



NICHOLAS SCHOOL OF THE
ENVIRONMENT AND EARTH SCIENCES
DUKE UNIVERSITY

IRidium

A program to model melt
Infiltration and Reaction
through porous rock

User Instructions

Current to version 6

A. Boudreau

Division of Earth and Ocean Sciences, Nicholas School of the
Environment, Duke University, Durham, NC 27708 USA
Boudreau@duke.edu

June 2006

IRidium - Instructions

IRidium

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

A. Boudreau – Duke University

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 at Duke University has led to an increasing need to incorporate more realistic and quantitative models for mineral-liquid equilibria into transport-reaction models.

To this end, the **IRidium** program has been developed for use on windows-based PC's. The mineral-liquid equilibrium calculations are based on the **MELTS** algorithm of Ghiorso and co-workers (Ghiorso and Sack, 1995 and others). 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 and C-O-H-S gas percolate 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.

Because one has mass movement in a pressure field, advective mass and heat transport is assumed to be adiabatic (constant entropy). Entropy change is calculated following the thermal

IRidium - Instructions

diffusion step. Phase equilibration is then done using free energy minimization with a constant entropy constraint, in which the stable phase assemblage and temperature are calculated at each node for the local bulk composition and pressure. For modest pressure gradients, this approach produces results that are indistinguishable from similar but perhaps more familiar heat content (enthalpy) calculations done in a similar stepwise fashion. However, the completeness of the MELTS algorithm on which IRidium equilibration engine is based makes this more thermodynamically rigorous approach possible.

Program Output

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.

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 entropy error remains while in attempting to find the stable assemblage.

XXX.tab - These are optional “snapshots” of an individual iteration that can be saved at any time during the running of the program. For example the file **13.tab** would be results from iteration #13. Data is stored in a more usable form than is the Iroutput.txt file, and the tab-separated values can be easily imported into a spreadsheet to make plots, for example.

IRidium - Instructions

General Steps to Setup and Run the Program

On first opening 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. If doing compaction, setup the compaction parameters.
- 3) Set mass liquid diffusion coefficients, trace element partition coefficients, and other 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. When completed, 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.

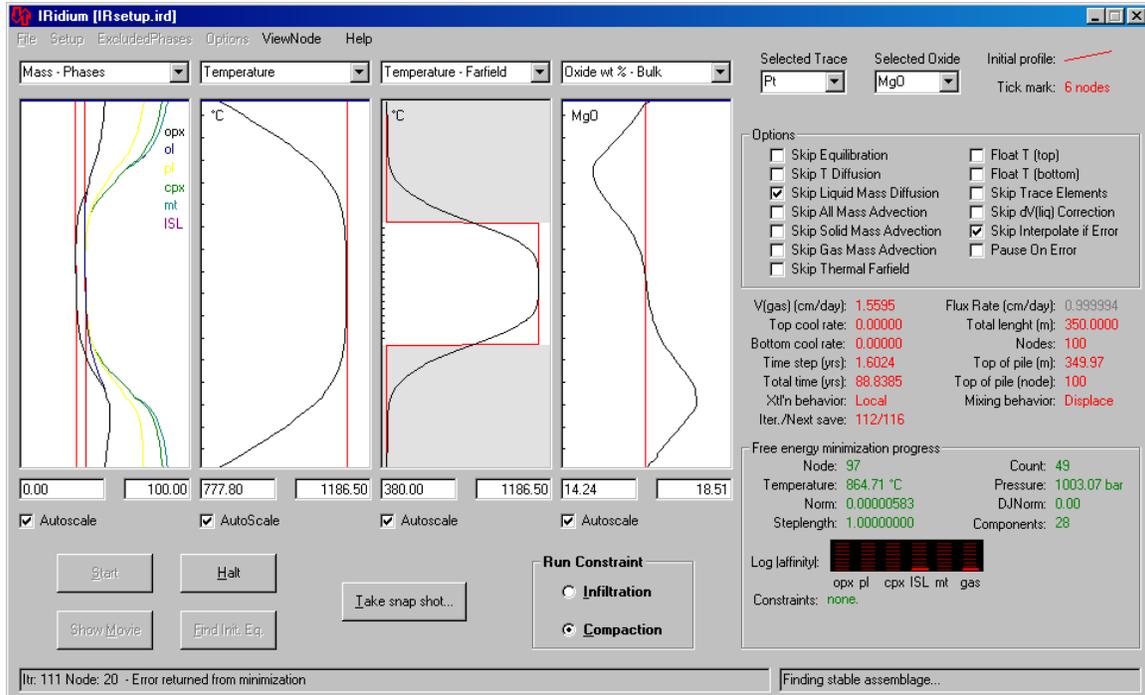
C) Select the "Start" button (Infiltration or Compaction) and watch the simulation run.

