IRidium

A program to model silicate liquid infiltration and reaction through porous rock

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Although modeling of magma-rock interactions are becoming increasingly sophisticated, there have not been until now general models that include equilibrium reactions of major phases (minerals and silicate liquid), trace element modeling and reactive transport. Our work on layered intrusions has led to an increasing need to incorporate more realistic and quantitative models for mineral-liquid equibria into transport-reaction models.

To this end, the IRIDIUM program has been developed for use on windows-based PC's. The mineral-liquid equilbrium calculations is based on the MELTS algorithm of Ghiorso and co-workers (Ghiorso and Sack, 1995 and others). (Currently, only olivine and orthopyroxene use the same solid solution models as does MELTS, other phases are modeled as ideal solutions using simple endmembers.) It is coupled with standard diffusion and advective one-dimensional mass transport equations. The program is expected to be a useful tool to a broad range of igneous studies. This program is general enough so users can specify a range of starting compositions (including inhomogeneous host rock compositions). The program allows calculation of reaction and chromatographic fronts as silicate liquid percolates through a porous solid matrix.

General Program Notes

Iridium has two main operation modes, of which the user must select one:

Infiltration: Liquid is infiltrated into a liquid + solid assemblage from the bottom.

Compaction: Bottom is closed to mass transfer; differential liquid and solid movement is by compaction of the crystal pile.

The program has several different input/output data files associated with it:

Irsetup.ird - This stores the initial setup information, including bulk compositions, T, P and trace element distribution coefficients, and the composition of the infiltrant liquid. It is loaded automatically on program startup and updated each time the “Start” or “Find Init” buttons are selected.

MassDCoef.csv – This is a comma-separated values (csv) file containing the mass diffusion coefficients for the major elements used by the program. Also, one element must have a diagonal element set to zero; the concentration of this element is then found by difference form 100%. This file is loaded automatically on program startup

IRidium - Instructions

NOTE: while one can enter off-diagonal diffusion coefficients, currently only the diagonal elements are used by the program.

Iroutput.txt – This stores the result of the simulation after each complete iteration. The time "0" iteration is the initial stable phases in the assemblage. In case of a program crash, one can load the last completed iteration and correct individual nodes if there is a simple problem.

Irliquid.txt - This stores just the liquid composition of the topmost node after each complete iteration. This is useful, say, when the "mix liquid" option is active to see the average composition of the liquid above the crystal pile.

Irlog.txt - This stores any errors that were detected during the last run. Most commonly the errors are associated with finding isenthalpic equilibrium state in which some minor enthalpy error remains while in attempting to find the stable assemblage.

General Steps to Setup and Run the Program

On first running the program after installation, a default dataset should be loaded automatically and step 'A' below can be skipped.

A) Enter initial parameters in all of the setup windows:

1) Set the number of nodes, total length, the initial bulk composition, T and P of each node. For infiltration, the program assumes that liquid will enter at the bottom (1st) node. It also assumes that any crystal-free liquid, if present, will be at the top. Thus you should make sure your T and composition gradients are such that the solids are concentrated at the bottom of the graphics window.

2) If doing infiltration, setup the composition and thermodynamic properties of the infiltrant liquid.

3) If doing compaction, setup the compaction parameters.

4) Set miscellaneous parameters.

B) Find the initial stable state of the system:

Once the bulk composition, T, P etc. have been set, you need to calculate the initial equilibrium state of the system. This calculates the stable phases at each T and P. This is stored in the file ***Iroutput.txt*** as iteration "0".

