

COMPUTER METHODS AND MODELING IN GEOLOGY

RADIOACTIVE DECAY AND GEOCHRONOLOGY - ANSWER KEY

The parts of this exercise for students are in normal text, whereas answers and explanations for faculty are italicized.

Decay of naturally occurring radioactive isotopes in minerals provides a means by which we can date rocks and geological processes. Several elements have between 1 and 3 radioactive isotopes, for a total of 70 radioisotopes. Decay occurs primarily by emission of a helium nucleus from the radioisotope, a process called alpha decay, or by conversion of a neutron to a proton and electron followed by loss of the electron, called beta decay. Both forms of decay release energy, and this energy has contributed to keeping the interior of the Earth warm over the 4.5 billion years of its history.

Because the rate of decay of a particular radioisotope to a stable daughter product is fundamental to that isotope, and because that rate has remained invariant over geologic time, we can use the abundance of radioisotopes and their daughter products in rocks to determine the time of their formation. Radiometric dating works most reliably in igneous rocks, and the age derived generally marks the time of crystallization of the magma. However, radiometric dating has also been applied in special cases to sedimentary rocks. Conditions necessary for accurate radiometric dating include:

- 1) The rock containing the radioisotope and its daughter products has forever remained closed to those atoms, and
- 2) The original abundance of daughters in the rock before radioactive decay began is either zero, or can be known.

In today's class we will model the radioactive decay process, and then learn how the special radioactive series $^{238}\text{U} \rightarrow ^{206}\text{Pb}$ and $^{237}\text{U} \rightarrow ^{205}\text{Pb}$ can be used even when condition 1 is violated to determine both the time when a rock initially crystallized and when it underwent a recrystallization. I want you to answer all of the questions below. Open up Microsoft Word at the same time that you have STELLA running. You can write the answers to your questions as you go along. You can also paste any graphs you would like to use to answer your questions into your Word document to hand in to me.

Readings

Dalrymple, G.B., 1991, *The Age of the Earth*, Stanford, CA: Stanford University Press, p. 79-90, 99-102, 115-119, and 122-124.

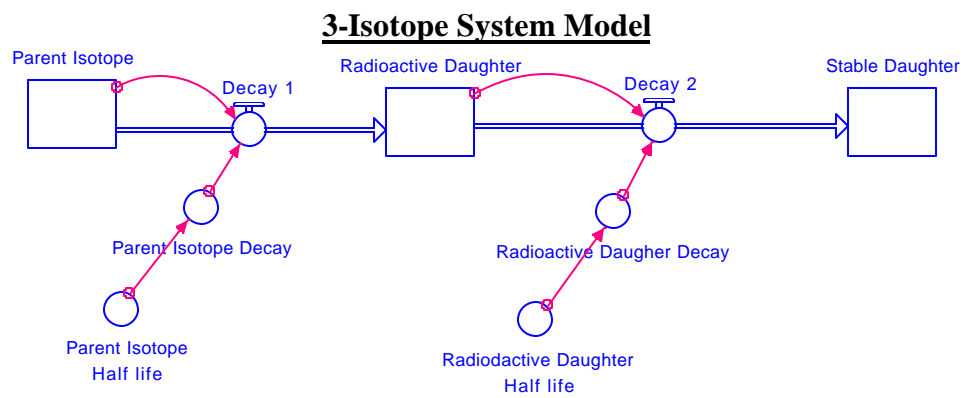
Faure, G., 1986, Principles of Isotope Geology, 2nd Edition, New York: John Wiley and Sons, p. 38-45 and p. 283-296.

Exercises

General Problems

- 1) Create a STELLA model of a 3isotope system in which a parent isotope decays to a radioactive daughter that in turn decays to a stable daughter. You may name your isotopes anything you like.

This model can be found in the file named "Documented_Isotope_Model.stm."



3-Isotope Model code - provided in the event that you are using an older version of STELLA than we're using or if you have problems downloading and opening the model

$$\text{Parent_Isotope}(t) = \text{Parent_Isotope}(t - dt) + (- \text{Decay_1}) * dt$$

$$\text{INIT Parent_Isotope} = 100$$

OUTFLOWS:

$$\text{Decay_1} = \text{Parent_Isotope} * \text{Parent_Isotope_Decay}$$

$$\text{Radioactive_Daughter}(t) = \text{Radioactive_Daughter}(t - dt) + (\text{Decay_1} - \text{Decay_2}) * dt$$

$$\text{INIT Radioactive_Daughter} = 0$$

INFLOWS:

$$\text{Decay_1} = \text{Parent_Isotope} * \text{Parent_Isotope_Decay}$$

OUTFLOWS:

$$\text{Decay_2} = \text{Radioactive_Daughter} * \text{Radioactive_Daughter_Decay}$$

$$\text{Stable_Daughter}(t) = \text{Stable_Daughter}(t - dt) + (\text{Decay_2}) * dt$$

$$\text{INIT Stable_Daughter} = 0$$

INFLOWS:

$$\text{Decay_2} = \text{Radioactive_Daughter} * \text{Radioactive_Daughter_Decay}$$