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

Remember - Garbage in, garbage out!

IRidium - Instructions

Main Program Window



Descriptions of command buttons:

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

Start - Starts the calculation. This will first calculate the initial assemblage if not already done.

Halt - Stops the calculation at any time.

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

Load Iteration - loads the saved iteration number entered in the textbox above the button. This allows one to stop the program, load the last (or an earlier) stored iteration, make changes to some run parameters if desired, and then restart at the loaded iteration.

Descriptions of Drop-down list boxes:

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

IRidium - Instructions

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:

These 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, and not when the program is calculating the initial stable assemblage.

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

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 Liquid 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 All Mass Advection – Causes the program to skip mass advection of liquids, gas, and solids. Useful if you wish to test or use the mass diffusion module alone.

Skip Solid Mass Advection – Causes the program to skip calculation of solid advection caused by compaction.

Skip Gas Mass Advection – Causes the program to skip calculation of gas advection.

Skip Thermal farfield – Causes the program to assume temperature is controlled by boundary conditions and not by a surrounding thermal buffer (i.e., country rock). See discussion of the thermal farfield in the *Setup – Miscellaneous* menu item description.

Float T (top) and Float T (bottom) – Only active if thermal farfield is inactive. When checked, temperatures at top and/or bottom are calculated from bulk entropy during equilibration. Otherwise T will change as determined by the top and bottom cooling rates entered in the Setup – Miscellaneous window.

Skip Trace Elements – Causes the program to skip the calculation of trace element distribution between solids, liquid and gas.

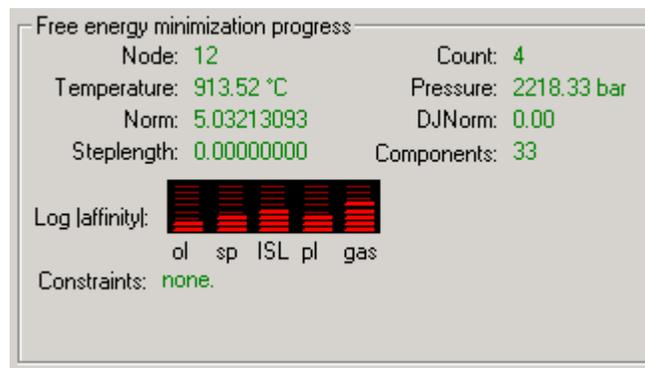
Skip Interpolate if Error – If unchecked, the program will interpolate between nodes for any node for which phase equilibration was unsuccessful.

IRidium - Instructions

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 mass balance correction.

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 entropy 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.

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

IRidium - Instructions

Setup Menu Item

The “Setup” menu selection on the main window is where one selects from several windows to setup the initial bulk compositions and other parameters the program needs. These are explained individually below.

Setup - Setup Bulk...

Setup Initial Bulk Composition

Bulk Oxide Wts.

SiO2	55.53
TiO2	0.42
Al2O3	8.68
Fe2O3	1.48
Cr2O3	0.00
FeO	9.29
MnO	0.00
MgO	16.34
CaO	5.92
Na2O	1.31
K2O	0.55
P2O5	0.04
H2O	0.40
CO2	0.01
S	0.03

Total **100.00**

Bulk Trace Conc.:

Cl	1.00	Nb	1.00	Tm	1.00
F	1.00	Cs	1.00	Yb	1.00
Sc	1.00	Ba	1.00	Lu	1.00
Ti	1.00	La	1.00	Hf	1.00
V	1.00	Ce	1.00	Ta	1.00
Cr	1.00	Nd	1.00	Pb	1.00
Co	1.00	Sm	1.00	Th	1.00
Ni	1.00	Eu	1.00	U	1.00
Zn	1.00	Gd	1.00	Re	1.00
Rb	1.00	Tb	1.00	Os	1.00
Sr	1.00	Dy	1.00	Ir	1.00
Y	1.00	Ho	1.00	Pt	1.00
Zr	1.00	Er	1.00	Au	1.00
				Cu	1.00

