PELE

PELE – USER INSTRUCTIONS

SYSTEM REQUIREMENTS

PELE requires Windows 95 or Windows NT version 4.0 or later in order to run. Disk requirements are modest, 4 MB should be plenty, but perhaps it may need 8-10 for temporary installation files.

IMPORTANT: there is a minimum screen resolution requirement of 800 x 600 with small screen fonts. To check or to change your screen resolution, you need to go to the "Display" settings window. You can get to this window in one of three ways:

1) Click on "My Computer", then select "Control Panel", and then select "Display".
2) Click on the "Start" button, then select "Settings", then "Control Panel", and then select "Display".
3) With the mouse pointer on a free (uncovered) area of the desktop, click the RIGHT mouse button, then select "Properties".

Once you have the "Display" window open, select the "Settings" tab to view and/or change the properties of the monitor display. Using the "Desktop Area" Slider control, make sure that the display shows a resolution of 800 x 600 or higher. Using the "Font Size" pulldown list, select "Small fonts" if using 800 x 600 resolution. At higher screen resolution, you can use either small or large fonts. Selecting "Large fonts" causes the PELE main window to take up more screen real estate, but is otherwise a user preference.

INSTALLING PELE

1. Download the accompanying file PELExxx.EXE (where 'xxx' is the version number), a self-extracting ZIP file. It can be downloaded from the web at
        http://www.nicholas.duke.edu/people/faculty/boudreau/DownLoads.html.

2. Run PELExxx.EXE to unzip the setup files. They will be placed in your TEMP directory.

3. Run SETUP.EXE to install the program after files are unzipped; follow the on-screen instructions. In some instances, the installation program may need to install/update some system files, then asks you to reboot your computer to continue with the installation. Do not be afraid, this is normal.

4. When done with the installation, the PELE icon will appear in your "Start" button "Programs" list.

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STARTING PELE

After the program has been setup and started, a default data set is loaded for testing the program. Simply press *Execute* and watch the system perform a fractional crystallization of a MORB composition (or something similar). Select a graph and watch the results as they are computed graphically.

- Press *Halt* to stop the calculation at any time
- Press *Reset* to reset the input data to the state prior to the last beginning of execution.
- Select an option under *Select Output* to view either text or one of four graphical outputs
- Select the menu item *File - View Output* to see the results from each step.

PROGRAM OUTPUT:

The program produces four output files:

Reset.ple: This data file is used by PELE to return the program to its initial state to either
a) The last time the files was manually saved (by menu option *File-Save Input File*)
b) The state prior to pressing the *Execute* button.
These parameters are loaded when then program is first started and whenever the *Reset* button is pressed. You can save this data under a separate file name if desired using the menu option *File-Save Input File As…*.

Note: If you have a problem loading the program, it may be that this file is corrupt. (This problem was noted in a Danish installation). If you experience problems, try deleting the Reset.dat file and restarting the program.

Output.txt : This is a text file with the results of the last computational run. It can be opened through the *File-View* menu option or any text editor. It is overwritten each time the *Execute* button is pressed.

Liquid.tab : This is a tab-delimited file with the composition of the liquid of the last computational run. It can be opened with any common spreadsheet such as Microsoft Excel. It contains the major element, trace and isotopic composition of the liquid at each step of the run. It is overwritten each time the *Execute* button is pressed.

Solids.tab : This is a tab-delimited file with the composition of the solid phases of the last computational run. It can be opened with any common spreadsheet such as Microsoft Excel. It contains the mole fraction of the solid phase components at each step of the run. It is overwritten each time the *Execute* button is pressed.

The following pages contain a brief summary of the windows and output for PELE. While

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attempts have been made to correct or limit entry of invalid input parameters, it is very possible that the wrong combination of options can lead to a program crash.

Garbage in - garbage out!

Finally, while this program was based on published algorithms of the much more sophisticated MELTS program, it is not a direct port of that program. Users should determine if it is suitable for their usage. It does, however, have a number of enhancements including trace element and isotope modeling, sulfur phases and a six species gas phase.

ENJOY!

Any problems or comments, or to be notified of upgrade availability, you can contact me by e-mail at boudreau@duke.edu

Alan Boudreau
July 2005

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MAIN WINDOW - SETUP MODE

When the program is first started, you will see the window shown below. The various command buttons and options are explained below. Menu items along the top are explained separately.

The initial liquid composition is entered into the boxes in the "Oxide Wts." field. One also enters pertinent values in the "Intensive Variables" field. For example, for isobaric crystallization, one would enter a start and stop temperature or, optionally, a start and stop pressure. One can also enter a "dP/dT" value so that the pressure changes as temperature changes for polybaric, polythermal crystallization.

Command Buttons:

 Find Liquidus - Finds the liquidus temperature for the given bulk composition in the *Oxide Wts.* field. Note that the liquidus is calculated based on solid phases only, the gas phase is ignored and thus the liquid may be vapor-saturated at the calculated liquidus temperature.

 Compute Redox - Computes the equilibrium Fe^{2+}/Fe^{3+} based on selected oxygen buffer

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(optional). The FeO and Fe_2O_3 concentrations in the *Oxide wts.* box are adjusted accordingly. When the program is running, Fe^{+2}/Fe^{+3} is adjusted to the selected buffer by addition or loss of O_2 at each step prior to calculating the equilibrium assemblage.