$Parent_Isotope_Decay = \text{LOGN}(2)/Parent_Isotope_Half_life$
 $Parent_Isotope_Half_life = 1$

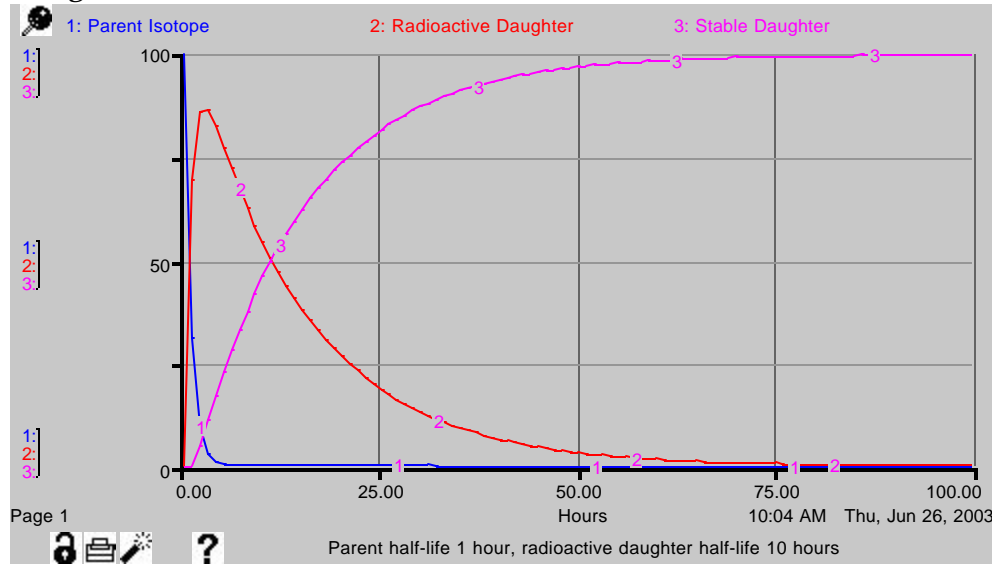
$Radioactive_Daughter_Decay = \text{LOGN}(2)/Radioactive_Daughter_Half_life$
 $Radioactive_Daughter_Half_life = 10$

2) Now that your model is created, assign the following values:

Initial number of radioactive parents = 100
Initial number of radioactive daughters = 0
Initial number of stable daughters = 0
Half life of radioactive parent = 1 hr
Half life of radioactive daughter = 10 hrs

3) Run your model for about 50 hours and keep track of the number of radioactive parents, radioactive daughters, and stable daughters as a function of time. **Describe and explain** what you observe. In particular, explain the graph representing the number of radioactive daughters as a function of time.

-Range = 0 – 50 hours, DT = 1 hour

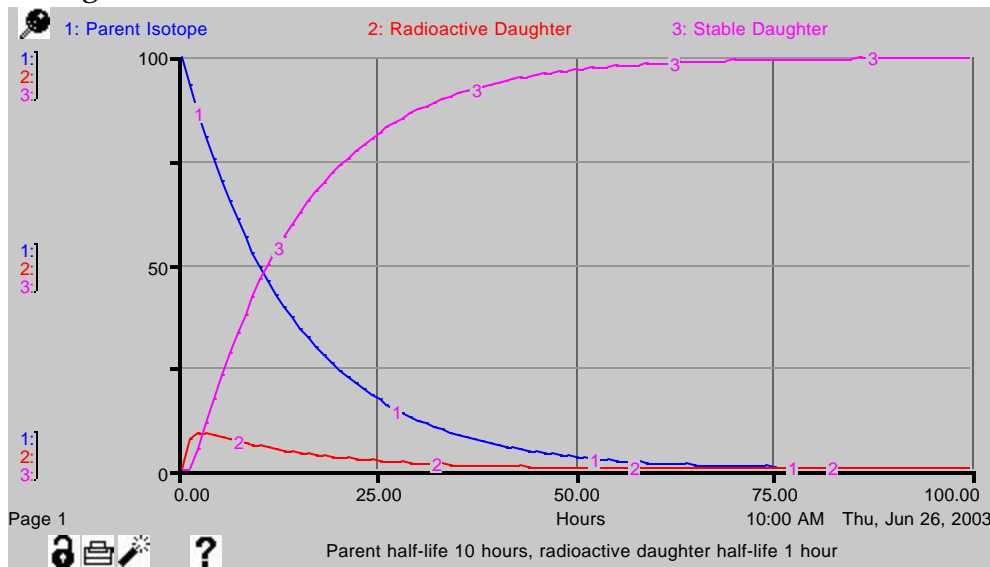


The amount of the parent isotope decreases and levels off to nearly 0 quickly because it has a very short half-life of 1 hour. As the parent isotope decays, the radioactive daughter initially experiences a rapid rate of growth equal to the rate of decay of the parent. However, the radioactive daughter then begins to decay itself, and therefore never reaches the number of atoms of the original parent reservoir. As the radioactive daughter decays,

the stable daughter starts to grow. Since the decay flow of isotopes depends on the number of isotopes in the reservoir (i.e., $dP/dt = -\lambda P$ where dP/dt is the change in the number of atoms per time, P is the number of atoms, and λ is the decay constant), the number of parents asymptotically approaches 0, and the number of stable daughters asymptotically approaches a value equivalent to the initial number of parents.