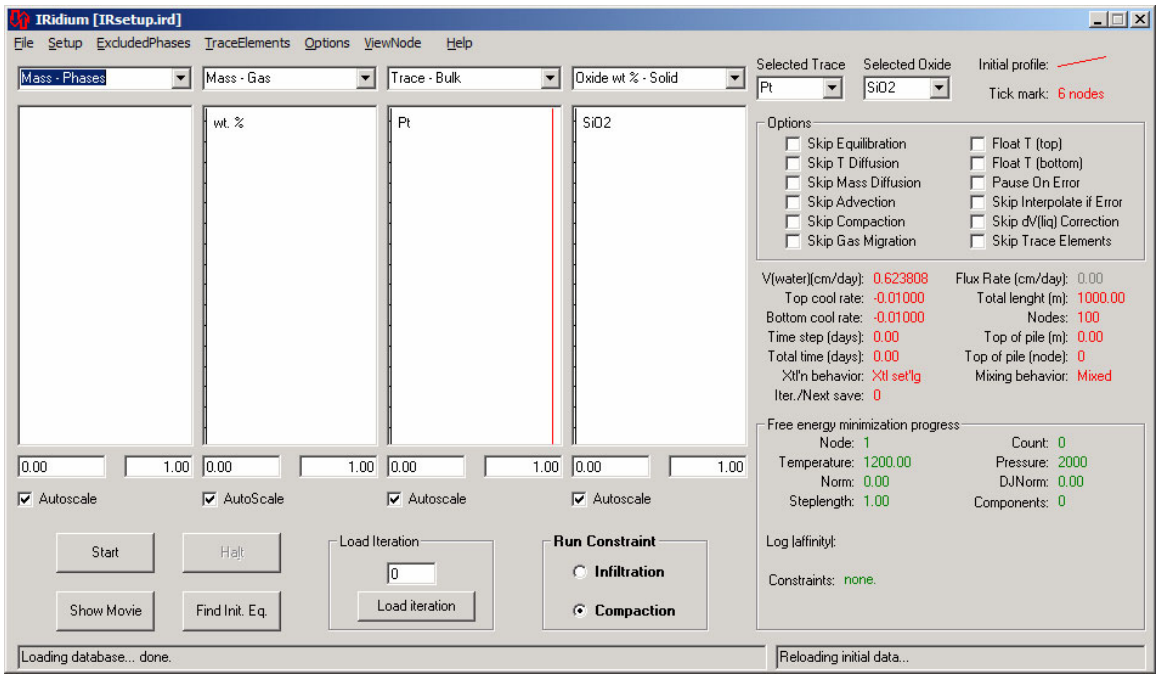
If the initial conditions are not such that the stable state is all liquid, then one should see stable phase assemblages and other physical parameters being displayed at each node as the calculation progresses. The program will halt once the stable state has been found. If there are problems during this stage, you may have to adjust your setup parameters. For example, you may want to open the "Excluded Phases" window to exclude any minor problem phases.

C) Select the "Start" button (Infiltration or Compaction) and watch the simulation run.

D) After the run, select the "Show movie"… option to show the saved results.

Remember - Garbage in, garbage out!

Main Program Window



Descriptions of command buttons:

Start - starts the calculation

Halt – stops the calculation

Find Init. Eq. – Calculates the in initial stable phase assemblages based on the input bulk composition, T and P of each node.

Show Movie – plots successively the results of the last run (stored in the file "Iroutput.txt"), one iteration at a time.

Load Iteration – loads the saved iteration number shown in the textbox above the button.

Descriptions of Drop-down list boxes:

List box above each plot - Selects the data to be plotted in one of the four graphics windows

Select Trace – Selects the trace element to be plotted in the graphics window when plot trace element is also selected

Select Oxide – Selects the major element oxide to be plotted in the graphics window when plot oxide is also selected

Checkbox Options:

Theses options allow one to skip various calculation options during the run. They are useful for checking that various pieces of the calculation are being done correctly and that you have the input values set correctly. They are only active during the run, not when the program is calculating the initial stable assemblage.

Skip equilibrium – Causes the program to skip calculation of the new equilibrium phase assemblage at each step.

Skip advection – Causes the program to skip mass advection of liquids, gas, and solids (if compaction active). Useful if you wish to test or use the mass diffusion module alone.

Skip T diffusion – Causes the program to skip thermal diffusion. This is useful if one is interested in understanding the thermal effects of the heat of reaction of an infiltrating liquid.

Skip Mass diffusion – Causes the program to skip mass diffusion in the liquid. Useful if your problem involves high rates of infiltration or compaction velocities such that mass diffusion is relatively unimportant.

Skip Compaction – Causes the program to skip calculation of liquid and solid velocities caused by compaction.

Skip gas migration – Causes the program to skip calculation of gas advection.

Float T (top) and **Float T (bottom)** – When checked, temperatures at top and/or bottom are calculated from bulk enthalpy during equilibration. Otherwise T will change as determined by the top and bottom cooling rates entered in the Setup – Miscellaneous window.

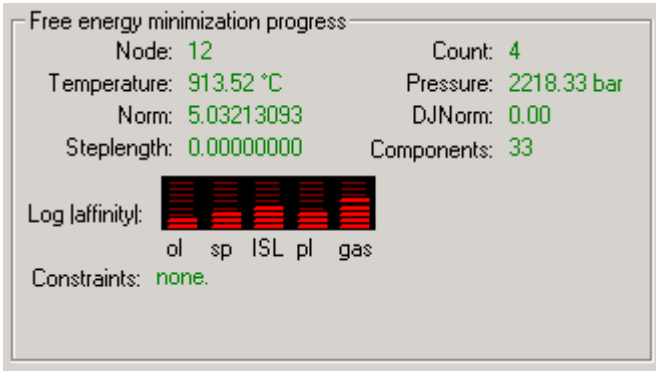
Pause on Error – Causes the program to stop if an error condition is encountered. Otherwise the error is simply logged into the file "Irlog.txt" and the program simply ignores the error (if it is a minor enthalpy adjustment error) or uses previous values (if unable to find a stable equilibrium assemblage). A serious error will result in an error message in any event.

