. The sub-directory "Models" contains the data for the different compositional models. The Models directory is therefore very large (~0.7 Gb after zipping), but it is a static component of HyMaTZ that can be copied into the directory of future versions so that there would be only one "Models" folder on the computer. The current tester's version of HyMaTZ (2.1) can be downloaded by clicking on the following icon (Northwestern Box Link), and, in the near future, can also be download from GitHub.



Usage

Warning: First save work and results that you want to keep before running this program. This program uses a graphical user interface (GUI) as a convenient way to rapidly examine how changes in the thermodynamic variables and elastic physical properties affect the seismic velocities. Bringing up the GUI might kill the console kernel, so all the objects in the current namespace will be lost. At the conclusion of this program, when the GUI is closed, the Python console might restart (some IDEs need you to do a manual restart). The use of the GUI may lead to a warning message from the Python interpreter. This can be ignored as the GUI will work regardless as will the restarted Python shell.

Executing Main.py brings up the following screen. Note: On some screen settings, the GUI that first appears may be drawn too low such that the "Plot Update" button cannot be seen. If you do not see a "Plot Update" button at the bottom left of the GUI, use the mouse to drag the GUI slightly upwards until the "Plot Update" button appears or click the Maximize button on the top right.

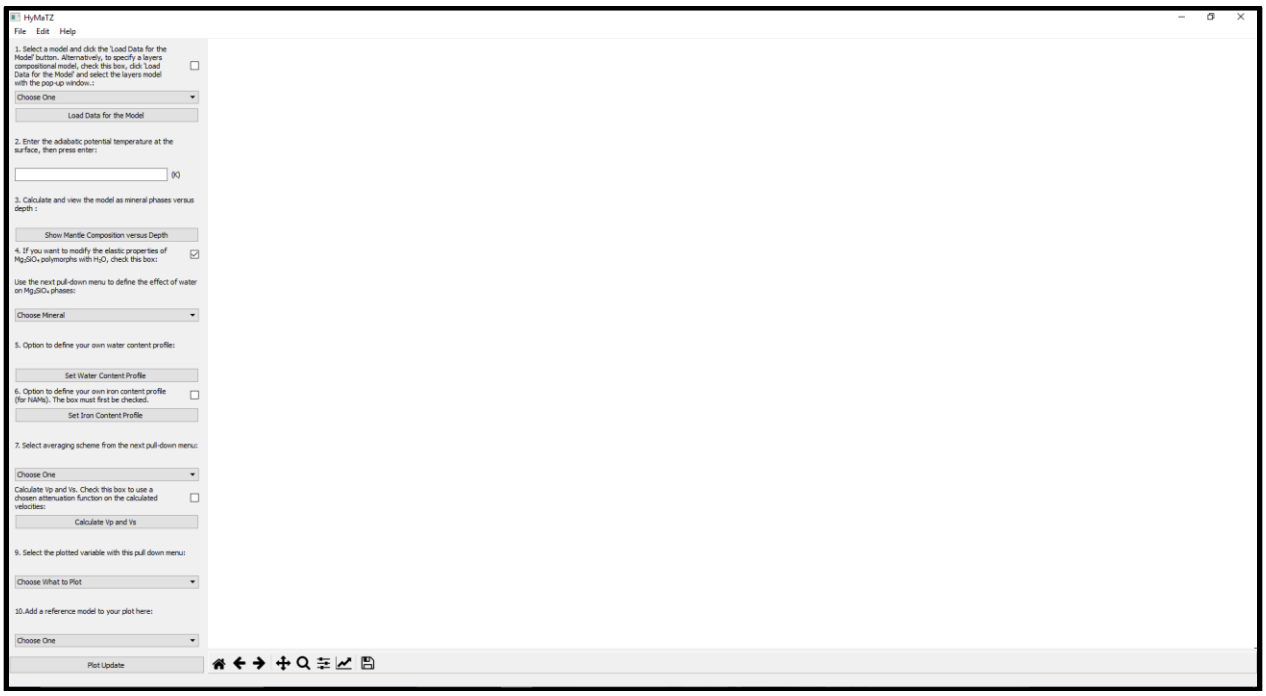


Figure 1. Interface to HyMaTZ. This window shows the state of the program upon launching.

Notice how the left-hand column of the program window appears as a set of instructions. The blank white space on the right will be used for plots. The flow-through can be summarized as a series of steps, numbered 1-10, as shown on the left side of the HyMaTZ window:

1) Select a model composition
2) Enter the adiabatic foot temperature (surface reference) and press enter
3) Display phase proportions
4) Modify elastic properties of hydrous Mg_2SiO_4 phases
5) Define water content profile
6) Define iron content profile (Option)
7) Select averaging scheme
8) Calculate V_p and V_s
9) Plot results
10) Compare results with reference models

1. Select mantle composition (can also be a mixture or a stratified model)

The compositional models were calculated using the Perple_X software, which is a collection of Fortran programs for calculating phase diagrams and phase equilibria. More information on it can be found on the Perple_X website http://www.perplex.ethz.ch. A number of pre-calculated compositional models, obtained using Perple_X, are contained in the program. These models implement numerous versions of pyrolite from various authors, harzburgite, basalt, and an example of piclogite. The user can also elect to describe the mantle as a "mechanical mixture", which uses the specification of different proportions of any two different models as the composition of the mantle. The idea for this model is due to [*Xu et al.*, 2008]. To choose this option, the user selects "Mechanical Mixture" from the pulldown button in Step 1. Figure 2 shows an example of how to define a mechanical mixture.