- 4) Now change the half-lives so that the radioactive parent is 10 hrs and the radioactive daughter is 1 hr. What impact does changing the half-lives have on the abundance of the different isotopes as a function of time?

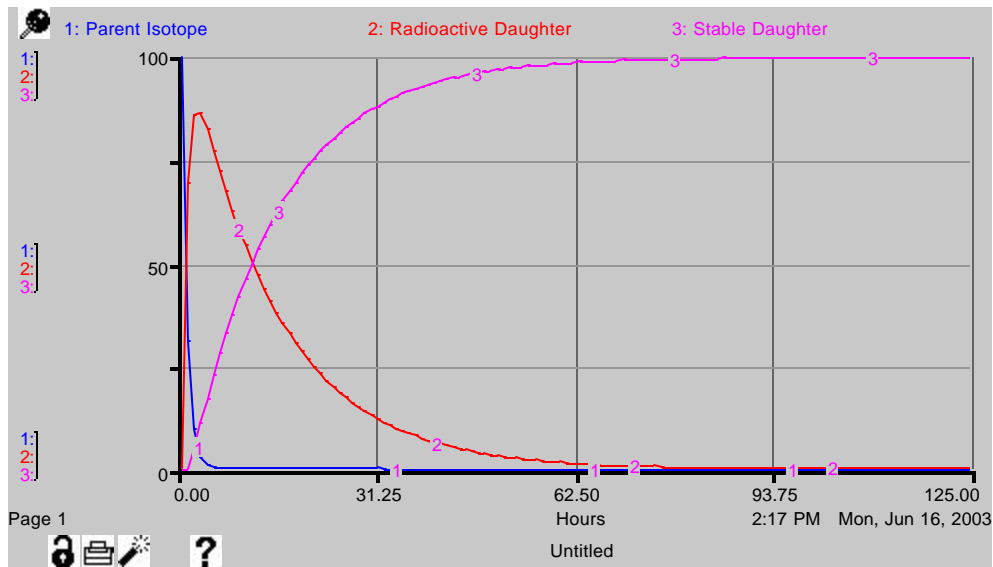
- Range = 0 – 50 hours, DT = 1 hour



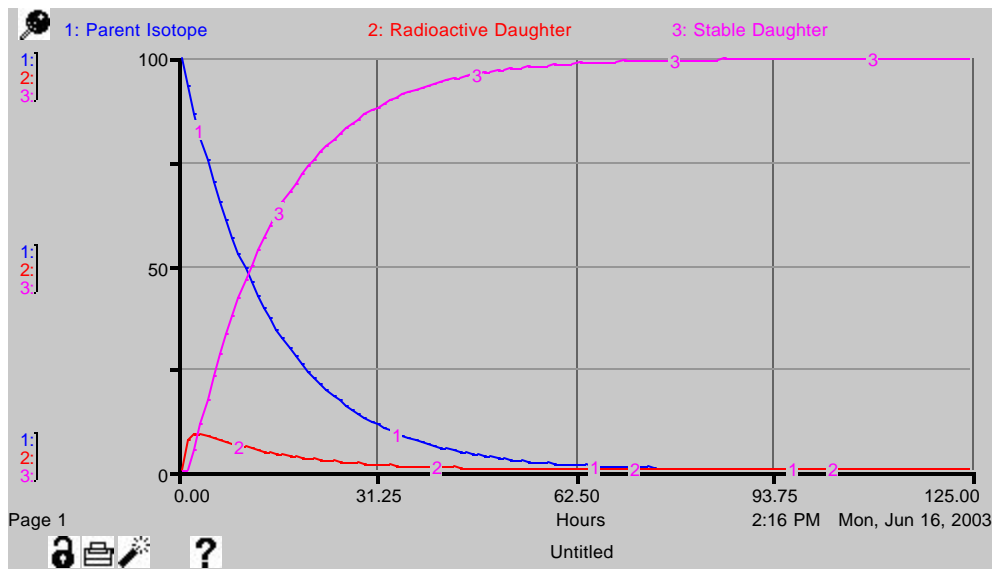
Increasing the half-life of the parent causes it to decay much more slowly. The radioactive daughter isotope concentration still peaks at about the same time, but has a much lower peak value because it now decays much faster (shorter half-life).

- 5) How do the final results of the isotopic decay compare to the final results of the decay in problem 2-3? Does the decay come to completion at the same time? Why or why not? Note: you may need to extend your simulation period to answer this question.