Skip interpolate on error – If unchecked, the program will interpolate between nodes for any node for which phase equilibration was unsuccessful.

Skip trace elements – Causes the program to skip the calculation of trace element distribution between solids and liquid.

Skip dV(liq) Correction – Any volume changes on crystallization are assumed to be balance by liquid migrating in to or out from adjacent nodes. When checked, the program will not make this minor mass balance correction.

Free energy minimization progress window:

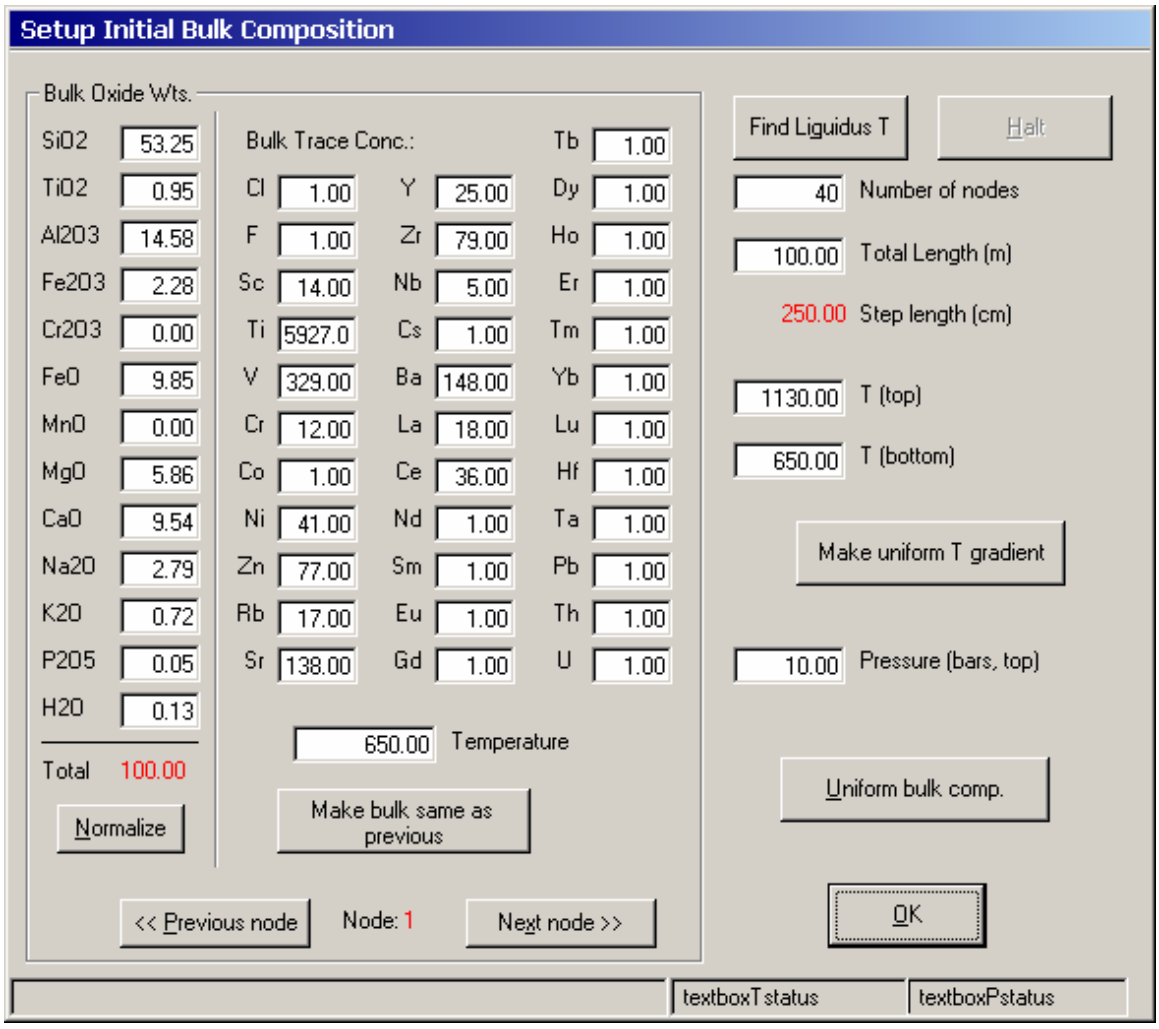


The window at the bottom right corner of the main program window (shown in detail above) shows data from the free energy minimization routine as the program is running.

The 'LED" display shows the evolving affinity of the minerals as liquid and mineral compositions are adjusted. At equilibrium, the LED's should be zero. A phase that stays high could be a problem phases

Setup Menu Item

Setup - Bulk Menu Item



This is the window where one sets the number of nodes in the simulation (currently limited to 300), the starting bulk composition of each node (major oxides as well as 34 trace elements) as well as the initial T and P of each node.