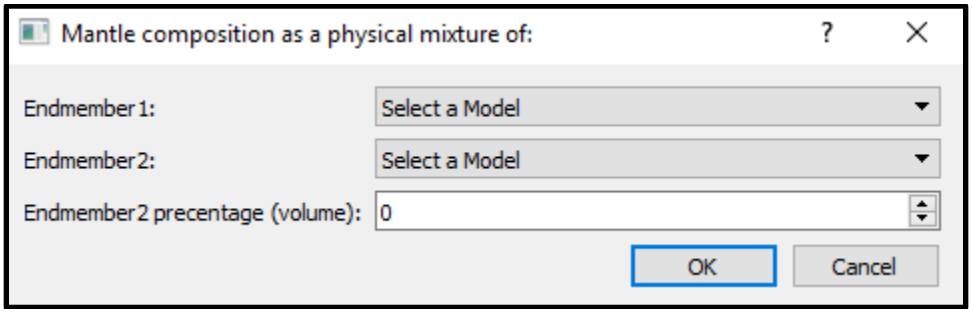


Figure 2. Mechanical mixture window used to set the two different models, which will form the mechanical mixture that models the mantle.

Additionally, there is an option to use a user-defined model using the output from Perple_X saved in the program. This provides a function to transfer Perple_X output to a txt file which HyMaTZ will use as the data file of the user-defined model. In using this option input, the user has to make sure that the Perple_X calculation follows the instructions given on the Perple_X website (http://www.perplex.ethz.ch/perplex_66_example_24.html). The only exception is that the user can include Na_2O as a thermodynamics component and also include Gt-mgj in a solution model.

Alternatively, the user can also define a "layer model" in which the user would define layers of different thickness in the model, and each layer can have a different composition. At the

moment, HyMaTZ supports up to six different layers. To use this function, the user has to first check the box in Step 1 and click the "Load Data …" button. Figure 3 shows an example of how to define the layers.

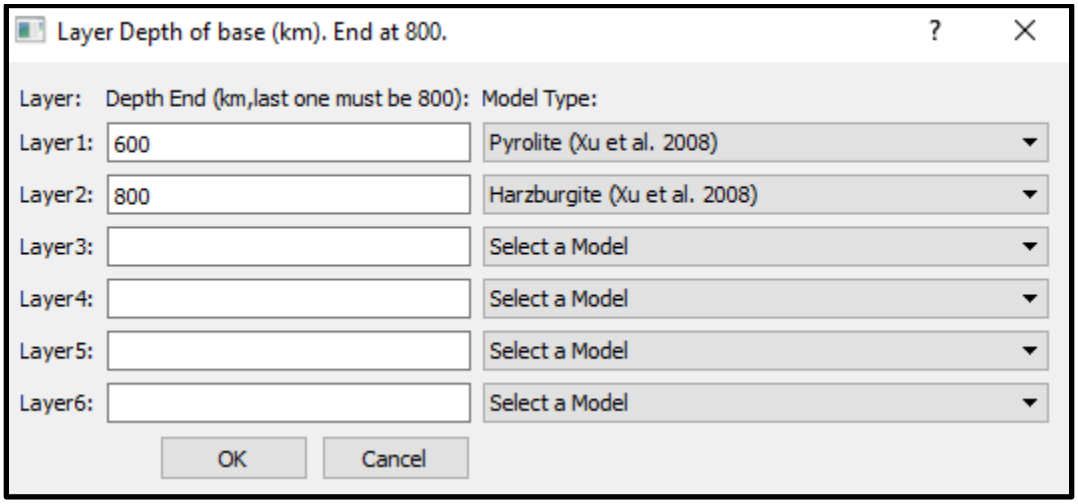


Figure 3. Layers control window used to set the composition of the different layers. The first layer starts at depth 0 and has a thickness in km that is the number that the user inputs. Each layer has a thickness in km that is the difference between the number input at that layer and the previous layer. The last utilized layer MUST end at the depth of 800 km. The right hand side is used to choose the composition of the layer.

After choosing a compositional model to work with, click the "Load Data for the Model" button. It will take a few seconds to load. So, what exactly are you loading here? The model specifies the minerals present in the mantle and the loaded data are their phase proportions, calculated by Perple_X, at the grid points defined by steps of 0.05 GPa and 5 K in P-T spaces for the range of pressures and temperatures from 0-30 GPa and 773-2773 K. This is why the Models are large, but, having all the phase proportion data available in HyMaTZ allows the user to select any isentropic temperature profile to work with, which is the next step.

2. Select an isentropic

Enter the foot (or reference) temperature in degrees K at the Earth's surface (at the bottom of the crust) to define an isentropic mantle temperature profile for the 10-800 km depth region, then press Enter. The temperature profile is then calculated, which is done by extracting the information already calculated and saved from Perple_X and using the requirement that the nodes of the profile have the same entropy.

3. Display the phase proportions of the chosen model

After you have chosen the foot temperature, then click the "Show Mantle Composition versus Depth" button to see the phase diagram of your model. A confirmation window will appear, e.g. "You are using the pyrolite model"; to agree to use this, just confirm. The details of the model given as the bulk composition in mol% and wt%, the literature reference of this model, and the

foot temperature are shown on the status bar at the very bottom of the window (Note: This information are not shown if the user is using the layers model).