- Range = 0 – 125 hours, DT = 1 hour, parent half-life = 1 hour, rad. daughter half-life = 10 hrs.



- Range = 0 – 125 hours, DT = 1 hour, parent half-life = 10 hours, rad. daughter half-life = 1 hr



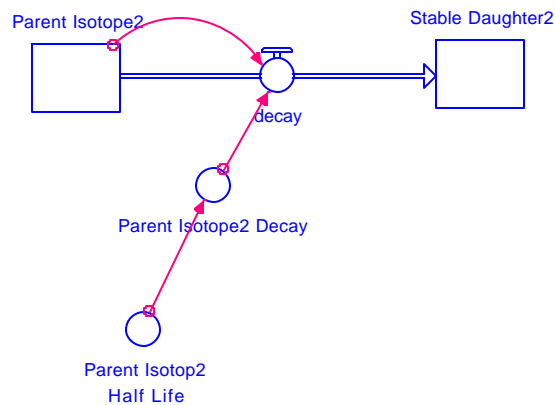
It takes about the same amount of time for nearly all of the atoms to become the stable daughter for both cases. However, for the first case, the parent is used up much faster than in the second case, and the radioactive daughter takes much longer to decay completely. This is simply a reflection of the changed half-lives (longer half-life takes longer to decay, and vice-versa).

6) Geochronologists discovered that isotopic decay series in which the parent isotope has a much longer half life than the daughter products can be

modeled as a decay straight from the radioactive parent to the final stable daughter product, a concept known as "secular equilibrium." Create a STELLA model on the same page as your existing model and prove that in fact this is the case. **Explain** your proof.

Note: STELLA will not allow you to have 2 reservoirs with the same name, so you will need to modify the names of the components in your second model somewhat.

Secular Equilibrium Model - placed on same STELLA model page below original 3-isotope model



Secular Equilibrium Model code

$$Parent_Isotope2(t) = Parent_Isotope2(t - dt) + (- decay) * dt$$

$$INIT Parent_Isotope2 = 100$$

OUTFLOWS:

$$decay = Parent_Isotope2 * Parent_Isotope2_Decay$$

$$Stable_Daughter2(t) = Stable_Daughter2(t - dt) + (decay) * dt$$

$$INIT Stable_Daughter2 = 0$$

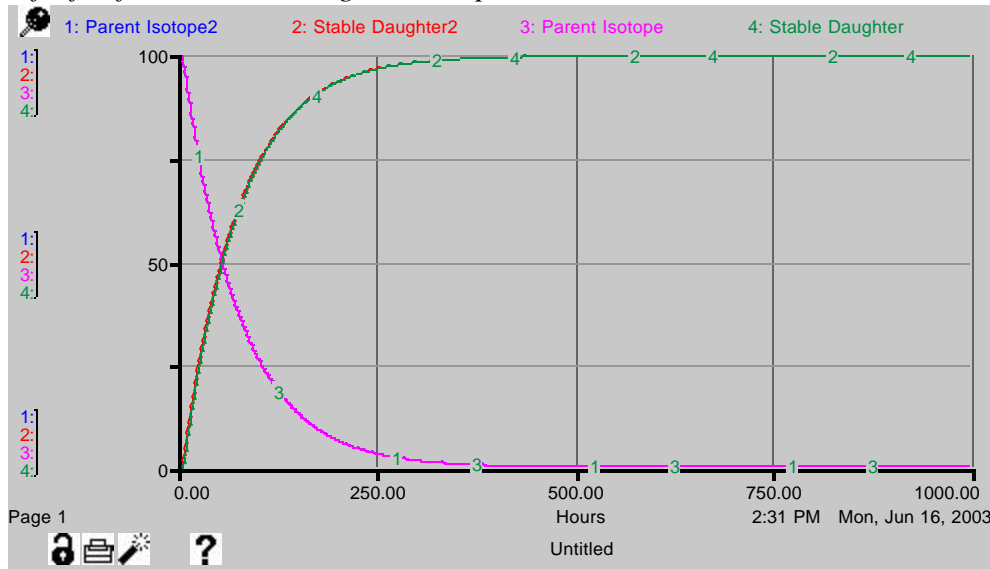
INFLOWS:

$$decay = Parent_Isotope2 * Parent_Isotope2_Decay$$

$$Parent_Isotop2_Half_Life = 100$$

$$Parent_Isotope2_Decay = LOGN(2)/Parent_Isotop2_Half_Life$$

- Range = 0 – 1000 hours, DT = 1 hour, half-life of both parent isotopes = 100 hours, half-life of radioactive daughter isotope = 1 hr.