Show Output - Shows either text or one of four graphs (described below) in the output window.

Execute - Begins the calculation. The initial input data is saved in the file RESET.DAT

Continue - Active only when the *Step* box is checked; allows the computation to proceed after pausing after each computational step.

Halt - Aborts the computation, active while computation is running.

Reset - resets the input to the state prior to pressing the Execute button, (or when RESET.PLE was last manually saved via the menu options *File – Save input file of File-Save input file as…*)

The input data is automatically save as the file 'RESET.PLE' each time the *Execute* button is pressed. You can also save your input data under a file name of your choice by selecting the menu item *File – As input File as…*

Option buttons:

Iosbaric/Isenthalpic/Isentropic/Isochoric - Select one option. Shaded fields are not used by the selected option; any data shown is not used to constrain the calculation but one can still enter data into those fields.

Once an option is selected, fill in optional fields in the *Intensive Variables* field. For example, for isenthalpic option, enter optional enthalpy change between steps (*Inc*). Note that you can enter either *dP/dH* or a *Pinc* for changing pressure at each step. However, entering a value in one field will zero the value in the other.

Fractionation/Equilbrium - Select one option for fractional crystallization or equilibrium crystallization. For fractional crystallization, all solids/gas are removed from the bulk assemblage at the end of each step.

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MAIN WINDOW - EXECUTION MODE

Once the calculation has started, a portion of the main window shows both calculation progress and results from the calculation after each step as either a selected graph or as text. The *Free Energy Minimization Progress* field, which appears only during program execution, shows the following information as the program finds the minimum in free energy:

Count – current iteration in the minimization loop.

Temperature and *Pressure* – T and P of current step.

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DJNorm - result of each minimization attempt (= 0 if calculation is finding minimum at each point successfully, a negative number indicates an ill-conditioned problem)

Norm - Comparison of new with previous estimate of stable phase compositions (should approach zero as iterations increase)

Steplength. Fraction of estimated optimal change in phase compositions (should approach 1.00 as iterations increase)

Components - total number of components for which minimization is being attempted.

ln|affinity| - "LED"-type graphical display of phases currently being considered in the minimization routine. This graph shows the natural log of the absolute values of the individual phase affinity at each iteration as free energy is minimized. One can use this graph to help to identify problem phases during the run, which may then be excluded on subsequent runs.

Constraints (none shown in above figure) – These are the active liquid constraints (i.e., those liquid components that are held constant to prevent them from falling below a minimum trace value). These start to show up when there is not much of a liquid component left!

If the ***Show Output – Text*** option has been selcted, then in the lower window are shown the results of the last successful minimization step:

   Step number, and ***constrains/options*** on the calculation.

   Temperature and ***Pressure*** at each step.

   Bulk system properties.

   Liquid properties and it composition.

   Saturated phases, their affinity for the liquid (should be 0.00), mass precipitated at this step, total mass precipitated, and composition of the phases.

   Problem phases - if any phases cause problems and were excluded from the reaction, the will be listed in this optional output section.

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Undersaturated participating phases and their affinity.

This data, is also saved in an output file OUTPUT.TXT that can be viewed by selecting the menu item *File – View last execution* or any text editor. Optionally, you can save the result of the last run to a file name of your choice using the *File – Save last execution as…* menu option. One can print out the result by selecting the menu item *File – Print last execution…*

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GRAPHICS OPTIONS

Show Output - AFM
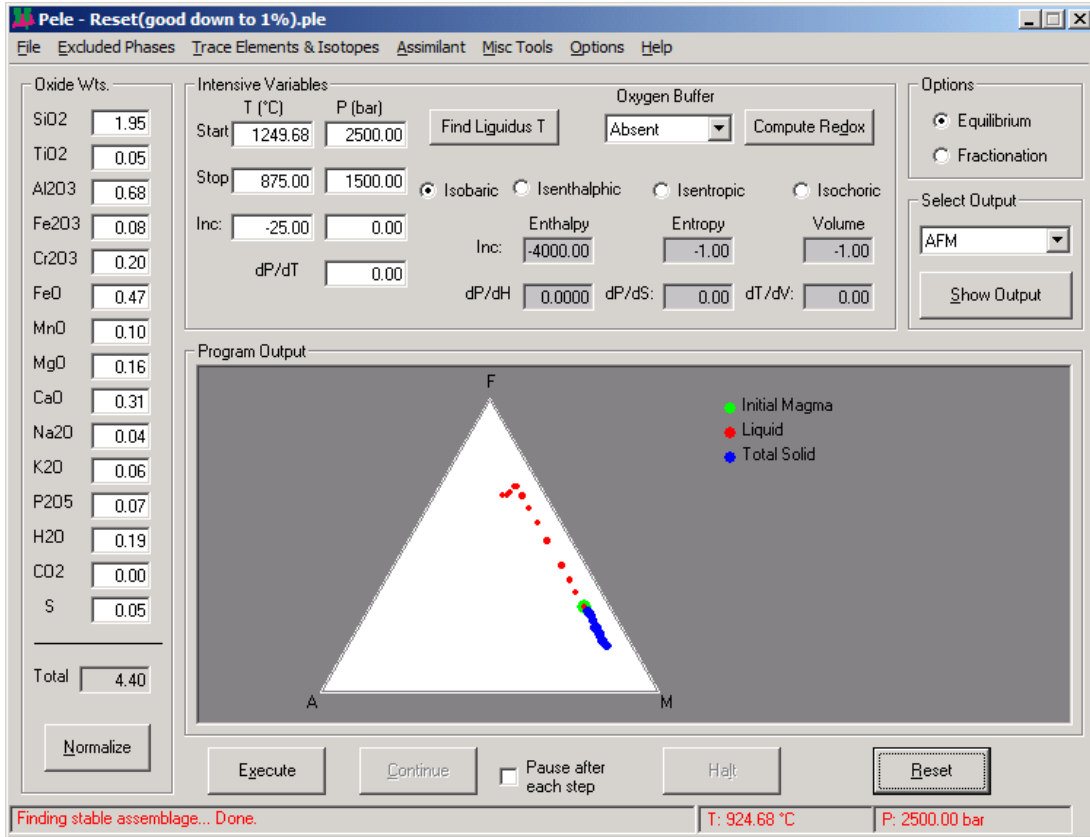
This is a standard weight percent AFM plot showing the initial bulk composition (green), the liquid composition after each calculation step (red), and the bulk total solid composition (blue) after each calculation step. If the *Assimilation* option is selected, then the bulk composition of the solid and liquid assimilants are also plotted (filled black = solid, unfilled circle = liquid). This and the other graphs are selected from the main window. They can be viewed or changed while the computation proceeds.