Before on can enter the data, one must enter the total number of nodes, or steps, that the total length will be subdivided into. This is entered into the textbox labeled "Number of nodes". One also enters the total length of the system, from which the program calculates the size of each node.

Once this is done, one enters the bulk composition for each node. Note that there are two buttons to make this easer to enter for initially uniform-composition systems. The ***"Uniform bulk comp."*** command button on the right-hand side will make all nodes the same composition as the currently listed node. This will make the bulk composition the same for all nodes. Alternatively, once can select the command button located below the trace element input boxed labeled ***"Make bulk same as previous"***. By pressing the ***"next node"*** and then the ***"make bulk same as***

previous", one will copy the composition of the previous node into the current node. This is useful, say, for making a layer of different bulk composition from that of the host.

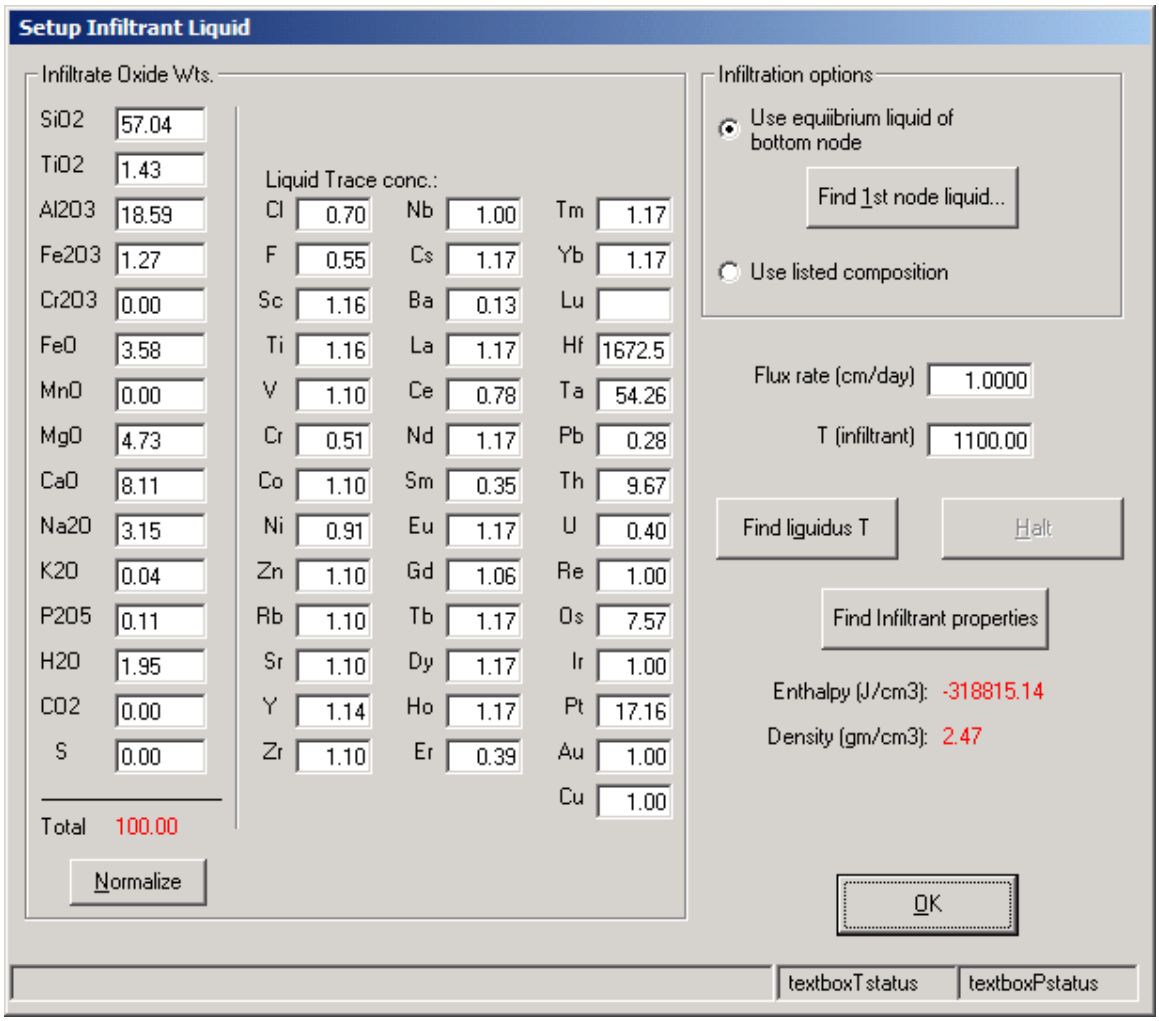
Temperature can be entered individually for each node (in the box below the trace elements). More typically, however, on will enter the top and bottom temperatures in the text boxes at left, then press the ***"Make uniform T gradient"*** button and the program will calculate a uniform thermal profile between the top and the bottom.