Temperature: 1130.00

Number of nodes: 100

Total Length (m): 350.0000

Step length (cm): 350.00

T (top): 1130.00

T (bottom): 1130.00

Pressure (bars, top): 1000.00

Buttons: Find Liquidus T, Halt, Make uniform gradient, Uniform bulk comp., OK

Node: 1

Navigation: << Previous node, Next node >>

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.

IRidium - Instructions

Before one 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 three buttons to make this easier to enter for initially uniform-composition systems. The "**Uniform bulk comp.**" command button on the right-hand side will make all nodes the same bulk composition as the currently listed node. Alternatively, one can select either command button located below the trace element input box labeled "**Make bulk same as previous node**" or "**Make bulk same as next node**" to make the current node the same bulk composition as the previous node (Node - 1) or next node (Node + 1), as desired. 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, one 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 calculated based on bulk density and step length.

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

IRidium - Instructions

Setup - Setup Infiltrant...

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. One can either enter a liquid composition (both major oxides and trace elements) or, optionally, one 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 your 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.

IRidium - Instructions

Setup - Setup Compaction...

Setup Compaction Parameters

0.0500 Minimum liquid fraction (0.001 - 0.05 typ.)

0.30 Grain radius (mm)

5.00E+14 Solid 'compaction' viscosity (Pa s)

11.00 Liquid viscosity (Pa s)

Use constant liquid viscosity

1.50E-03 Permeability constant (Ko)

0.30 Density difference (g/cc)

Use constant density difference

Characteristic dimensions

Compaction length scale (m): 78.33

Compaction time scale (days): 25,127.74

Compaction velocity (cm/s): 3.61E-05

Use Shirley... OK

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 equilibrium 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.

IRidium - Instructions

Setup - Setup Diffusion Coefs...

Setup Diffusion Coefficients

Diffusion Coefficients	Soret Coefficients			
SiO2	1.00E-06	SiO2	-1.70E-03	Enter or edit diffusion and optional soret coefficients at left. Off-diagonal diffusion coefficients are not currently implemented. One component (e.g., SiO2) must be set to zero. This one component, highlighted in red, is calculated by mass balance. If none are set to zero, then the diffusion coefficient for SiO2 is set to zero and SiO2 is calculated by mass balance. If more than one component is set to zero, then the first entered D = 0.0 component is found by mass balance.
TiO2	5.00E-07	TiO2	2.00E-03	
Al2O3	0.00E+00	Al2O3	0.00E+00	
Fe2O3	1.00E-06	Fe2O3	2.70E-03	
Cr2O3	1.00E-06	Cr2O3	2.00E-03	
FeO	1.00E-06	FeO	2.70E-03	
MnO	1.00E-06	MnO	2.00E-03	
MgO	1.00E-06	MgO	3.10E-03	
CaO	1.00E-06	CaO	2.20E-03	
Na2O	5.00E-06	Na2O	-8.00E-04	
K2O	3.00E-06	K2O	-1.40E-03	
P2O5	1.00E-07	P2O5	0.00E+00	
H2O	1.00E-05	H2O	0.00E+00	
CO2	0.00E+00	CO2	0.00E+00	
S	0.00E+00	S	0.00E+00	

1.00E-07

D(liquid) - trace elements

0.00E+00

D(gas) - major and trace elements

Include Soret diffusion

OK

Cancel

This window allows one to set mass diffusion coefficients, D, for mass diffusion in the liquid. Note that one component must be entered as zero (0.00): this component is found by mass balance and will be highlighted in red.

Optionally, one can also set soret diffusion, σ , for mass diffusion in a thermal gradient. If active, the total diffusion flux, J, is calculated from the following:

$$J = -D \frac{\partial C}{\partial z} - \sigma DC \frac{\partial T}{\partial z}$$

Starting with version 6.03 this data is no longer saved in a separate file, but is now saved as part of the Irsetup.Ird file.