Note: If you wish to print this or any other window, press the key combination *Alt-PrtScrn*. This will copy the window to the clipboard, where it can then be copied into any common bit-map editor such as **Paint**. The graphic can then be manipulated and printed from the paint program.

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Show Output - Isotopes
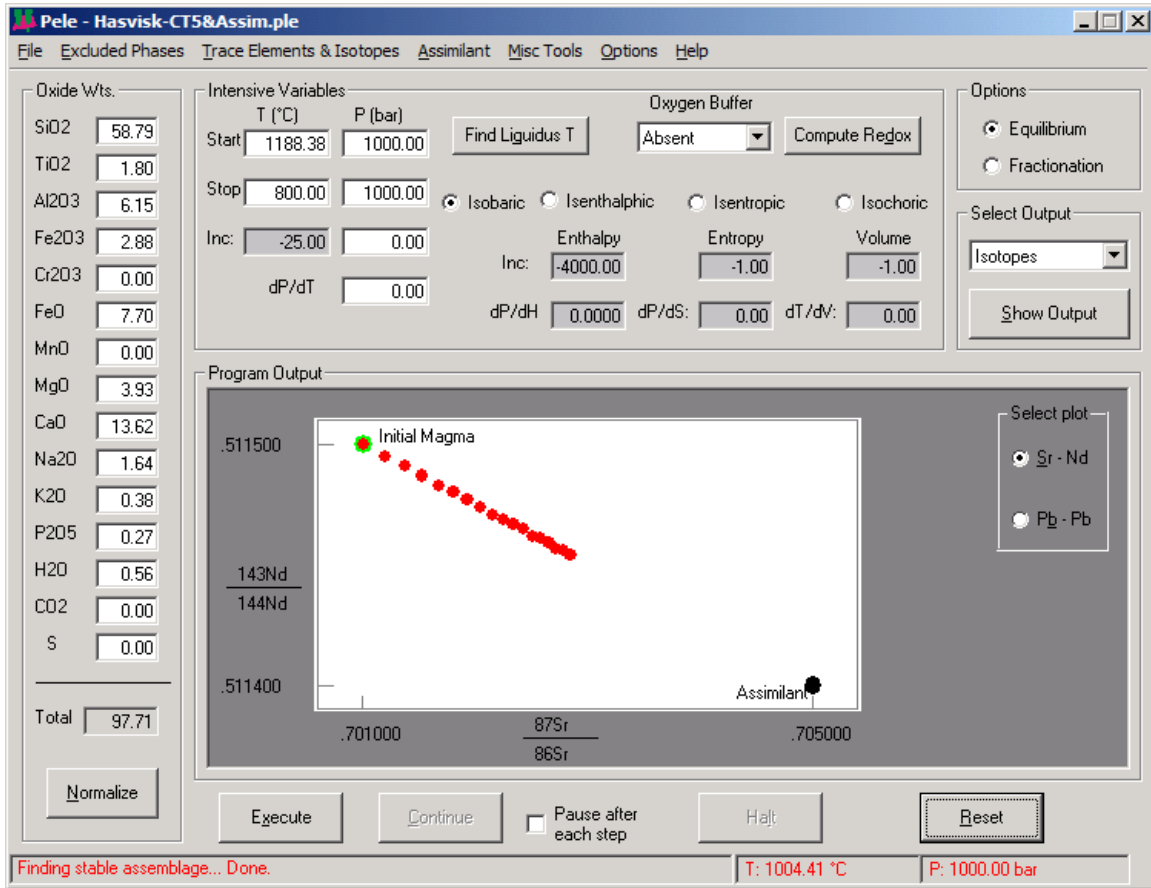
This graph plots the changing isotopic composition of the liquid when assimilation option has been selected. The program plots Sr vs. Nd or two Pb isotopic ratios. However, a cleaver user can change the mineral trace element distribution coefficients and isotopic concentrations through the *Isotopes and Trace Elements* menu item to plot other isotopes as well.