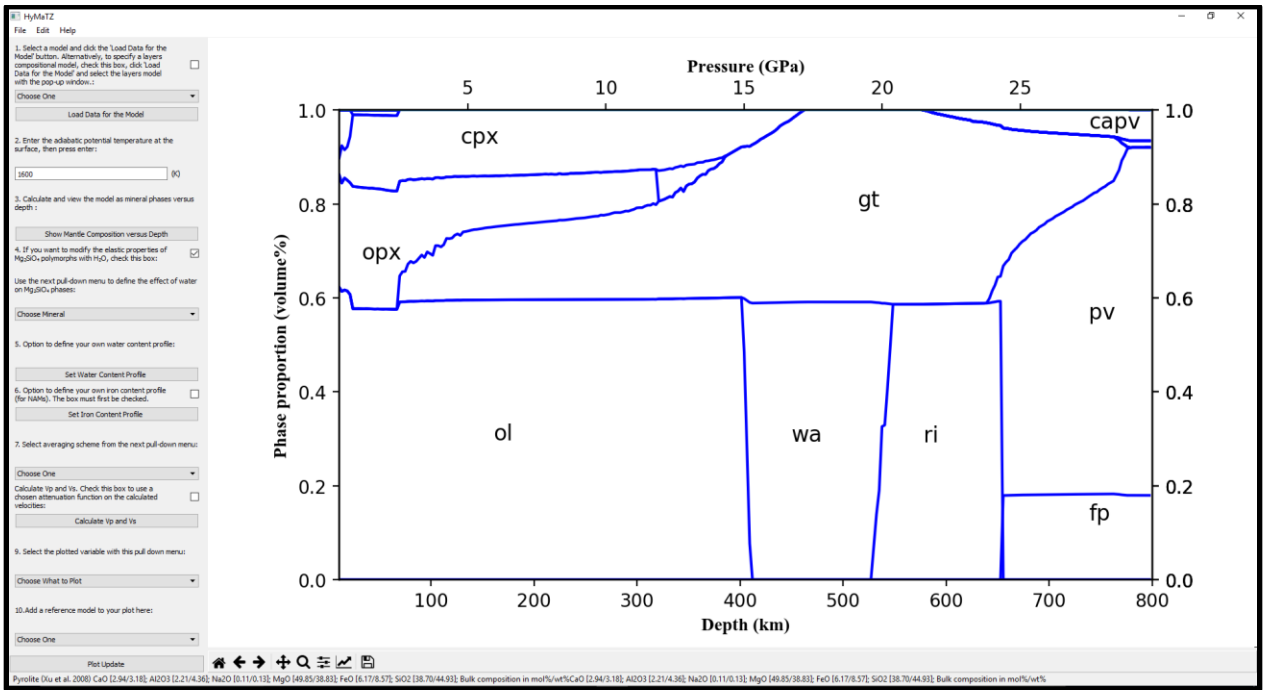


Figure 4. A display of the phase proportions of the minerals for a chosen model (pyrolite after *Xu et al.* [2008]) and foot temperature. The bulk composition is displayed at the very bottom in both weight percent and mole percent.

4. Modify the elastic properties of the hydrous Mg_2SiO_4 phases

HyMaTZ allows the user to choose the effects of the water and iron contents on the elastic properties of the nominally anhydrous Mg_2SiO_4 phases (olivine, ringwoodite, and wadsleyite). To do this, check the box provided in Step 4 of the GUI. The default is to have the box checked. If you want to remove the effects of water and iron, then simply uncheck the box and the thermoelastic properties used by Perple_X will be used for the elastic properties of Mg_2SiO_4 phases.

Use the pull-down menu labeled “Choose Mineral” to pick one of the phases and to see how the elastic properties are modified by the H_2O content in the default case, which uses an equation obtained by regression analysis to experimental data. In the current example, we will select olivine.

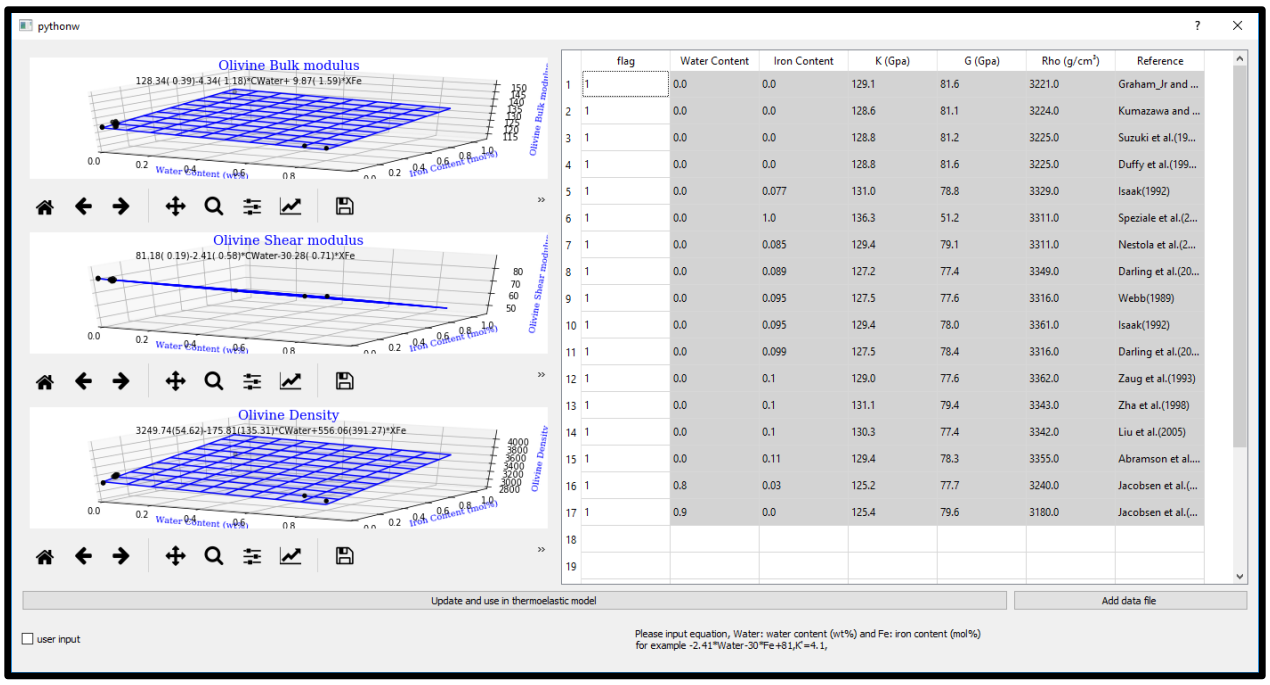


Figure 5. Regression window used to modify the properties of hydrous Mg_2SiO_4 phases from experimental data.