For trace elements, all are assumed to have a fixed diffusion coefficient; if set to zero, trace element diffusion is not calculated. Diffusion for both trace and major elements in a gas phase is similar.

IRidium - Instructions

Setup - Setup Partition Coefs...

Partition Coefficients			
Cl	0.0000	Sr	0.0000
F	0.0000	Y	0.0000
Sc	0.1600	Zr	0.0000
Ti	0.0000	Nb	0.0000
V	0.1900	Cs	0.0000
Cr	1.2500	Ba	0.0000
Co	3.2000	La	0.0000
Ni	10.0000	Ce	0.0000
Zn	0.8300	Nd	0.0000
Rb	0.0000	Sm	0.0000
Eu	0.0000	Ta	0.0000
Gd	0.0000	Pb	0.0000
Tb	0.0000	Th	0.0000
Dy	0.0000	U	0.0000
Ho	0.0000	Re	0.0000
Er	0.0000	Os	0.0000
Tm	0.0000	Ir	0.0000
Yb	0.0100	Pt	0.0000
Lu	0.0100	Au	0.0000
Hf	0.0000	Cu	0.0000

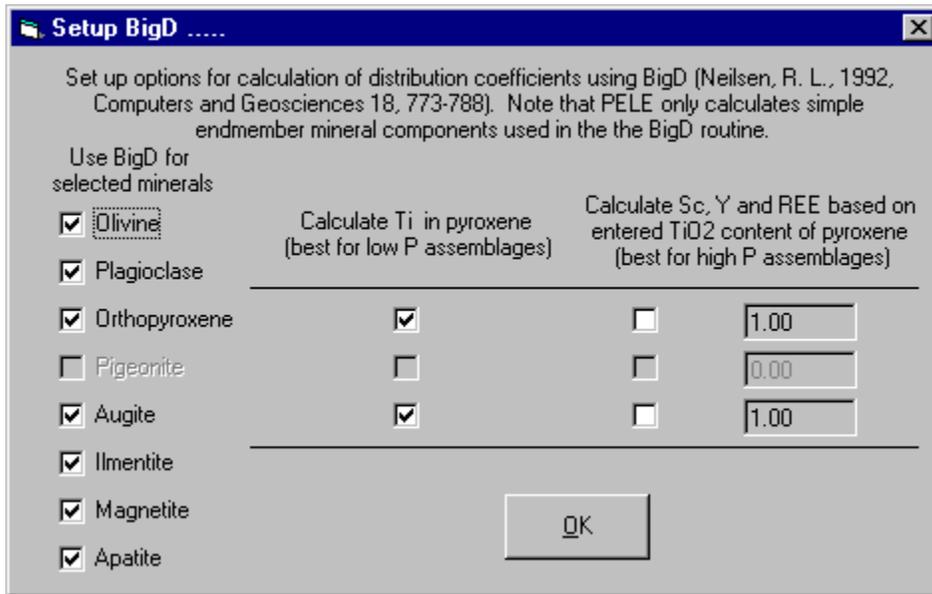
Trace element partitioning can be calculated by assuming either constant partition coefficients or, for those elements and phases where it is valid, using the subroutine BigD (Neilsen, R.L., 1992, Computers and Geosciences 18:773-788). This later option can be disabled by checking the **Disable BigD** 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 as part of the Irsetup.Ird file, or it can be saved manually through the menu item **File – Save as**.

IRidium - Instructions

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



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

IRidium - Instructions

Setup - Setup Miscellaneous...

Thermal Properties

Diffusivity (cm² sec⁻¹)

Allowable equilibration entropy error (0.01 J/C typical)

Thermal Farfield:

Relative thickness (0 - 3)

Top	Bottom	Initial T Farfield (0 - 2500 C)
<input type="text" value="950.00"/>	<input type="text" value="800.00"/>	
<input type="text" value="0.00E+00"/>	<input type="text" value="0.00E+00"/>	T Step (C/day)
<input type="text" value="2000.00"/>	<input type="text" value="2000.00"/>	Maximum T
<input type="text" value="500.00"/>	<input type="text" value="500.00"/>	Minimum T

Mixing behavior

Displace magma Mix magma

Magma crystallization behavior

Local equilibrium

Crystal settling Initial liquid fraction

Drip off top F(liq) for drip

Time step multiplier (0.01 - 1.0 typical)

Min. F(liq) for equilibration (0.10 typical)

Vapor velocity parameter

Record save interval (1-10 typical)

iterations between equilibration (1 typical)

Thermal Properties: Thermal diffusion can be calculated in one of two ways. They are illustrated in the two plots shown on the next page.