Needless to say, the plot will not be very interesting if the assimilation option has not been selected. Up to 100 points can be plotted, after which no more point are plotted.
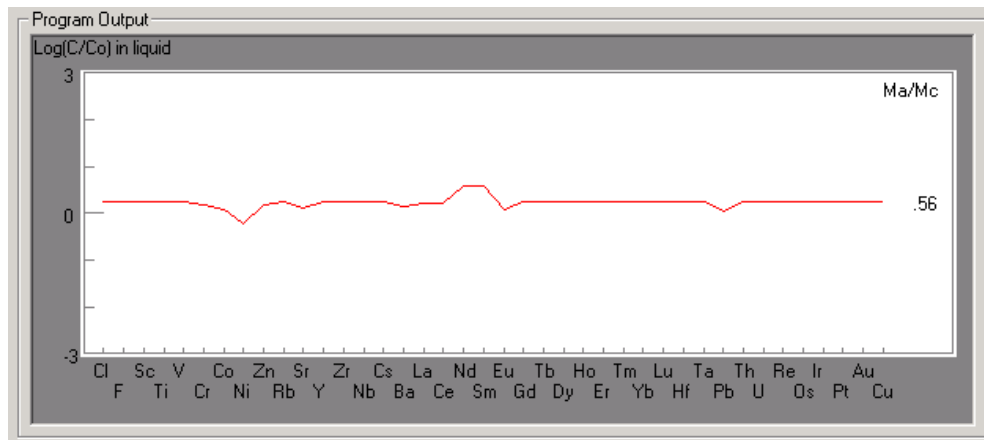
Note: If you wish to print this or any other window, press the key combination *Alt-PrtScrn*. This will copy the window to the clipboard, where it can then be copied into any common bit-map editor such as **Paint**. The graphic can then be manipulated and printed from the paint program.

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Show Output - Mass Solids
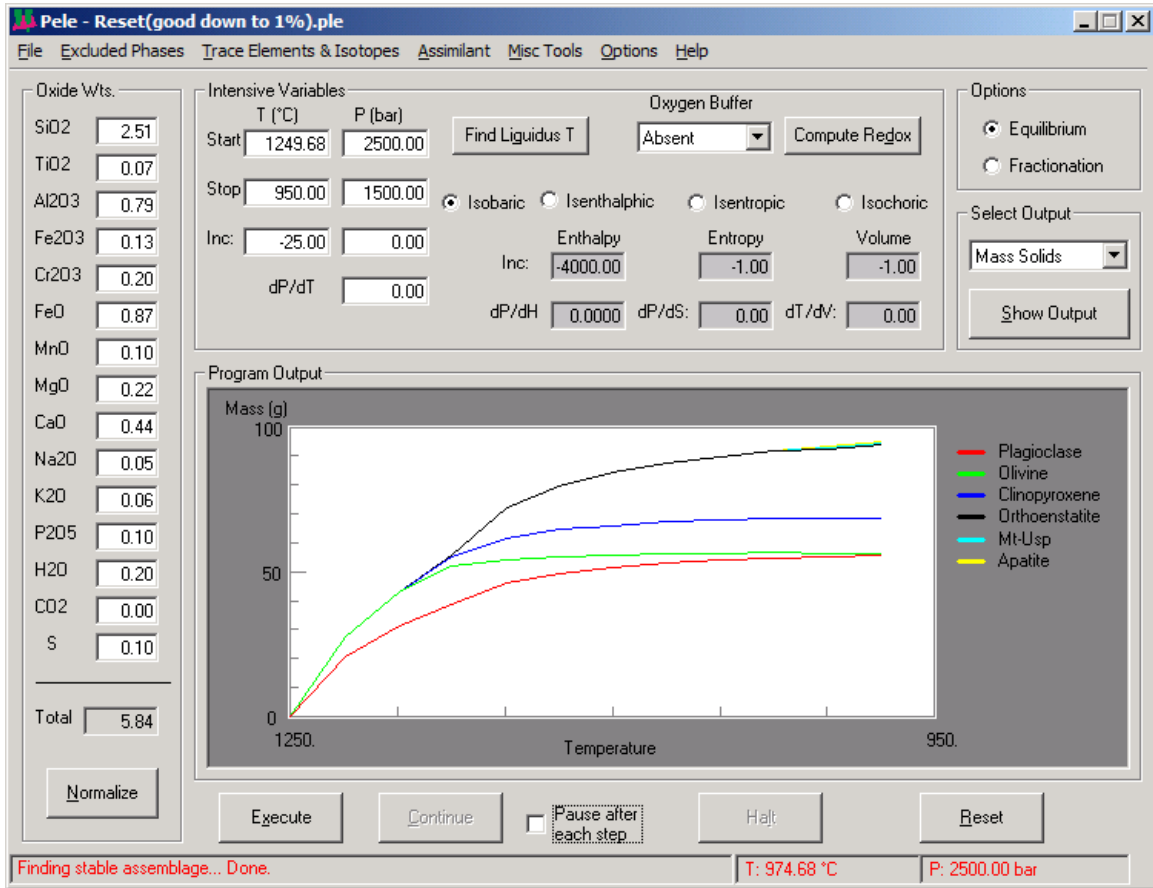
This graph plots the total mass of solids precipitated at each step in the reaction. Up to 100 points can be plotted, after which no more point are plotted.