This window shows the elastic properties of the chosen mineral phase obtained by regression analysis using experimental results reported in the literature. A compilation of existing data as of June 2017 is saved in the program and shown on the Table on the right. The user can select which references to use in the regression analysis by using the flag in the first column of the data table. A value of 1 indicates the data point will be used in the regression analysis and a value of 0 indicates the data point will not be used. The user can also add new data by clicking on the "Add data file" button and typing the new values into the text file. Click the save button and close the window to update.

Note: These datasets are available in the folder HyMaTZ\Mineral_Physics\EXPDATA (see e.g. Olivine.txt).

A planar relationship is used to express the density, bulk modulus, and shear modulus as a function of water content and iron content. The fitted regression equation is displayed at the top of each plot, where the water content is given in wt% H_2O, and the iron content is given as X_{Fe} = Fe/(Fe+Mg). Note: Although the effect of Fe content is being modified, the amount of iron in all the phases (partitioning) are from the Perple_X output, or are specified by the user (see below).

The program also gives you the option to use your own function to define how water and iron contents determine the density, bulk modulus, and shear modulus. To do this, at the bottom of the current window (Figure 5), check the box "User Input". In the pop-up edit boxes, you can enter your own equation for the functional dependence on water and iron contents, along with the values for the pressure derivative of K and G, so if you just want to play with K_0' and G_0', you

can do so here. The default is to use the fitted regression equations obtained by fitting to the experimental data and K_0' and G_0' values from *Stixrude and Lithgow-Bertelloni* [2011].

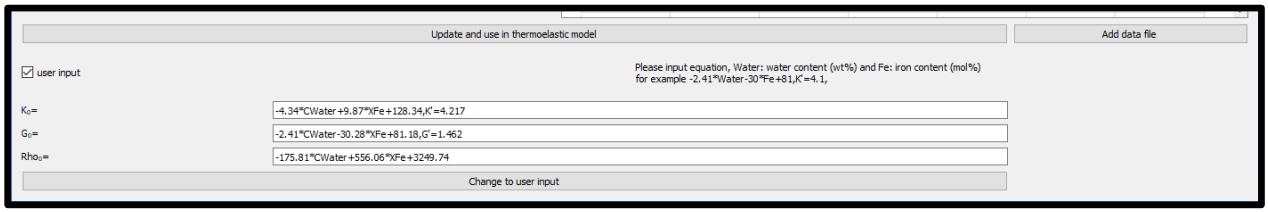
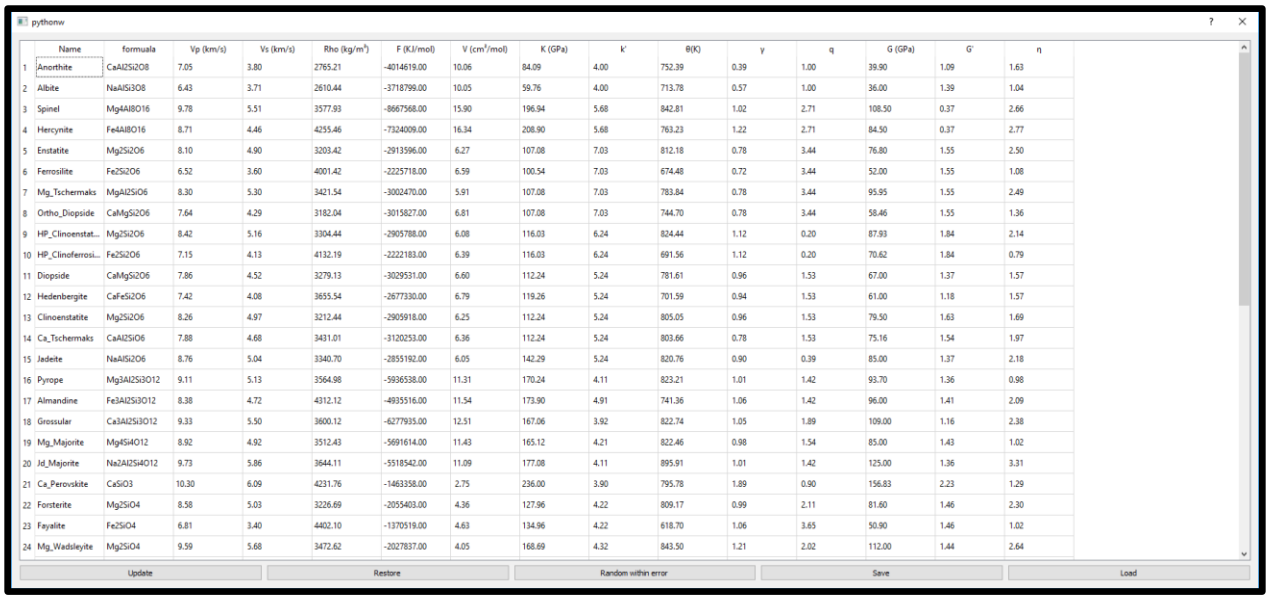


Figure 6. View of the "User Input" Window for changing the equations that determine the density, *K*, and *G* as functions of the water and iron contents. The default entries are the equations from the regression analysis of the selected experimental data. Here, at the end of the line, you can also use your K_0' and G_0' values.