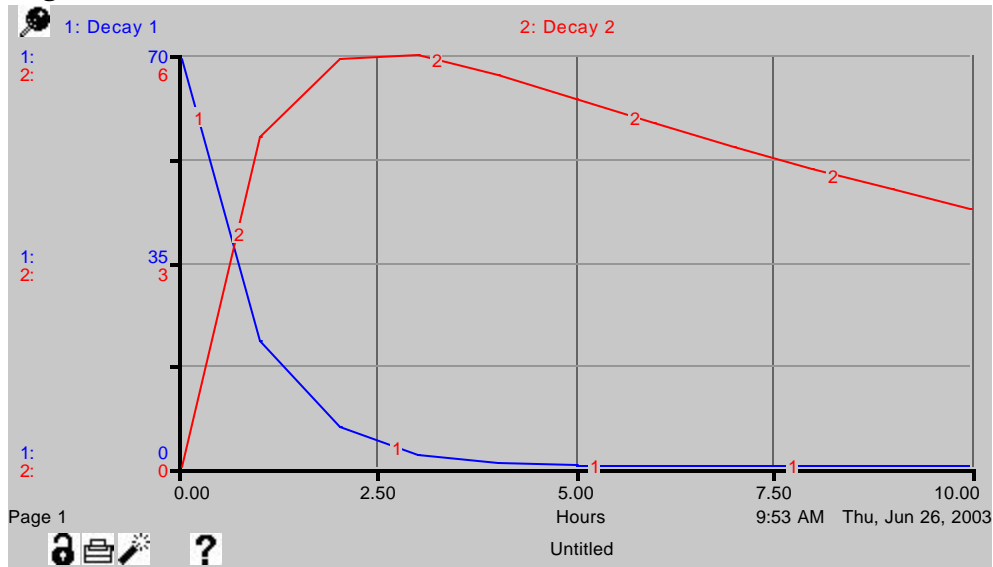
The above graph shows the amount of radioactive parent and stable daughter as a function of time for both the 3-isotope (variable names Parent Isotope and Stable Daughter) and the 2-isotope secular equilibrium (variable names Parent Isotope2 and Stable Daughter2) models. In each case, the half-life of the parent isotope has been set at 100 hours, and in the 3-isotope model, the half-life of the radioactive daughter has been set to 1 hour. Since the curves for the 2 models coincide, the model that eliminates the intermediate radioactive daughter still captures the behavior of the parent and stable daughter of the more complex system. The half-life for the parent isotope is so much bigger than the half-life of the radioactive daughter that the radioactive daughter doesn't get a chance to build up to a significant amount and can be ignored.

7) In secular equilibrium,

$$I_1 N_1 = I_2 N_2 \dots = I_n N_n$$

Where N_1 , N_2 and N_n are the quantities of the radioactive parent (subscript 1) and its radioactive daughters (subscript 2 ... n), and λ_1 , λ_2 and λ_n are the decay constants. Modify your STELLA program to graph $\lambda_1 N_1$ and $\lambda_2 N_2$ over time, and then set the half-life of the parent to 1 hour and that of the radioactive daughter to 10 hours. Run your model for about 10 hours. Are the values you achieve at the end of the run consistent with the equation above?

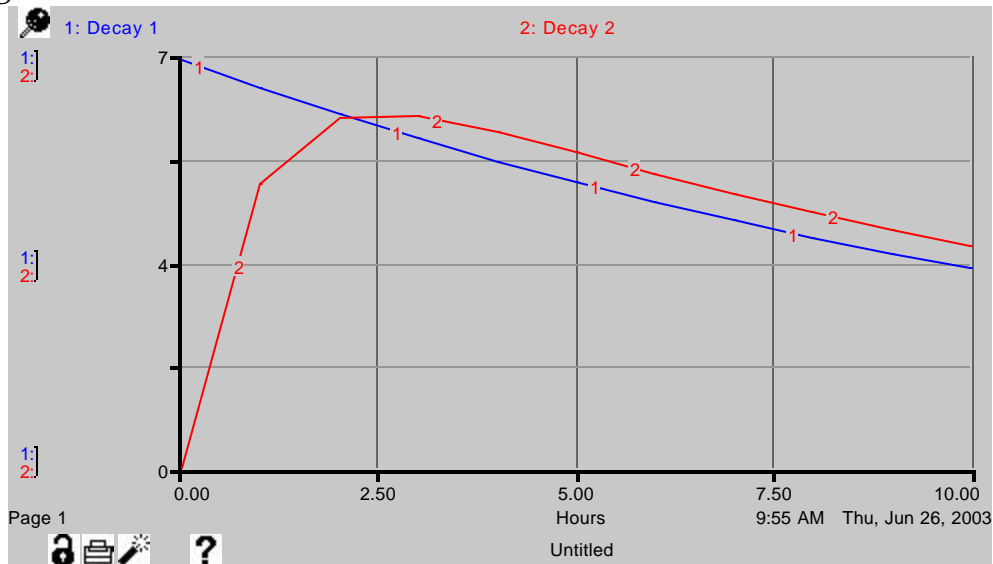
- Range = 0-10 hours, DT = 1 hour



I_1N_1 and I_2N_2 are simply the decay fluxes, so this question can be answered by graphing them. With a parental half-life of 1 hour and radioactive daughter half-life of 10 hours, secular equilibrium is not achieved by the end of the run.