The ***"Find liquidus T…"*** command button will find the liquidus temperature for the currently selected node. This value is optionally placed in the ***"Temperature"*** box for the currently selected node. This is useful for finding the maximum T you may want to have for your assemblage. Again, you should generally have T hotter at the top.

Pressure is only specified at the top. P at all other steps is based on bulk density and steplength.

This data is saved as part of the Irsetup.Ird file.

Setup - Infiltrant Menu Item



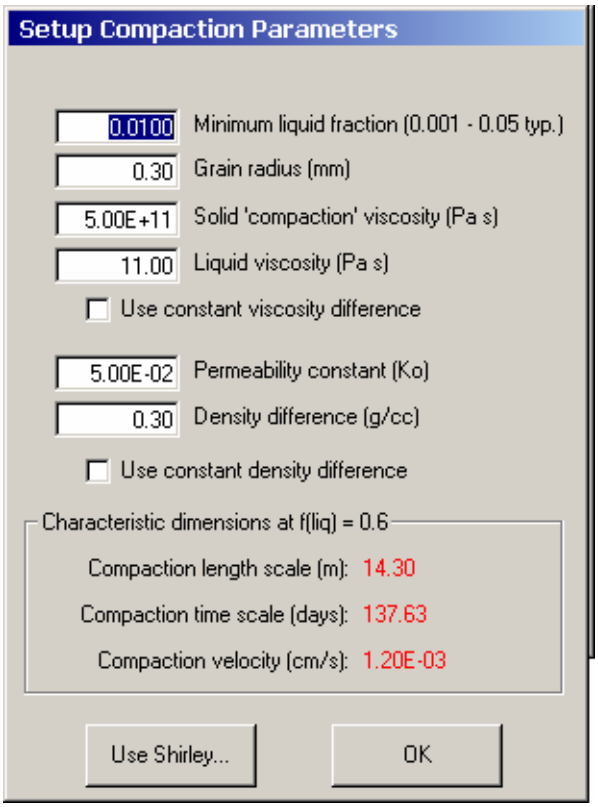
In this window one sets up the composition of the liquid that will be infiltrating upwards from the base, as shown in the graphics windows of the main program window. Once can either enter a liquid composition (both major oxides and trace elements) or, optionally, once can calculate the liquid in equilibrium with the solid assemblage at the bottom node and use this one. This latter option is useful if you have a "layer" of different composition higher in you column and want liquid from the surrounding rock to infiltrate through this layer.

If you enter a liquid, you should then press the command button ***"Find Liquidus T"***, which will enter this temperature in the T (infiltrant) text box.

Also, if you enter a composition, you will need to calculate the infiltrant properties by pressing the ***"Infiltrant properties"*** command button. This then calculates the enthalpy and density of the liquid.

This data is saved in the Irsetup.IRD file.

Setup - Compaction Menu Item



The compaction routines used in the program are from Shirley, and are based on the compaction equations of McKensie

Minimum liquid fraction - This values is the limit at which compaction (and calculation of equlibrium phase assemblages) will assume the node to be fully solidified.

Grain radius – Grain size used in equations of Shirley.

Solid and **liquid viscosity** – Enter viscosities in Pa-s.

Permeability constant – Constant used in permeability expressions of Shirely.

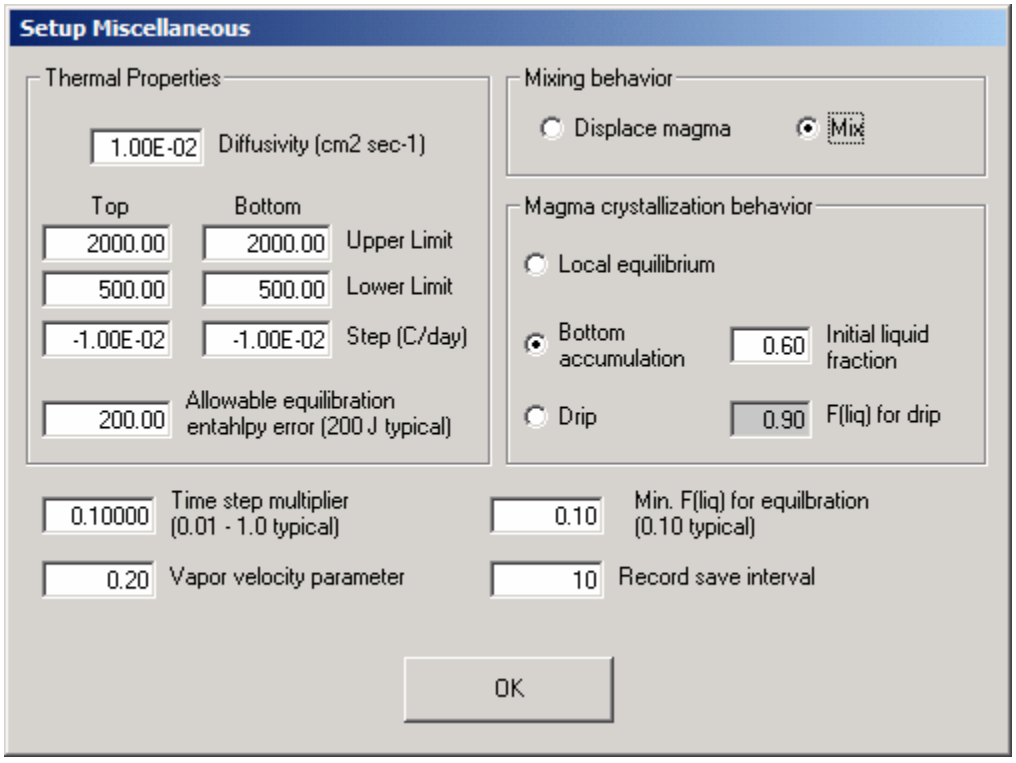
Density difference – Solid - liquid density difference, if using a constant density difference. In some instances, using the actual calculated density difference may result in some nodes having a negative difference in which case the crystals in that node may actually float!