Note: If you wish to print this or any other window, press the key combination *Alt-PrtScrn*. This will copy the window to the clipboard, where it can then be copied into any common bit-map editor such as **Paint**. The graphic can then be manipulated and printed from the paint program.

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Show Output - Spider
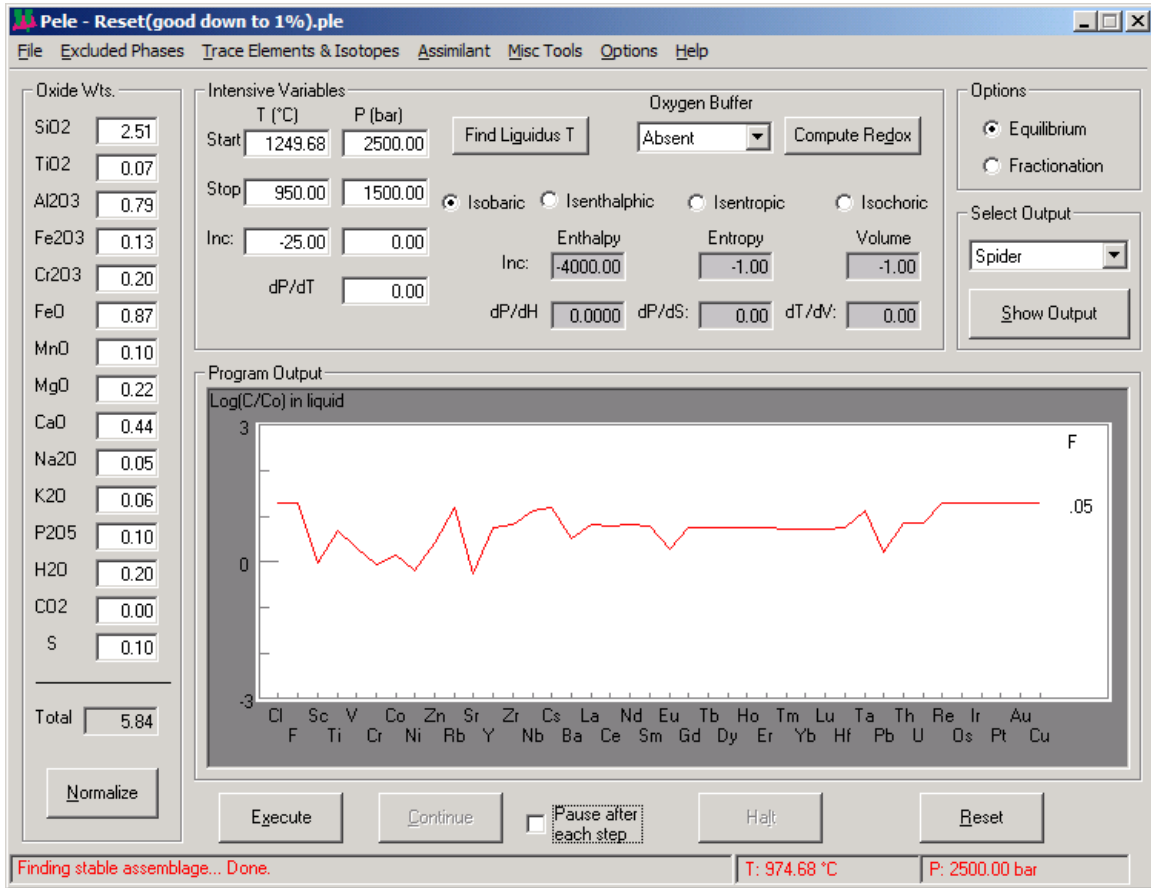
This plot shows the concentration of 40 trace elements (normalized to their initial bulk concentration) at the current/last step in the calculation. Data is plotted as element concentration as a function of F, the fraction of liquid remaining (as shown), or as a function of the mass assimilated/mass crystallized (Ma/Mc) if the assimilation option is selected (shown below).

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PELE MENU OPTIONS

MENU ITEM - *ExcludedPhases*

Use this window to exclude phases from being considered in the calculation. Checked phases are excluded. Shaded check boxes are phases not currently available. Note that you can select from two spinel models (either eight components or mt-usp only) and three rhombohedral oxide models (either four components, hm - ilm, or pure ilm). You cannot select more than one of each type!

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MENU ITEM – *Assimilation-Eruption-Recharge*

        PELE allows one to add a liquid and solid assimilant as well as an option to remove some of the remaining mamga after each step and then find the stable assemblage under the same constraints as for an inital liquid alone. This allows one to model the effect on phase porportions, trace elments and isotopes that result from the combined effects of assimilation, magma mixing, magma recharge and mass loss to eruption.