Modify other elastic properties:

You can also view or change any of the thermoelastic data for any mineral by bringing up the thermodynamic database that was used by Perple_X to calculate the phase proportions. To do so, go to the menu item, Edit -> View/Modify Thermodynamic Data:



	Name	formuala	Vp (km/s)	Vs (km/s)	Rho (kg/m³)	F (KJ/mol)	V (cm³/mol)	K (GPa)	k'	θ(K)	γ	q	G (GPa)	G'	η
1	Anorthite	CaAl2Si2O8	7.05	3.80	2765.21	-4014619.00	10.06	84.09	4.00	752.39	0.39	1.00	39.90	1.09	1.63
2	Albite	NaAlSi3O8	6.43	3.71	2610.44	-3718799.00	10.05	59.76	4.00	713.78	0.57	1.00	36.00	1.39	1.04
3	Spinel	Mg4Al8O16	9.78	5.51	3577.93	-8667568.00	15.90	196.94	5.68	842.81	1.02	2.71	108.50	0.37	2.66
4	Hercynite	Fe4Al8O16	8.71	4.46	4255.46	-7324009.00	16.34	208.90	5.68	763.23	1.22	2.71	84.50	0.37	2.77
5	Enstatite	Mg2Si2O6	8.10	4.90	3203.42	-2913596.00	6.27	107.08	7.03	812.18	0.78	3.44	76.80	1.55	2.50
6	Ferrosilite	Fe2Si2O6	6.52	3.60	4001.42	-2225718.00	6.59	100.54	7.03	674.48	0.72	3.44	52.00	1.55	1.08
7	Mg_Tschermaks	MgAl2SiO6	8.30	5.30	3421.54	-3002470.00	5.91	107.08	7.03	783.84	0.78	3.44	95.95	1.55	2.49
8	Ortho_Diopside	CaMgSi2O6	7.64	4.29	3182.04	-3015827.00	6.81	107.08	7.03	744.70	0.78	3.44	58.46	1.55	1.36
9	HP_Clinoenstat...	Mg2Si2O6	8.42	5.16	3304.44	-2905788.00	6.08	116.03	6.24	824.44	1.12	0.20	87.93	1.84	2.14
10	HP_Clinoferrosi...	Fe2Si2O6	7.15	4.13	4132.19	-2222183.00	6.39	116.03	6.24	691.56	1.12	0.20	70.62	1.84	0.79
11	Diopside	CaMgSi2O6	7.86	4.52	3279.13	-3029531.00	6.60	112.24	5.24	781.61	0.96	1.53	67.00	1.37	1.57
12	Hedenbergite	CaFeSi2O6	7.42	4.08	3655.54	-2677330.00	6.79	119.26	5.24	701.59	0.94	1.53	61.00	1.18	1.57
13	Clinoenstatite	Mg2Si2O6	8.26	4.97	3212.44	-2905918.00	6.25	112.24	5.24	805.05	0.96	1.53	79.50	1.63	1.69
14	Ca_Tschermaks	CaAl2SiO6	7.88	4.68	3431.01	-3120253.00	6.36	112.24	5.24	803.66	0.78	1.53	75.16	1.54	1.97
15	Jadeite	NaAlSi2O6	8.76	5.04	3340.70	-2855192.00	6.05	142.29	5.24	820.76	0.90	0.39	85.00	1.37	2.18
16	Pyrope	Mg3Al2Si3O12	9.11	5.13	3564.98	-5936538.00	11.31	170.24	4.11	823.21	1.01	1.42	93.70	1.36	0.98
17	Almandine	Fe3Al2Si3O12	8.38	4.72	4312.12	-4935516.00	11.54	173.90	4.91	741.36	1.06	1.42	96.00	1.41	2.09
18	Grossular	Ca3Al2Si3O12	9.33	5.50	3600.12	-6277935.00	12.51	167.06	3.92	822.74	1.05	1.89	109.00	1.16	2.38
19	Mg_Majorite	Mg4Si4O12	8.92	4.92	3512.43	-5691614.00	11.43	165.12	4.21	822.46	0.98	1.54	85.00	1.43	1.02
20	Jd_Majorite	Na2Al2Si4O12	9.73	5.86	3644.11	-5518542.00	11.09	177.08	4.11	895.91	1.01	1.42	125.00	1.36	3.31
21	Ca_Perovskite	CaSiO3	10.30	6.09	4231.76	-1463358.00	2.75	236.00	3.90	795.78	1.89	0.90	156.83	2.23	1.29
22	Forsterite	Mg2SiO4	8.58	5.03	3226.69	-2055403.00	4.36	127.96	4.22	809.17	0.99	2.11	81.60	1.46	2.30
23	Fayalite	Fe2SiO4	6.81	3.40	4402.10	-1370519.00	4.63	134.96	4.22	618.70	1.06	3.65	50.90	1.46	1.02
24	Mg_Wadsleyite	Mg2SiO4	9.59	5.68	3472.62	-2027837.00	4.05	168.69	4.32	843.50	1.21	2.02	112.00	1.44	2.64

Figure 7. View of the thermodynamic dataset from *Stixrude and Lithgow-Bertelloni* [2011] used to calculate the phase proportions, isentropic temperature, and seismic velocities. Note: If you choose to modify a parameter such as K_0 or K_0', it will affect the calculated velocity and density in Step 7, but it will not affect the phase proportion model, which has already been calculated in Step 3 and is immutable once the temperature and model are set. The buttons along the bottom of the current window function like this:

'Update' – click this button to apply changes to the thermoelastic data
'Restore' – restores parameters to original Perple_X output

‘Random within error’ – generate random values for all parameters within 1σ.
‘Save’ – save thermoelastic data to an ASCII text file
‘Load’ – load thermoelastic data from an ASCII text file into the data table.

4. Define the water content profile

HyMaTZ allows the user to define a water content profile in the mantle. Clicking on the “Set water content profile” brings up the following window.