8) Now change the half-life of the parent to 10 hours, and that of the daughter to 1 hour. Describe and explain what you see.

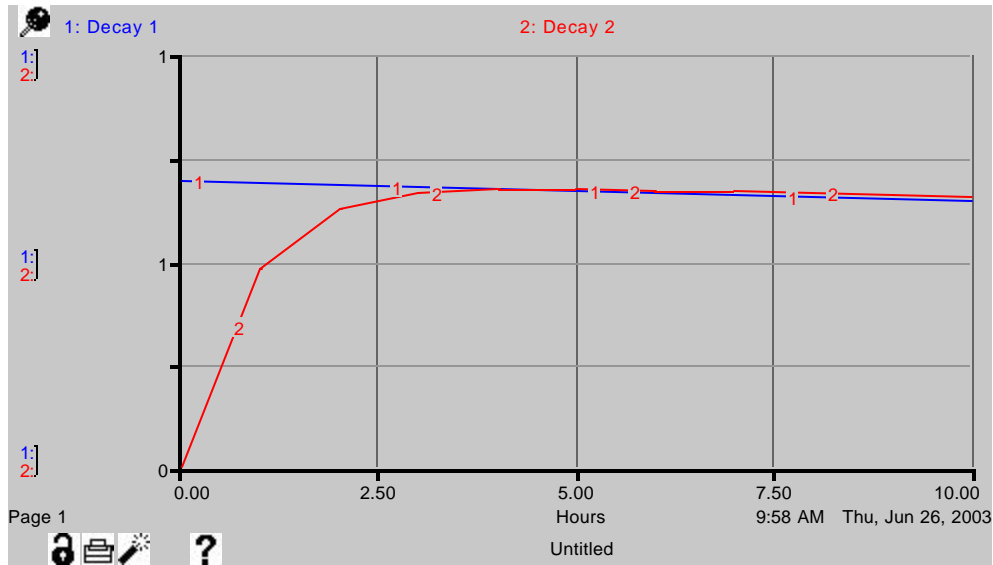
- Range = 1-10 hours, DT = 1 hour



With this combination of half-lives, the decay fluxes are much closer to one another by the end of the model run, suggesting that secular equilibrium is near.

What would have to be changed for the secular equilibrium assumption to be correct? Run some experiments and see what it takes to reach secular equilibrium.

To cause the system to approach secular equilibrium, the ratio of parent half-life to daughter half-life must be increased. The figure below shows what happens when the half-life of the parent is increased to 100 hours while the half-life of the radioactive daughter remains 1 hour.



U-Pb Dating

We're now going to start working with a real isotopic system used in geochronology. In this system, radioactive uranium isotopes decay to produce stable lead isotopes. You can find diagrams of these decay series in your readings from Faure (1986) on pg. 285-286.

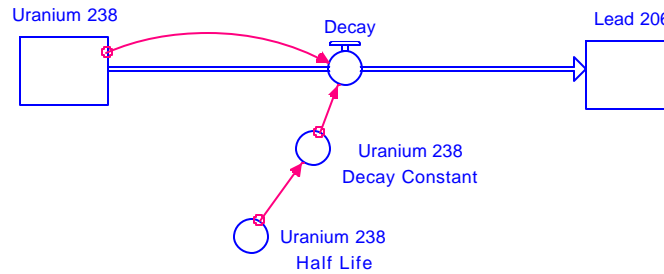
The table below lists the half-lives of each of the isotopes in the chain for the decay of ^{238}U to ^{206}Pb .

isotope	half-life
Uranium 238	$4.468 \cdot 10^9$ years
Thorium 234	24.5 days
Protactinium 234	1.14 minutes
Uranium 234	$2.33 \cdot 10^5$ years
Thorium 230	$8.3 \cdot 10^4$ years
Radium 226	1590 years
Radon 222	3.825 days
Polonium 218	3.05 minutes
Lead 214	26.8 minutes
Bismuth 214	19.7 minutes
Polonium 214	$1.5 \cdot 10^{-4}$ seconds
Lead 210	22 years
Bismuth 210	5 days
Polonium 210	140 days
Lead 206	Stable

- 9) Examine the half-lives carefully. How do you think you might go about modeling this system? Once you've decided, create a STELLA model on a new model page to show this decay system.

The half-lives of all of the radioactive daughter isotopes are very small in comparison to that of the parent isotope. As a result, the system should rapidly approach secular equilibrium. The system can thus be modeled as a direct decay from parent (U-238) to stable daughter (Pb-206). Many students will try to include U-234 and Th-230 in the decay series since these have long half-lives. Their half-lives are only tiny fractions of the U-238 half-life, however, and they also can be completely ignored.

Uranium 238 – Lead 206 Model



This model can be found in the file "Documented_UPb_Model.v.1.stm."