Compaction length and **time scales** - Calculated from the entered data, following Shirley.

Use Shirley command button - Use Shirley's values

This data is saved as part of the Irsetup.Ird file.

Setup - Miscellaneous Menu Item



Thermal Properties: Enter the thermal diffusivity. A cooling rate for the top and the bottom can also be specified, as well as limits. Cooling rates are per day and must be negative numbers if you wish temperature to drop with time. *Note: If the option boxes "T float (top)" or "T float (bottom)" in the main program window are checked, then these values are ignored and T is calculated from the bulk enthalpy during the equilibration calculations.*

One should also enter an "***allowable equilibration enthalpy error limit***". For the isenthalpic calculations done for most nodes, the program tries to find the stable assemblages based on total enthalpy to within 1.0 joule. However, nodes where phases are only marginally stable may cause larger errors. 200 J is a typical value.

Mixing behavior: The program will check to see if the uppermost nodes are all liquid. If so, one can select how magma escaping from the crystal pile will interact with this supernatant liquid. The **Displace magma** option simply displaces the existing liquid upward. The **Mix** option will cause the new magma to mix in with the existing magma to make a compositionally uniform liquid.

Magma crystallization behavior: the program allows for three different modes of crystallization behavior:

1) The **Local equilibrium** option is the default value; equilibrium phases are calculated for each node individually. Solids do not move unless the compaction option is active.

2) The **Bottom accumulation** option assumes that all solids that crystallize above the top of the crystal pile settle to the top of the crystal pile to produce a "cumulate" of fixed initial porosity as set in the ***Initial liquid fraction*** textbox. All liquid above the top of the pile is initially mixed to give a homogeneous composition prior to crystallization.

3) The **Drip** option allows the bulk composition of the topmost node to fall to the top of the crystal pile once the liquid volume fraction falls below the ***F(liq) for drip*** value. Unlike the Bottom accumulation option whereby only solids accumulate on the floor, in this case, the entire liquid and solid assemblage of the topmost falls to the floor. Liquid above the floor is then displaced upward.

Optimal time steps are calculated by the program. However, one can enter a "***Time step multiplier***" in the textbox provided. This number will be multiplied by the time step calculated by the program. Using a number less than 1.0 is useful if you notice the program is giving "saw tooth" results in the graphics window, or is otherwise giving poor results.

One should also enter a "***Minimum F(liquid) for equilibration***" value (typically between 0.01 and 0.10). This value determines the minimum liquid fraction for which stable phase assemblages will be attempted. At low values of f(liquid) the program can have a hard time finding the stable assemblage.