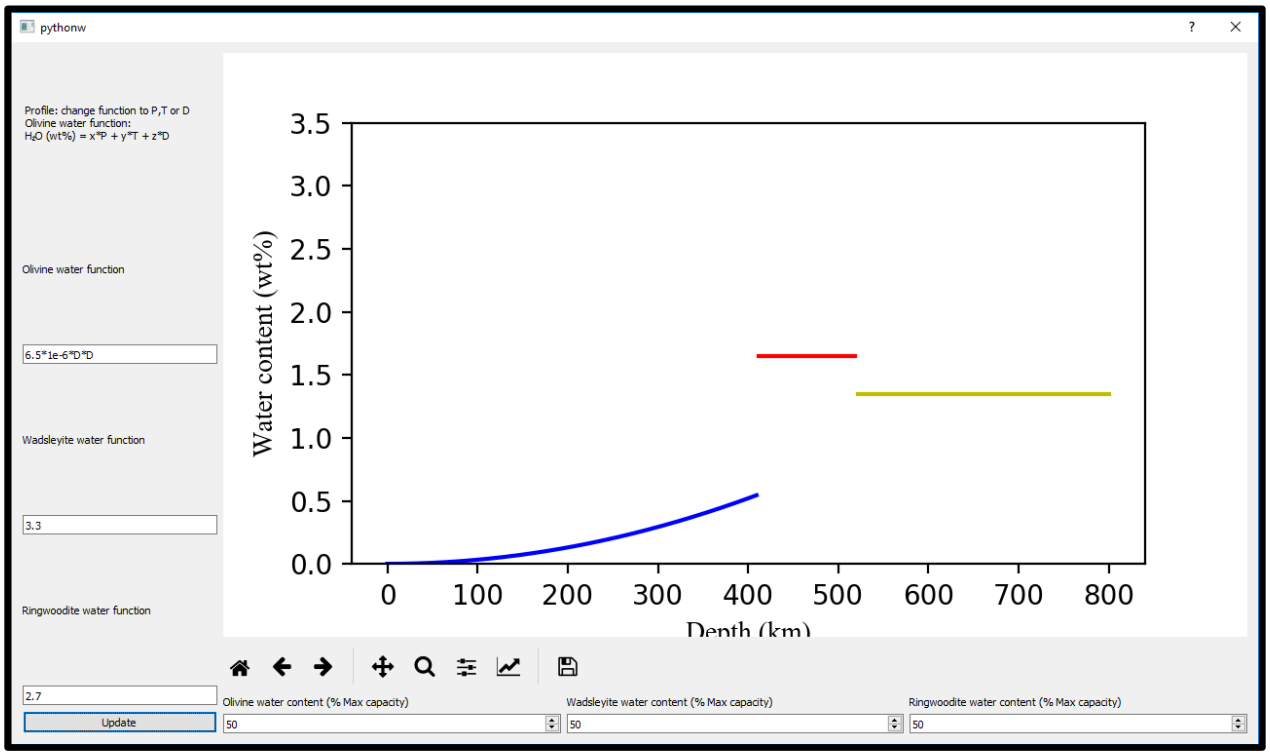


Figure 8. Water content profile window, with 50% of storage capacity for all phases selected.

The maximum storage capacity for wadsleyite is set to 3.3 wt%, and the partition coefficients of 6:30:15 for olivine:wadsleyite:ringwoodite from *Inoue et al.* [2010] are used to distribute the water content at 410 km and 520 km. The water content of wadsleyite and ringwoodite are constant versus depth, whereas the increase in water content of olivine with depth is defined by the curve given in *Hauri et al.* [2006]. In addition to simply specifying the percent of maximum storage capacity for each phase, one can also modify the water profile as a function of depth using a polynomial function on the left side bar. A single number, as shown by the example of 3.3 wt% H_2O for wadsleyite, produces a constant function. These functions can be edited by the user to define a user-preferred water content profile. The text in the upper left of the window shows an example of how to define the water content as a function of pressure (P) and temperature (T) or as a function of depth (D). The bottom panel allows the user to input the water content as a percent of the maximum capacity for each of the Mg_2SiO_4 minerals. After the user has defined the water content profile, click ‘Update’ and close the window.

5. Define the iron content profile

HyMaTZ allows the user to define an iron content profile for the mantle as the Fo number of olivine and its high-pressure polymorphs. Clicking on the "Set iron content profile" brings up the following window (first check the box in Step 6; the default setting is false):