U238-Pb206 Model code

```

Lead_206(t) = Lead_206(t - dt) + (Decay) * dt
INIT Lead_206 = 0
INFLOWS:
Decay = Uranium_238_Decay*Uranium_238
Uranium_238(t) = Uranium_238(t - dt) + (- Decay) * dt
INIT Uranium_238 = 1*10^9
OUTFLOWS:
Decay = Uranium_238_Decay*Uranium_238
Uranium_238_Decay = LOGN(2)/Uranium_238_Half_Life
Uranium_238_Half_Life = 4468.0

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10) Because the half-life of ^{238}U is so long, you will need to start with a very high number of ^{238}U atoms in order to see any isotopic decay at all. I would suggest using a billion atoms.

You will also need to run the model for a very long time. The longer your simulation period, the larger your time-step must be in order for the model to run. Note, however, that STELLA will not allow you to use a time-step longer than 1 million years. How might we deal with this problem? Answer: STELLA will allow us to create our own time units. I would suggest you create a time-unit called "millions of years" and then scale your simulation length and half-life accordingly. Make sure you use the "1/2 dt rule of thumb" to determine the proper time-step for these runs.

- To create the time-unit "millions of years," double click on the U-238 half-life converter, click the "units" button, and where it says "units of measure, unspecified units," pull down to the "unit editor." Here you can create your own unit of measurement. Once you've named the unit, add it to the list. The next time you go to select units, the new unit will appear under "my units" in the unit editor. Note,

the units have already been set for you in the documented model, but I'm providing the information on how to do it here in case you are unable to open our model and have to create your own.

Using the unit millions of years allows the user to run the model from 0 to 4500 millions of years to model the decay of U that would have occurred in rocks as old as the Earth. For such a simulation, STELLA will not allow a time step less than 1/4 (million years), because it has a limited iteration capacity. However, if one compares the results at the end of a run with a time step of 1/2 to that of a run with time step of 1/4, one finds that there is little difference, so a time step of 1/4 is probably sufficiently short to get reasonable results. Note that students may choose the longer time step of 1/2, so quantitative answers for this section may vary somewhat from student to student.

Suppose you were dating a zircon crystal that formed 3.8 billion years ago. What would be its $^{206}\text{Pb}/^{238}\text{U}$ ratio assuming that the crystal has remained closed to both the parent and daughter isotopes?

Using a time-step of 1/4 million years and running the model from 0 to 3800 million years results in a ratio of $^{206}\text{Pb}/^{238}\text{U} = 0.803$.

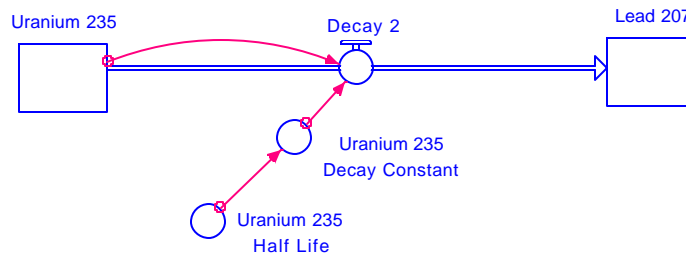
11) How many billion years will it take before all of the ^{238}U has decayed to ^{206}Pb ? How many times the current estimated age of the universe is this?