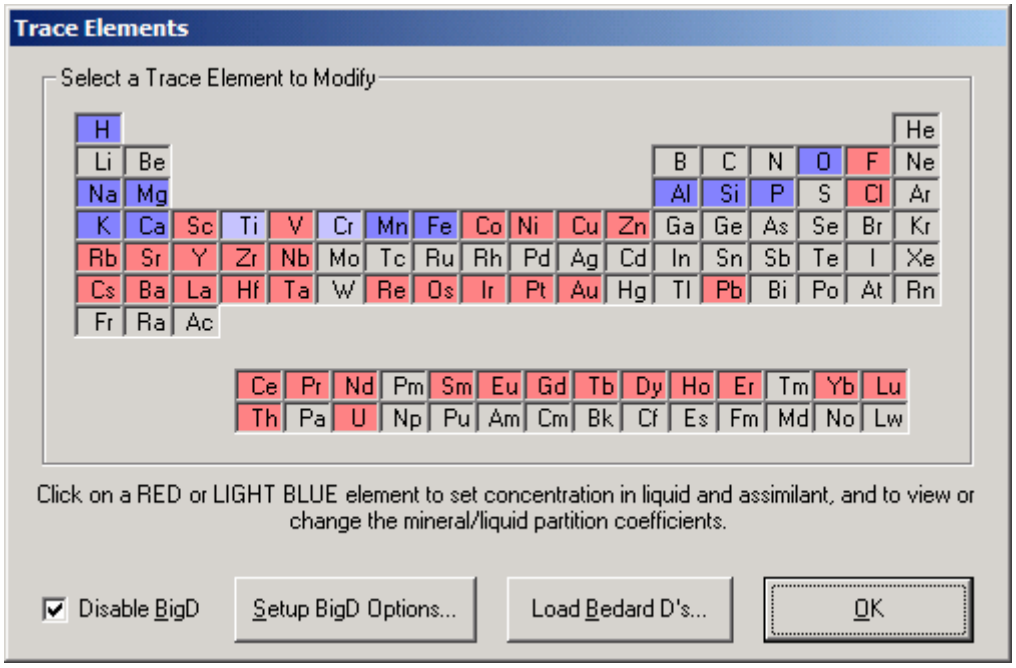
If one wishes a gas phase to migrate, one should enter a value > 0.0 for the ***Vapor velocity parameter***. Gas velocity is then calculated in one of two ways:

1) If compaction is active, then gas velocity is calculated as the characteristic compaction velocity scaled by vapor velocity parameter.

2) If infiltration is active, then gas velocity is calculated as the mass flux velocity (at f(liq) = 1.0) scaled by the vapor velocity parameter.

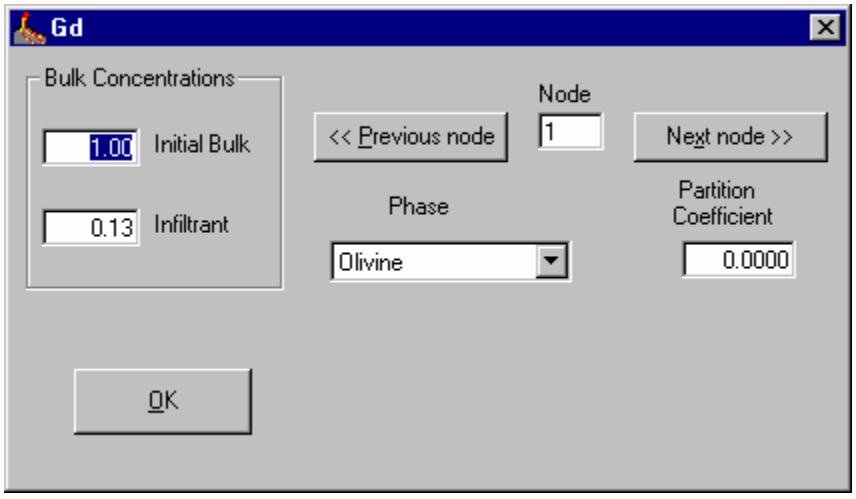
All data entered in this window is saved as part of the Irsetup.Ird file.

Trace Elements Menu Item



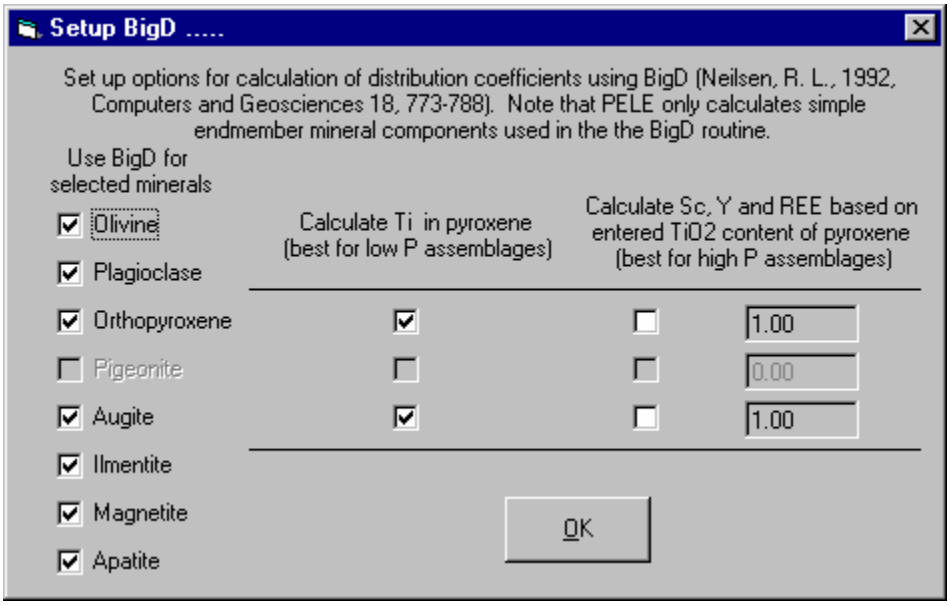
This window allows you to set the partition coefficients for up to 34 trace elements. There are two ways this can be done.