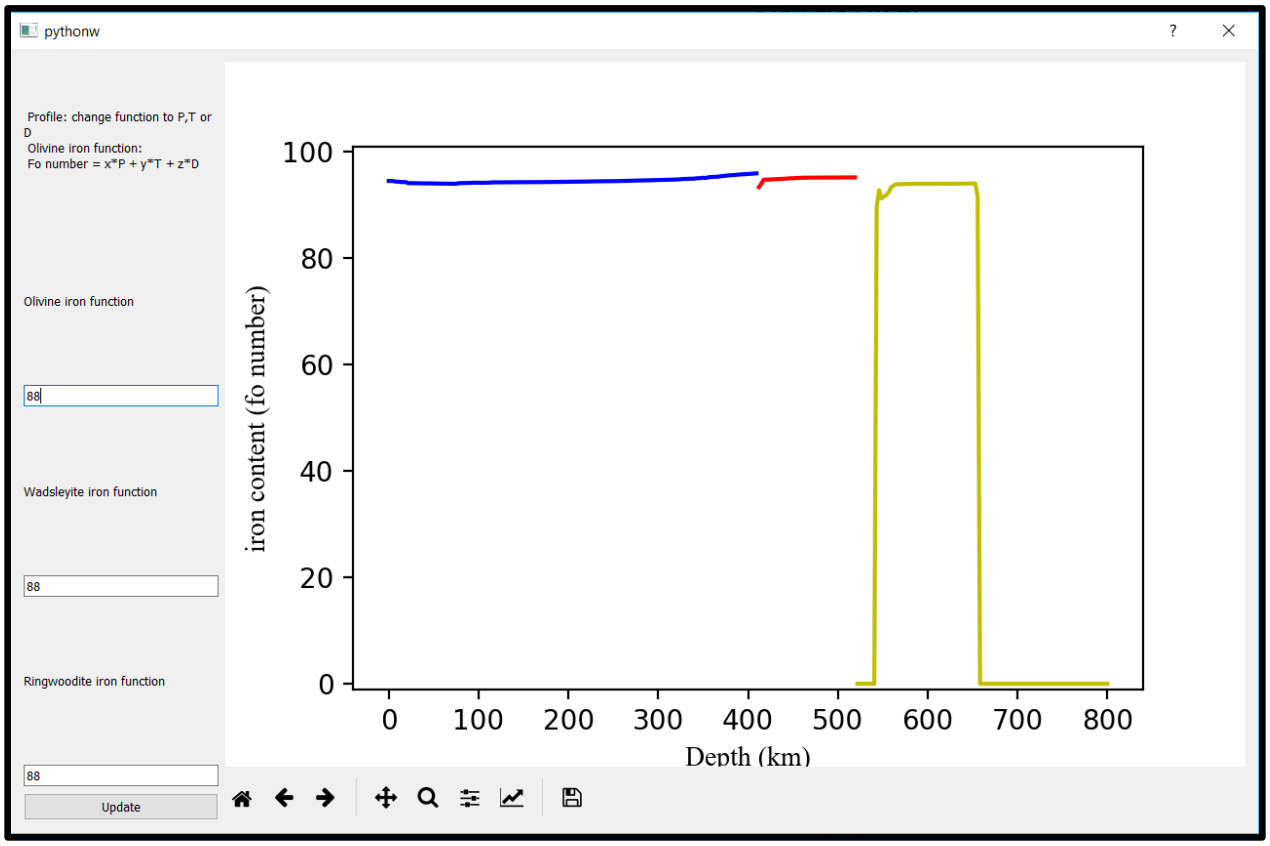


Figure 9. Iron content profile window. The default Fo number is that calculated by Perple_X.

These functions can be edited by the user to define a user-preferred Fo number profile. The text in the upper left of the window shows an example of how to define the iron content as a function of pressure (*P*) and temperature (*T*) or as a function of depth (*D*). After the user has defined the iron content profile, click 'Update' and close the window.

6. Select an averaging scheme

HyMaTZ allows the user to choose from a number of well-known averaging schemes for determining the bulk rock properties from an aggregate of individual minerals; for details, see *Cottaar et al.* [2014] and the references therein. Simply click on the pull-down menu and choose the appropriate averaging scheme. The authors recommend Voigt-Reuss-Hill as a first pass.

7. Calculate V_p and V_s

Once all the inputs are set, click "Calculate V_p and V_s" and the velocity profiles will be calculated based on the chosen input elastic data parameters. Here, we also provide a function to provide attenuation of the calculated seismic velocities. To choose an attenuation function, check the box in Step 8.

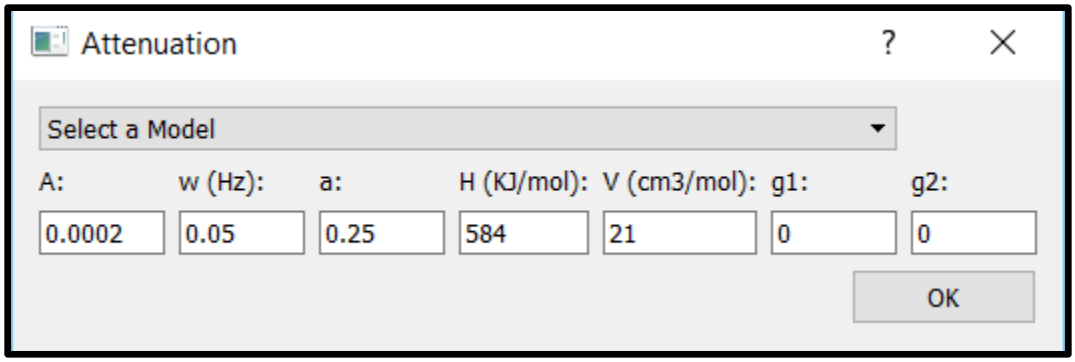


Figure 10. View of the "Attenuation" Window for choosing a modifying attenuation function. The available models are from *Goes et al.* [2000] and *Cammarano et al.* [2003].

8. Plot results

HyMaTZ plots the calculated results, e.g., seismic velocities, on top of the phase diagram. Use the pull down menu to select the quantity of interest, which can be V_p, V_s, temperature, bulk modulus, shear modulus, and density as well as the others, to be displayed on the diagram. After the item to be plotted is selected, click the "Plot update" button at the bottom of the window to display it. To begin anew with a clean plot, choose the "Clean" option and click "Plot update". An example plot is shown below.