1) **Fixed thermal boundary:** One can specify the temperature at the upper and lower boundaries of the system and the rates at which they can change. Initial temperatures at the boundaries are as set in the *Setup bulk...* window. The *Skip Thermal Farfield* checkbox on the main form should be *checked* to use this option, and/or the *thermal farfield relative thickness* should be set to 0.

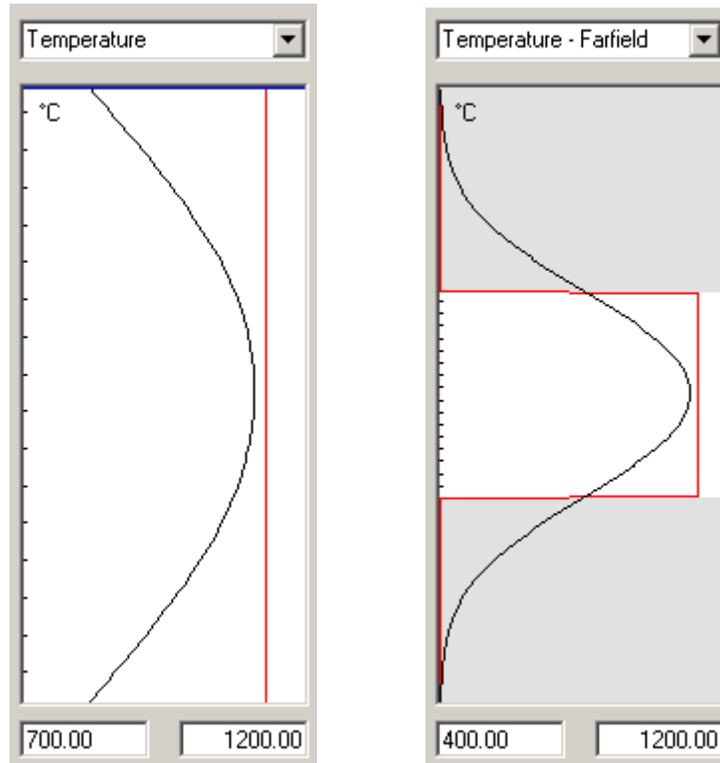
Note: If the option boxes *T float (top)* or *T float (bottom)* in the main program window are checked, as well as the **skip thermal farfield**, then these boundary rate values are ignored and T is calculated from the bulk entropy during the equilibration calculations.

2) **Thermal farfield:** Alternatively, one can have heat lost to a thermal buffer above and below the system (the *thermal farfield*). The only purpose of the thermal farfield is to act as a thermal sink to the system. It has no bulk properties other than a thermal diffusivity. The *Skip Thermal Farfield* checkbox on the main program window should be *unchecked* to use this option. One also set the *Thermal farfield relative thickness* to an integer value between 1 and 3.

A fixed thermal diffusivity is entered for both the system and thermal farfield. A cooling rate (*T step*) for the top and the bottom can also be specified, as well as minimum and

IRidium - Instructions

maximum temperature limits. This T step is applied to the top/bottom of the thermal farfield if it is active, otherwise it applies to the top/bottom of the system alone. Temperature change will stop once a boundary temperature reaches the set limit. Cooling rates are per day and must be negative numbers if you wish temperature to drop with time. These rates are typically set to zero if using the thermal farfield, but need not be.



*Examples of the two thermal profile plots that can be selected from the main program window. Right shows temperature distribution in the system alone. Left shows temperature distribution in the system (white area) and in the surrounding farfield thermal buffer (grey areas). The red line in both plots is the initial temperature distribution, in this case a opx-phyric magma at 1130 °C intruding country rock at 400 °C. The black line show the temperature profile after the system has evolved (crystallized) for some time. Note that the thermal farfield region will not change if **skip thermal farfield** is checked on the main window*

Properties of the thermal farfield include the **relative thickness**, which is the thickness of the thermal buffer above and below relative to the thickness of the system. For example, if the column is 100 m thick and the relative thickness parameter is set to 2, then the thermal buffer above and below the system will each be 200 meters thick.