Use this window to set the phase assemblage in a solid assemblage or the liquid composition for a liquid assimilant. One also sets the mass of the liquid and or solid assimilant to be added at each step. One can enter zero for the mass of either the liquid or solid assimilant added per step.

Bulk thermodynamic properties of the assimilant are also shown, and cannot be directly edited by the user except by editing the solid or liquid assimilant composition, temperature, or pressure. These thermodynamic properties are used depending on the options selected in the Main Window. For example, if the *isenthalpic* option is active (as is appropriate for assimilation), then the stable assemblage and temperature at each step is calculated assuming that the total enthalpy is equal to that of the remaining magma from the previous step plus that of the solid and liquids added.

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Enter a value in the ***Mass erupted at each step*** box to reduce the mass of bulk remaining magma prior to addition of the liquid and solid assimilants.

Check the ***Include assimilant*** check box if you wish assimilation-eruption-recharge constraint to be active in the calculation.

Press ***Clear All*** to clear all fields.

Selecting the ***Assimilant Trace Elements…*** button brings up the trace element window where up to trace element concentrations can be entered.

Selecting the ***Setup Solid Assimilant…*** button brings up the Setup Solid Assimilant window (see below) to setup the phases that actually make up the assimilant. The bulk composition (in wt. %), bulk enthalpy, bulk entropy, bulk heat capacity and bulk volume of the assimilant are calculated from this phase assemblage, based on 100g total mass of the assimilant.

Selecting the ***Setup Liquid Assimilant…*** button brings up the Setup Liquid Assimilant window (see below) to setup a liquid composition for magma mixing. The bulk composition (in wt. %), bulk enthalpy, bulk entropy, bulk heat capacity and bulk volume of the assimilant are calculated from an entered composition, based on a 100g mass of the assimilant liquid.

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Setup Solid Assimilant window

To set up the minerals that make up a solid assimilant, open the menu item *Assimilation-Eruption-Recharge,* then select the *Setup Solid Assimilant …* button to bring up the window shown above. Then:

1. Select a phase to add from the dropdown *Phase list* on the left in the above window.

2.   If it is a multicomponent phase, enter the mole fractions of the endmember components in the *Phase composition* area. At least one component must be non-zero, and the sum of all the components must add up to 1.0. Press *Normalize to 1.0* to normalize phase components normalize to 1.0

3. Enter mass % of phase in the assemblage. Phase mass % must be > 0.0 g.

4. If not already set, enter an assimilant temperature. Inital assimilant pressure is assumed to be the same as the liquid P set in the Main PELE window. (If pressure changers during execution, the solid assembalge thermodynamic prpoerties will be recomputed at each new pressre step.)

5. Press *Add/Update >>* to add the assimilant phase list shown on the right half of the above screen. Repete for each phase you wish to add. Press *"OK"* when done

Note: If you have a bulk assimilant that is in oxides weights and you do not know the solid phases that might make up this bulk composition, enter the weight % in the main window and use the *CIPW norm* option in the *Misc. Tools* menu to get the solid phase equivalent.

To remove or edit an assimilant phase:

1. Select a phase in the *Phases in assimilant* listbox on the righthand side.

2. To edit the selected phase composition or mass, change properties as desired.

3. To remove the selected phase, press *<< Remove Phase.*

4. If you wish to renormalize all phase component masses to a new total mass, then press *Norm to 100%.*

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Setup Liquid Assimilant window

To set up a liquid assimilant (to model magam mixing), open the menu item *Assimilation-Eruption-Recharge,* then select the *Setup Liquid Assimilant …* button to bring up the window shown above. Then:

1. Enter the composition of the liquid on the left in the above window. Normalize to 100%

2.   Enter the total mass to be assimilated, and the temperature of the liquid. Inital assimilant pressure is assumed to be the same as the liquid P set in the Main PELE window. (If pressure changers during execution, the liquid thermodynamic prpoerties will be recomputed at each new pressre step)

3. Press *Find Properties…* to calcuate the enthalpy, entropy and volume of the mass of liquid at the selected temperature. *Note:* If the liquid is below it's liqudus temperature, properites will be for a supercooled liquid.

Optionally, one can use the initial magma shown in the Main Window. Pressing *Use Initial Liquid* will load the oxides listed in the main Window, the temperatures, as well as trace elements and isotopes for this initial liquid.

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MENU ITEM – *Trace Elements*

Selecting this menu item brings up the above window. Select either the ***Initial Liquid***, the ***Liquid Assimilant***, or the ***Solid Assimilant*** option and enter the trace element composition of that component. Selecting the liquid assimilant will also bring up an option to set the liquid assimilant the same as the initial liquid.

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MENU ITEM – *Partition Coefficients*

Parition Coefficients

Phase	Partition coefficients
Olivine	Select a phase from the pull-down list at left to enter or edit the partition coefficients for that phase. Alternatively, you can set up to use BigD program of Roger Neilsen or those of Jean Bedard.