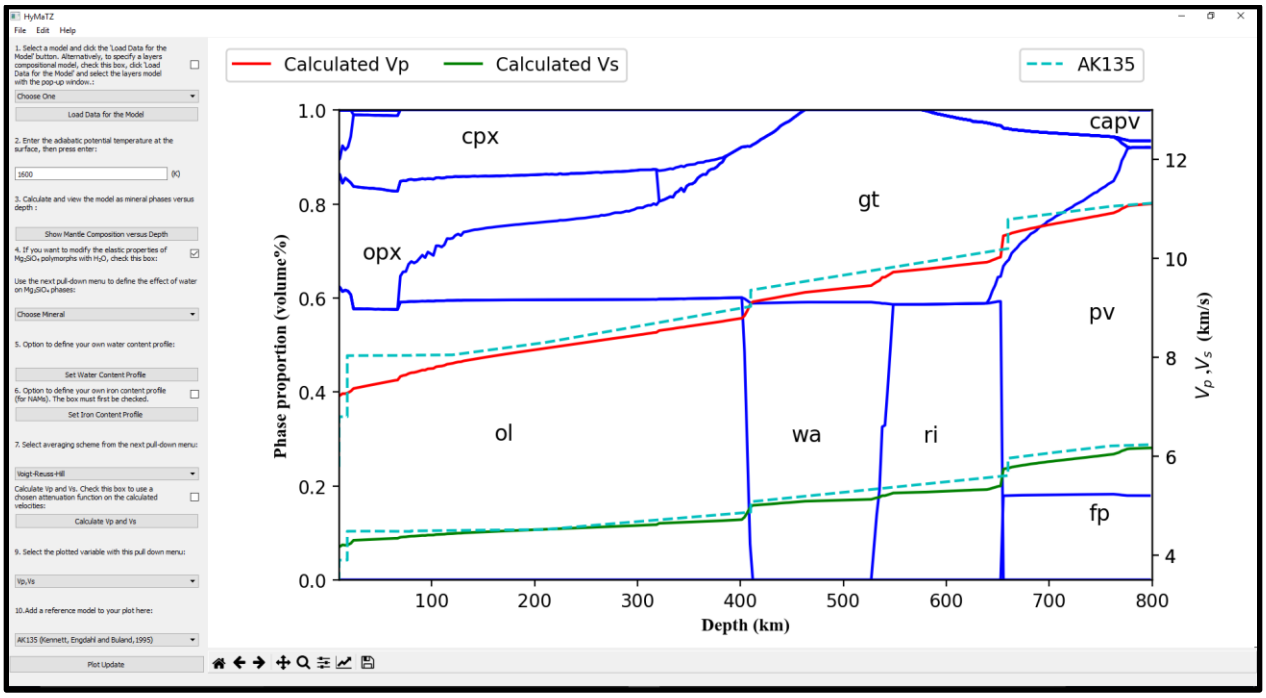


Figure 11. Final plot showing phase proportions, and our calculated velocities and the calculated velocities from the chosen reference model.

9. Compare with reference models

HyMaTZ contains a number of pre-loaded reference models with calculated results from published seismic models, including IASP91, AK135, PREM, and PEM-C, that can be compared with the calculated results from this program with the chosen mineralogical model. However, these reference models do not contain many of the physical properties used in the mineralogical model, and for now only V_p, V_s and V_p/V_s are available from the reference seismic models. Additionally, the program provides the option to import a user-defined velocity model from a local/regional model determined from travel time tomography. To use this, select the user-input option, which will bring up a file selection window. The selected file must be an ASCII text file with depth in km in column 1 and velocity in km/s in column 2.

All the calculated results from the program can be saved to be used for drawing curves for preparing publication-ready figures in the plotting program of your choice.

Additional Notes

The "File" menu contains the features to control the program.

File -> Open

Retrieves a Settings file to load a specific model with previously used parameters. Create the Settings file using the File -> Save option.

File -> Restart

Use this option to restore program defaults and start over to create new model.

File -> Export phase proportion

Exports a text file with phase proportion boundaries for plotting in other programs.

File -> Export V_p, V_s

Exports a text file with the calculated velocities for plotting and use in other programs.

File -> Save

Saves the current model settings to a file that can be loaded through the file menu.

File -> Save Temperature

Exports a text file with the calculated temperature profile for plotting and use in other programs.

Edit -> Mineral Plot

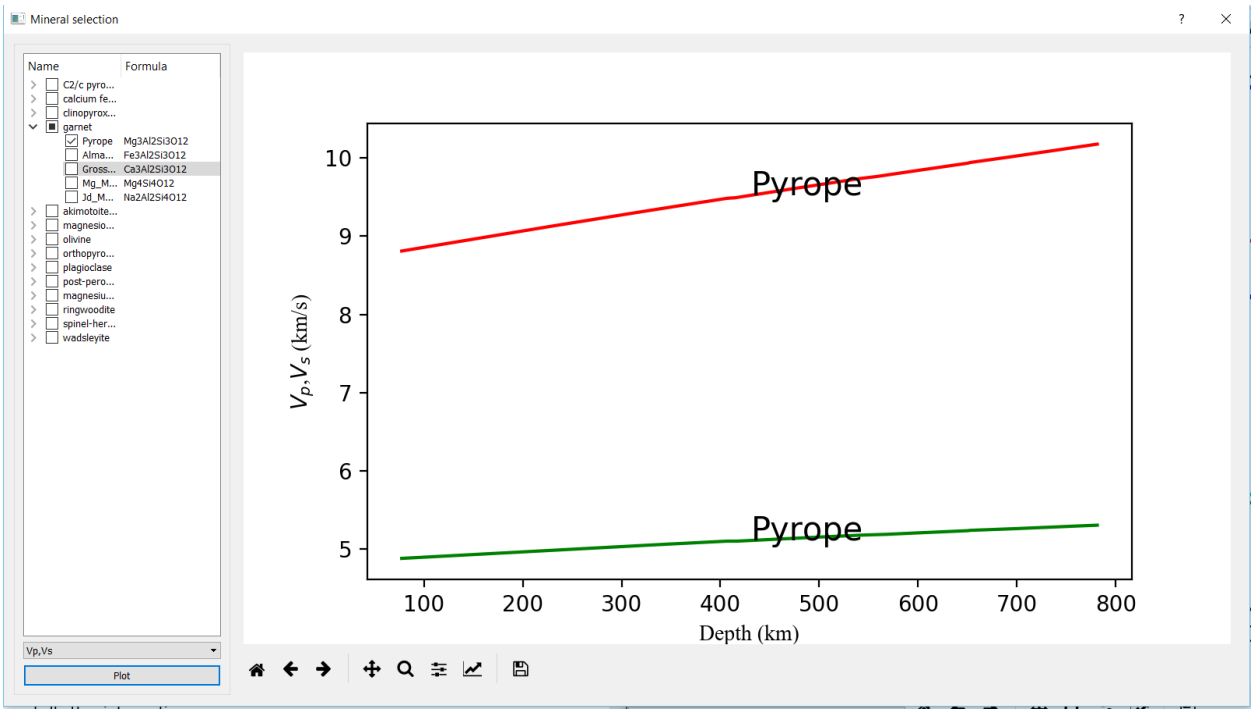


Figure 12. Window with the plots of the V_p, V_s and/or temperature of a single mineral.

Edit -> Change temperature profile

Inputs a temperature profile, which HyMaTZ will use to re-calculate the phase diagram and all the other information. Note: The temperature profile should be in the same format as the output of "Save Temperature".

Edit -> Export figure

Exports a figure that will be saved to a folder the user chooses.

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