One also sets the temperature of the top and bottom of the thermal farfield. Initial temperatures within the thermal farfield are assumed to be a linear gradient between the two, excluding the temperature of the system itself. For example, if the top and bottom farfield temperatures are set at 600 and 800 °C (to mimic a geothermal gradient perhaps?), then the initial temperature of the thermal farfield at the contact with the system will be 700 °C at both the bottom and top of the system. Note that within the system, the bottom and top nodes will have the initial temperatures as set in the **Setup**

IRidium - Instructions

bulk... window. This means there can be some initially large temperature changes during the first few iterations, and a small *time step multiplier* (see below) might be selected until the system smoothes out the thermal profile.

Finally, one needs to enter an "*allowable equilibration entropy error limit*". For the isentropic equilibrium calculations done for most nodes, the program tries to find the stable assemblages based on total entropy to within 0.0001 J/°C-100g. However, nodes where phases are only marginally stable may cause larger errors. 0.01 J/°C-100g 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 magma* option will cause the new magma to mix adiabatically 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 from liquid 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. The *mix magma* option should also be selected so that all liquid above the top of the pile is initially mixed to give a homogeneous composition prior to crystallization. The program assumes that heat is lost from the top, so only solids in the top node are calculated in the all-liquid part of the system if this option is active.
- 3) The *Drip off top* 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 top of the crystal pile. Liquid above the pile is then displaced upward. As for bottom accumulation, the program assumes that heat is lost from the top, so only solids in the top node are calculated in the all-liquid part of the system if this option is active.

For both the *Bottom accumulation* and *Drip off top* options, settling through a thick column of liquid (large pressure gradient) means that the solids will be out of equilibrium with the liquid at the top of the crystal pile. This is corrected during the next iteration when the solid-liquid assemblage of the pile is again computed.

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. For example, when using the thermal farfield with a sharp thermal break at the top and bottom boundaries, one might set the time step multiplier to an initially low value until the thermal profile smoothes out. Also, 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.

IRidium - Instructions

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 for the *Vapor velocity parameter*. There is no formal model for gas mass advection; gas velocity is arbitrarily calculated in one of three ways:

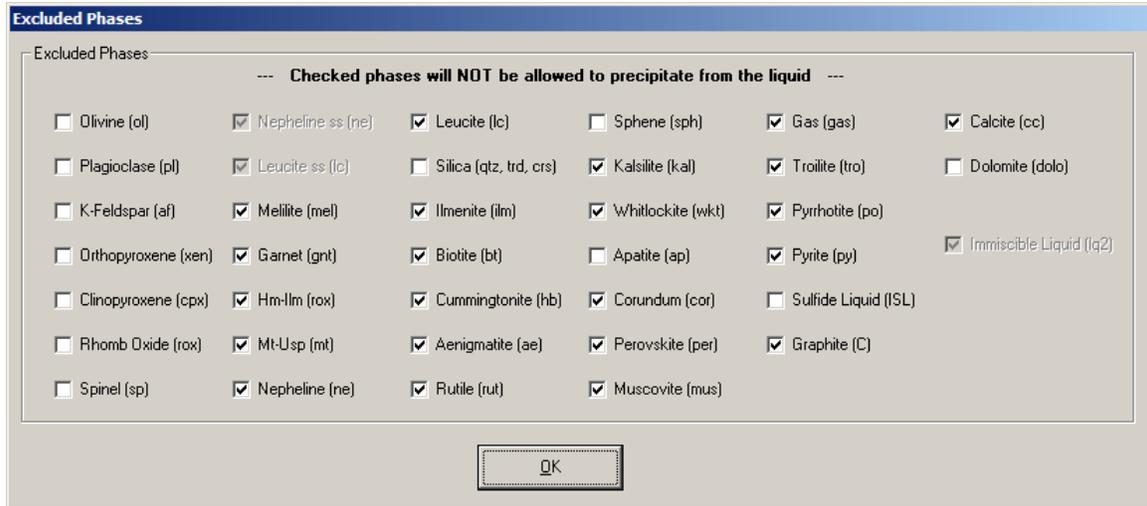
- 1) If compaction is active, then gas velocity is calculated as equal to the characteristic compaction velocity scaled by vapor velocity parameter, as long as this parameter is positive.
- 2) If infiltration is active, then gas velocity is calculated as equal to the mass flux velocity (at $f(\text{liq}) = 1.0$) scaled by the vapor velocity parameter, again as long as this parameter is positive.
- 3) If the vapor velocity parameter is set less than zero (e.g., -X), then the vapor will move X nodes upward at each iteration regardless of the infiltration or compaction option selected or calculated time step. For example, setting the parameter to -1 will move the gas upward one node at each iteration. This is perhaps the best choice, as this ensures that the gas does not move too fast and possibly move too far into vapor-undersaturated liquids.