Cl	0.0000	Sr	0.0004	Eu	0.0002	Ta	0.0010
F	0.0000	Y	0.0010	Gd	0.0003	Pb	0.0003
Sc	0.1600	Zr	0.0010	Tb	0.0005	Th	0.0003
Ti	0.0020	Nb	0.0010	Dy	0.0001	U	0.0003
V	0.1890	Cs	0.0002	Ho	0.0012	Re	0.0000
Cr	1.2500	Ba	0.0003	Er	0.0017	Os	0.0000
Co	3.2000	La	0.0003	Tm	0.0035	Ir	0.0000
Ni	10.0000	Ce	0.0003	Yb	0.0052	Pt	0.0000
Zn	0.8300	Nd	0.0002	Lu	0.0085	Au	0.0000
Rb	0.0002	Sm	0.0002	Hf	0.0029	Cu	0.0000

BigD

☑ Disable BigD

Setup BigD Options...

Load Bedard D's...   OK

Trace element partitioning can be calculated by assuming either constant partition coefficients or, for those elements and phases where it is valid, using the subroutine BigD (Neilsen, R.L., 1992, Computers and Geosciences 18:773-788). This option can be disabled by checking the **Disable BigD** checkbox.

For fixed values, one can enter these manually or you can load a data set supplied by Jean Bedard. The latter are loaded automatically by pressing the **Load Bedard D's...** button. Selecting the Bedard option disables the BigD option.

This data is saved in the file RESET.PLE that is saved each time the calculation is executed, or it can be saved manually through the menu item **File - Save**.

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BigD Options

To set up the options for the BigD subroutine, click on the *Setup BigD* in the *Trace Elements* window to get the following window:

Checked phases will have partition coefficients calculated by BigD. Note that for pyroxenes, Ti can be calculated by the BigD subroutine (best for low pressure crystallization), or an estimate of the pyroxene Ti content can be entered and this value will be used to calculate distribution coefficients for Sc, Y and the REE. This later option is best for high P crystallization. Note that you can only select either the low or the high P option for pyroxene; you cannot select both!

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MENU ITEM – *Isotopes*

The program allows one to model isotopic changes during assimilation for the above isotopic systems.

Although only Sr, Nd and two Pb isotopes are modeled, a cleaver user can adjust the distribution coefficients and isotopic concentrations of the elements Sr, Nd and Pb and use these elements as proxies to model other isotope systems. Isotopic modeling was new in version 3.10.

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MENU ITEM - *MiscTools*

MiscTools – Find Liquidus T

This finds the liquidus temperature for the composition in the main window at the desired start T and P. This temperature is then put into the Start T text box. The ***Find Liquidus T*** button in the main window does the same thing. Note that the liquidus is calculated based on solid phases only, the gas phase is ignored and thus the liquid may be vapor-saturated at the calculated liquidus temperature.

MiscTools – Find Vap Sat

This finds the maximum concentration of water at vapor saturation for the composition in the main window at the desired start T and P. The program then gives you the option of changing the default water content to this saturation value.

MiscTools – CIPW Norm

This gives a simple norm calculation of the listed bulk composition in the main window. Solid assemblages are calculated as dry (no H_2O)

MiscTools – Liquid Properties

This finds the thermodynamic and other properties of a liquid with the listed bulk composition in the main window and the listed start T and P. If the liquid is below the liquidus T, it is noted that the properties are for a supercooled liquid.

MiscTools - Plot Data
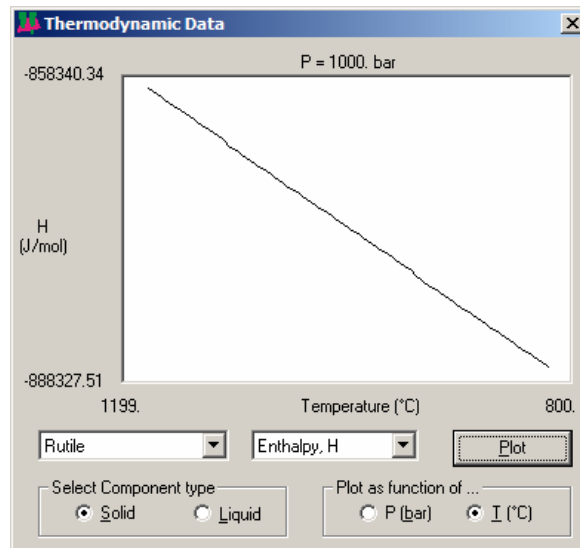
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Selecting this menu item bring up the above window in which one can plot the various thermodynamic parameters of the solid and liquid components. T and P range are as set in the start and stop T and P in the main window. To plot:

> - Select a component type (solid or liquid component)
> - Select whether to plot as a function of P or T
> - Select the component from the pull down list
> - Select the thermodynamic variable to plot from the pull down list
> - Press the Plot button

The program calculates 100 points between the start and stop T (or P) and plots the results in the window.

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MENU ITEM *Options*

       Options – Assimilation

       When selected (checked), assimilation is active. This has the same effect as checking the "Include assimilant" checkbox in the ***Assimilant*** window.

       Options – Melting

       When checked, program will first take the composition from liquidus temperature down to the desired "Start T" in steps before proceeding as usual.

       PELE works best when starting with an assemblage that is mostly liquid and then crystallizing. Starting the calculation at a temperature well below the liquidus where the first stable assemblage is a mostly solid assemblage may cause a program halt (unable to find a stable assemblage). If this option is selected (checked), the program will assume that the starting T is well below the liquidus. It will then try to first find the stable assemblage by taking the temperature down in steps from the liquidus to the desired starting temperature. If it is successful, the program will then proceed as usual.