Option 1: Manually enter partition coefficients. Check the check box "***Disable BigD***" and then elect an element from the periodic table. This will bring up the following window:



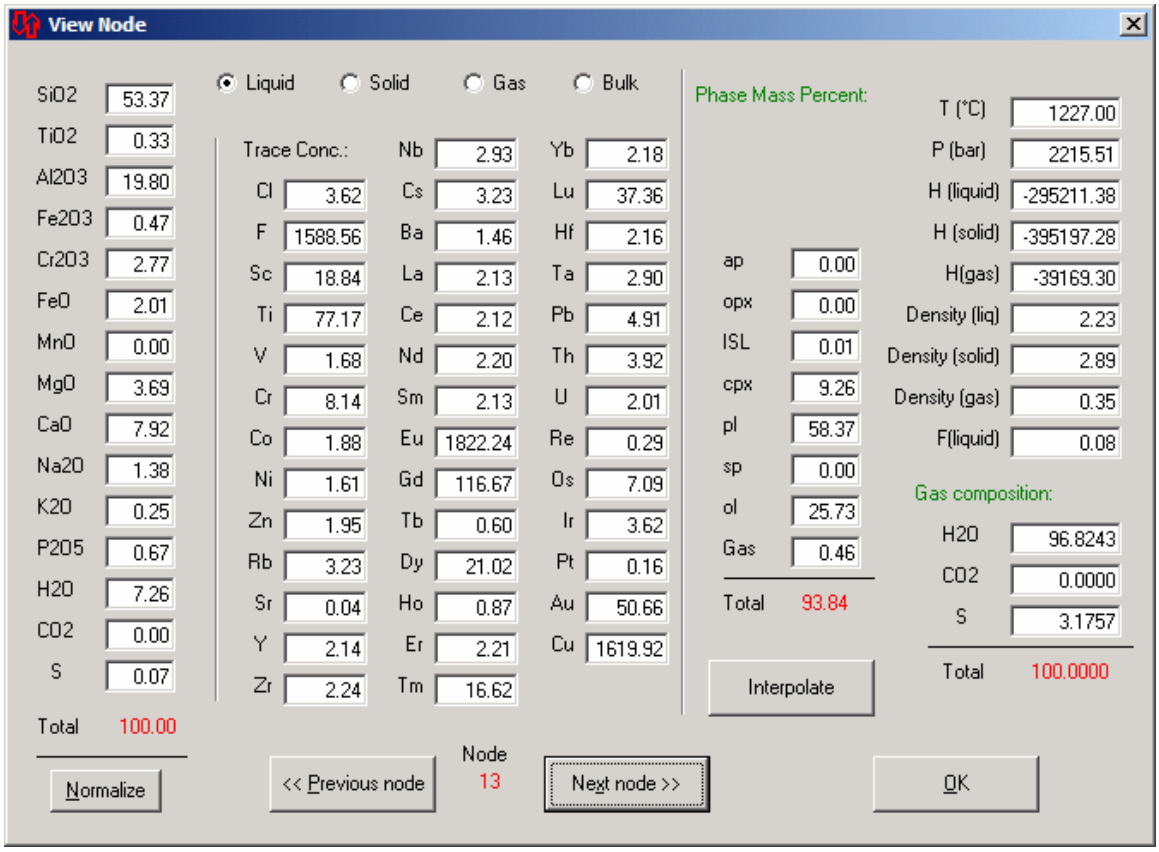
Select a phase and enter the desired partition coefficient. Note that you can also in the window enter the concentration of the trace element at each node. However, this is usually more readily done in the setup bulk windows

Option 2: For those minerals for which it is valid, you can press ***"setup BigD Options"*** to have partitions coefficients calculated by Roger Nielsen's BigD program:



All trace element parameters are saved as part of the Irsetup.Ird file.

View Node Menu Item



This window displays changing bulk compositions at any given node, and can be open while the program is running. It shows most of the data that is used by the program to calculate the stable state at each node. It is most useful for correcting a "bad node" calculation where, for various reasons, the program really screwed the pooch when attempting to find the stable assemblage.

To correct a bad node:

1) It is usually best to halt the program if it is running, and note the last completed iteration.

2) Using the ***load iteration*** on the main form, open to the first iteration that has the bad nodal calculation.

3) Use "***view node***", select a node and then select either ***solid***, ***liquid***, ***gas***, or ***bulk*** to correct or change any parameter for selected node.

4) Option: This is perhaps the best way to correct a minor problem: Find the bad node, then press the "***Interpolate***" button to interpolate values between adjacent nodes. Bulk properties are found by averaging liquid and solid properties from the surrounding nodes. This button is not active for the first or last nodes.