The limits on the vapor velocity parameter are -10 to +100.

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

IRidium - Instructions

ExcludedPhases Menu Item



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 component Rhomb Oxide, Hm - Ilm, or pure Ilmenite). You cannot select more than one of each type of oxide.

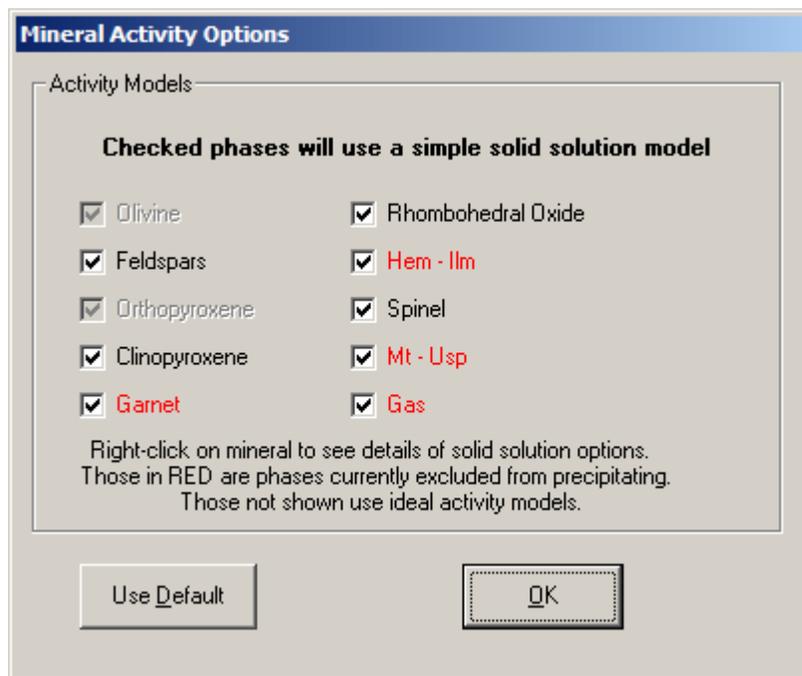
IRidium - Instructions

Options Menu Item

Options - Set current state as initial...

Selecting this option allows one to set the current state of the system as a new initial bulk composition, temperature profile, etc. This can then be modified through the various **Setup** options. This can be useful, say to mimic the effect of a new magma influx into a magma chamber.