       This option may help those interested in trying to model decompression melting, for example.

       Options – Solid solution models
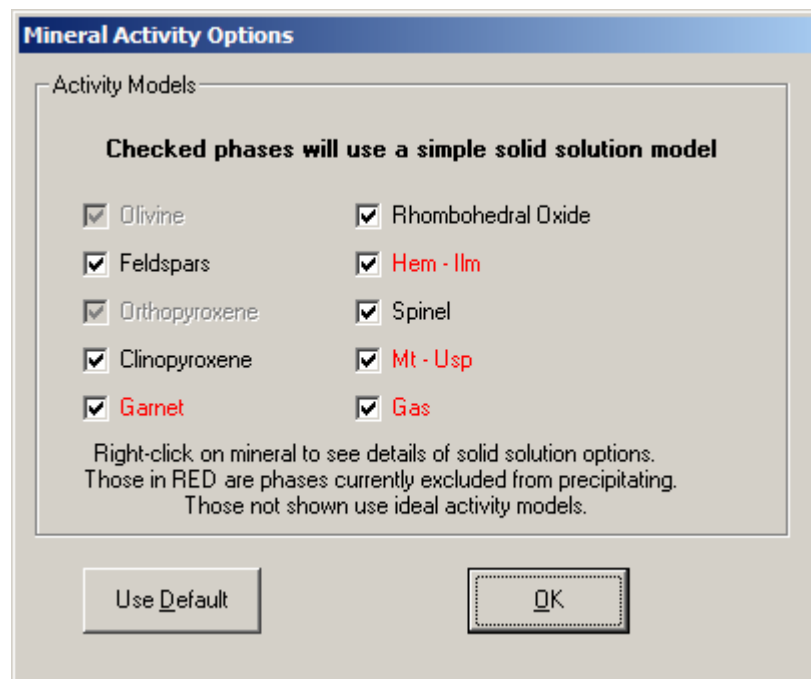
Beginning with version 4.0, more realistic solid solution activity models were added, similar to

the original MELTS program. Currently these include those listed in the above window. You can right-click on the phase name to see what the solid solution models are for that phase

Except for olivine and orthopyroxene, the code for both calculating and minimizing these non-ideal solid solutions is still being improved and debugged. Needless to say, using these non-ideal activity models can cause the program to halt prematurely.

Checking the check box causes the program to use ideal activity models for the phase and, in some cases, reduces the number of phases components (e.g., plagioclase is reduce from An – Ab – Or components to An - Ab components only)

For a gas, **PELE** can calculate the gas species based on either three possible components (H_2O, CO_2, H_2S) or six components (H_2O, CO_2, H_2S, SO_2, CO and CH_4). As SO_2, CO and CH_4 can be of very low abundance in some gases, they can cause problems in the minimization search. When the *Gas* option is checked, only three gas phase species are possible.

Options – Stop on Problem Phases

Occasionally a saturated phase will cause the program to be unable to find the stable assemblage. If this item is selected, the program will stop if there is a problem and give the user the option to continue or not. If this option is not selected (unchecked), the problem will simply continue with the calculation at the next T/P step.

Problem phases will be listed in the text window. Problem phases may be a trace phase if the affinity is small. Otherwise the most common offenders tend to be minor phases with high concentrations of a minor liquid component (e.g., Fe-Ti oxides).

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New in Version 5

Starting with version 5, CO_2 and S were added as additional system components. This allows one to exsolve both a C-O-H-S fluid and to precipitate sulfide and C-bearing phases from the liquid.

CO_2 solubility essentially incorporates the model of Papale (1999, Am Min 84:477-492). It has been modified as follows: the CO_2-oxide liquid interaction parameters have been recalibrated to the liquid components and interaction parameters used in PELE/MELTS. Also, the thermodynamic properties of pure CO_2 and all other gas species are now calculated by the general EOS for supercritical gases of Duan et al. (1996, GCA 60:1209-1216). Gases are otherwise assumed to mix ideally. Possible gas species include H_2O, CO_2, CO, CH_4, H_2S, and SO_2 . Graphite (C) is a possible precipitating solid.

The silicate liquid component for sulfur is FeS (liquid troilite).   An error will be generated if there is no FeO entered.

Sulfur fugacity is calculated by the method of Wallace and Carmichael (1992, GCA 56:1863-1874).

Immiscible sulfide liquid is assumed to be an ideal solution of two components, FeS and FeO. Other possible sulfide phases that can precipitate are pyrrhotite, pyrite and troilite.

FeS-oxide liquid interaction parameters were calibrated (with some arbitrary adjustment because of uncertain sulfide liquid compositions in the experimental data) from the data of O'Neill and Mavrogenes (2002, J Pet 43:1049-1087), Wentlandt (1982, Am Min 67:877-885); Mavrogenes and O'Neill (1999, GCA 63:1173-1180) and Haughton et al. (1974, Econ Geol 69:451-467). These are mostly of basalt-intermediate composition, but the lower solubility calculated for more acid compositions appear reasonable. Above ~10 kbar, sulfide saturation values are significantly lower than expected.