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

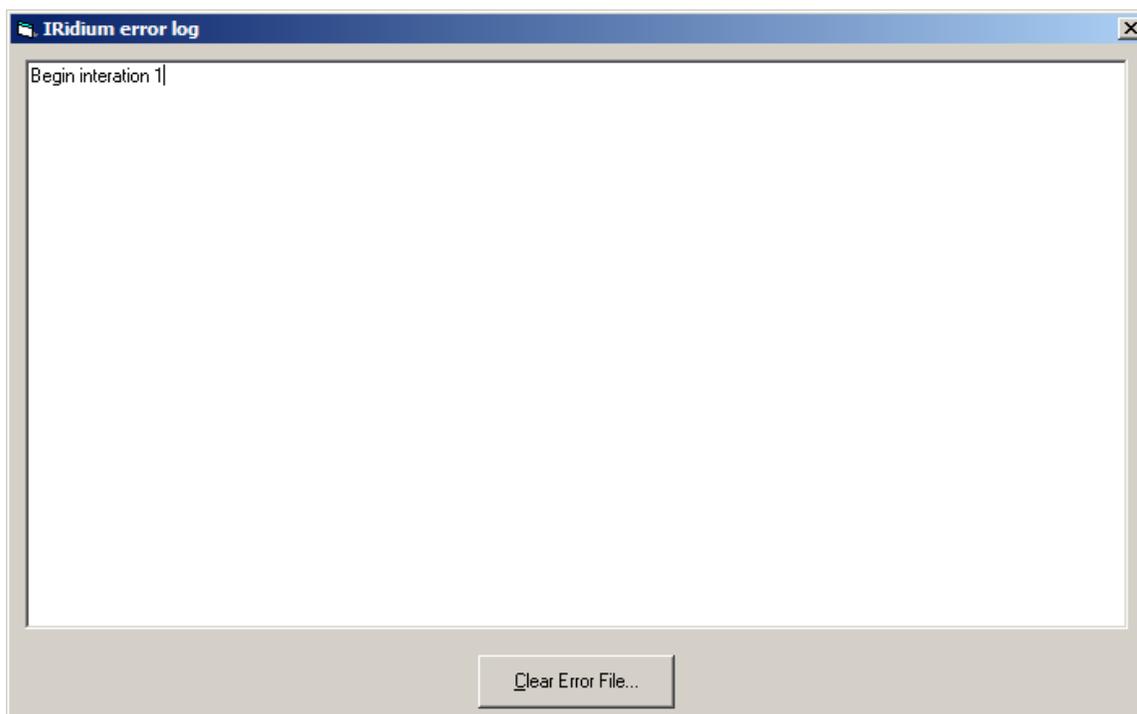
Except for olivine and orthopyroxene, the code for both calculating and minimizing these non-ideal solid solutions is still being improved and debugged. Needless to say, using these non-ideal activity models can cause the program to halt prematurely.

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)

IRidium - Instructions

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.

View Events Menu Item



This window displays any errors or other events logged by the program and stored in the file "IRlog.txt". You can clear the log file by clicking on the button "Clear event file..."

IRidium - Instructions

View Node Menu Item

The 'View Node' window displays a comprehensive set of input fields for defining a node's composition and state. On the left, a list of oxides and elements (SiO2, TiO2, Al2O3, Fe2O3, Cr2O3, FeO, MnO, MgO, CaO, Na2O, K2O, P2O5, H2O, CO2, S) has numerical input boxes. A 'Total' field shows 100.000. Below this is a 'Normalize' button. The central area features radio buttons for 'Liquid' (selected), 'Solid', 'Gas', and 'Bulk'. A 'Trace Conc.' section lists various elements (Nb, Yb, Cs, Lu, Ba, Hf, La, Ta, Ce, Pb, Nd, Th, Sm, U, Eu, Re, Gd, Os, Ir, Tb, Pt, Dy, Au, Ho, Er, Cu, Y, Tm, Zr) with their respective values. To the right, 'Phase Mass Percent' fields show S (liquid) at 73.28, S (solid) at 77.45, and S (gas) at 0.00. Physical properties like T (°C) at 1200.00, P (bar) at 2005.67, and densities for liquid, solid, and gas phases are also present. A 'Gas composition' section lists H2O, CO2, H2S, SO2, CO, and CH4, all at 0.0000. A 'Total' field for gas composition shows 0.0000. At the bottom, there are buttons for 'Use prev.', 'Interpolate', 'Use next', '<< Previous node', 'Node 2', 'Next node >>', and 'OK'.

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 the iteration that has the bad nodal calculation.
- 3) Use "***view node***", select a node and then select either ***solid***, ***liquid***, or ***gas*** to correct or change any parameter for selected node. The bulk will be undated automatically
- 4) Option: This is perhaps the best way to correct a minor problem: Find the bad node, and then press the "***Interpolate***" button to interpolate values between adjacent nodes. All properties are found by averaging liquid and solid properties from the surrounding nodes.

IRidium - Instructions

To correct the first or last node , this button will be labeled “*Extrapolate*” and will make a linear extrapolation from the previous or next two nodes.

Alternatively, one can select “*Use prev.*” or “*Use next*” to make all properties of the current node identical to the previous/next node.