It takes about 30-40 billion years for all of the ^{238}U to decay to ^{206}Pb . This is about 2-3 times the current estimated age of the universe (14 billion years). Note: to do this experiment requires setting the time-step to 1 (million years) because of STELLA's limited iteration capacity.

U-Pb Concordia problems

12) On the same model page you're using, create a second decay model representing the decay series $^{235}\text{U} \rightarrow ^{207}\text{Pb}$.

Uranium 235 –Lead 207 Model



U235-Pb207 Model code

$$Lead_{207}(t) = Lead_{207}(t - dt) + (Decay_2) * dt$$

$$INIT Lead_{207} = 0$$

INFLOWS:

$$Decay_2 = Uranium_{235} * Uranium_{235_Decay}$$

$$Uranium_{235}(t) = Uranium_{235}(t - dt) + (- Decay_2) * dt$$

$$INIT Uranium_{235} = 1 * 10^9$$

OUTFLOWS:

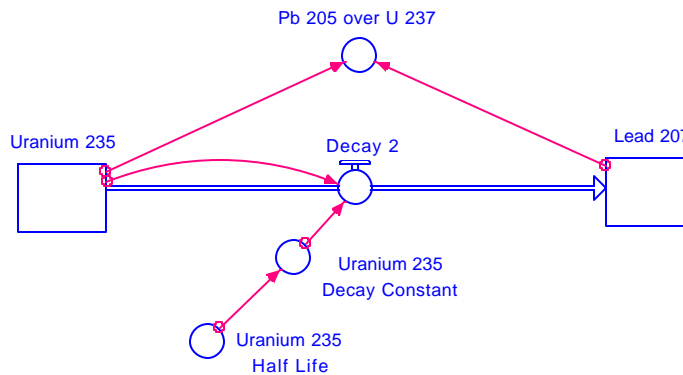
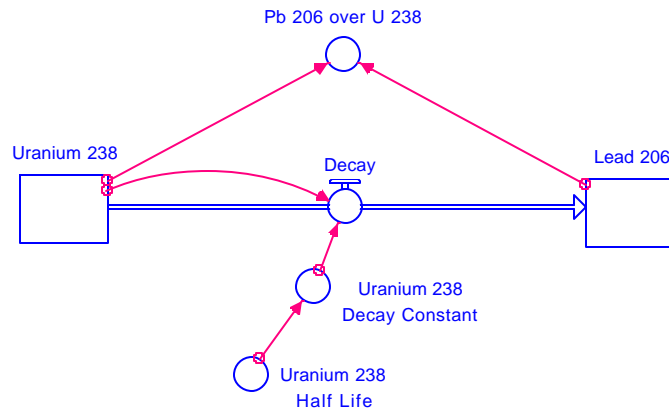
$$Decay_2 = Uranium_{235} * Uranium_{235_Decay}$$

$$Uranium_{235_Decay} = LOGN(2) / Uranium_{235_Half_Life}$$

$$Uranium_{235_Half_Life} = 703.8$$

Now create converters that will calculate the ratios $^{206}\text{Pb}/^{238}\text{U}$ and $^{207}\text{Pb}/^{235}\text{U}$.

U – Pb Models with Ratio Converters



Ratio Converters code

$Pb_{206_over_U_238} = Lead_{206}/Uranium_{238}$

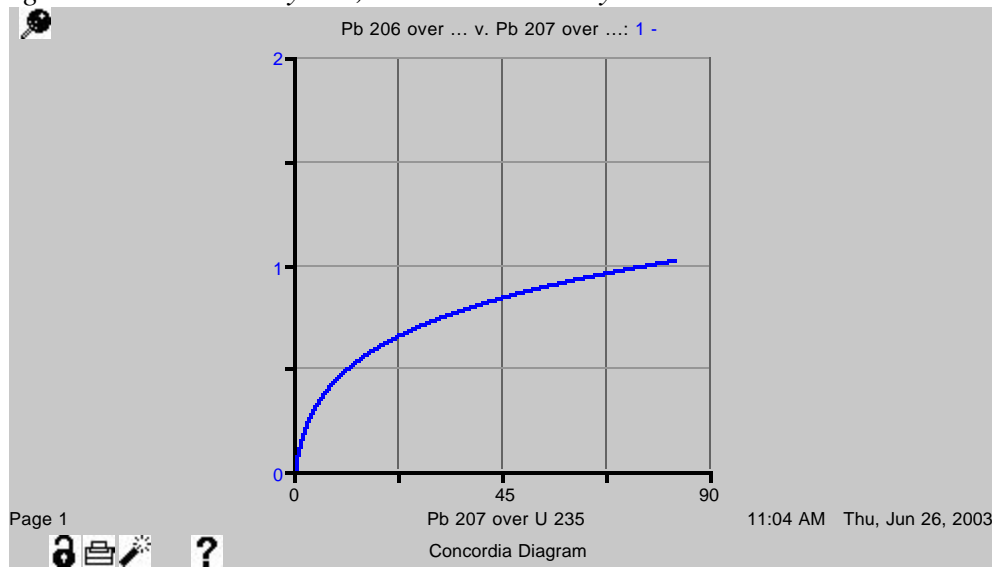
$Pb_{207_over_U_235} = Lead_{207}/Uranium_{235}$

Create a new graph on your page and choose scatter. On this graph choose the appropriate axes to make a concordia diagram such as you read about in Dalrymple and in Faure. Also create a table pad to output the ratios every time step.

Run your model for a time equivalent to the age of the Earth.

Concordia Graph

- Range = 0-4500 million years, $DT = 1/4$ million years



Explain what this graph means and how it works.

Note: The Y-axis here is the ratio Pb-206/U-238. Version 7 of STELLA does not allow this axis to be labeled (or we haven't figured out how anyway!).

The origin of the graph represents the isotopic ratios when the decay process begins (assuming that there was no initial daughter), and as one traces along the line, "time since decay began" increases. Since the half-life of U-235 is shorter than that of U-238, the ratio of Pb-207/U-235 increases more quickly than that of Pb-206/U-238. This can be seen in the higher numbers on the X-axis (scale goes from 0 to 90) compared to the Y-axis (scale goes from 0 to 2). The curve in the line also reflects the differing half-lives of U-235 and U-238. Early in the history of decay, the amounts of

Pb-206 and Pb-207 created are nearly identical. However, like in a running race, as time goes on, the speedier Pb-207 creation leads the ratio Pb-207/U-235 to increase more quickly than the ratio Pb-206/U-238, causing the line to curl over.

Students sometimes have a hard time understanding this. A way to have them think about it is to turn the graph 90 degrees. When viewed this way, they see that for every little increase in Pb-206/U-238, there's a very large increase in Pb-207/U-235.

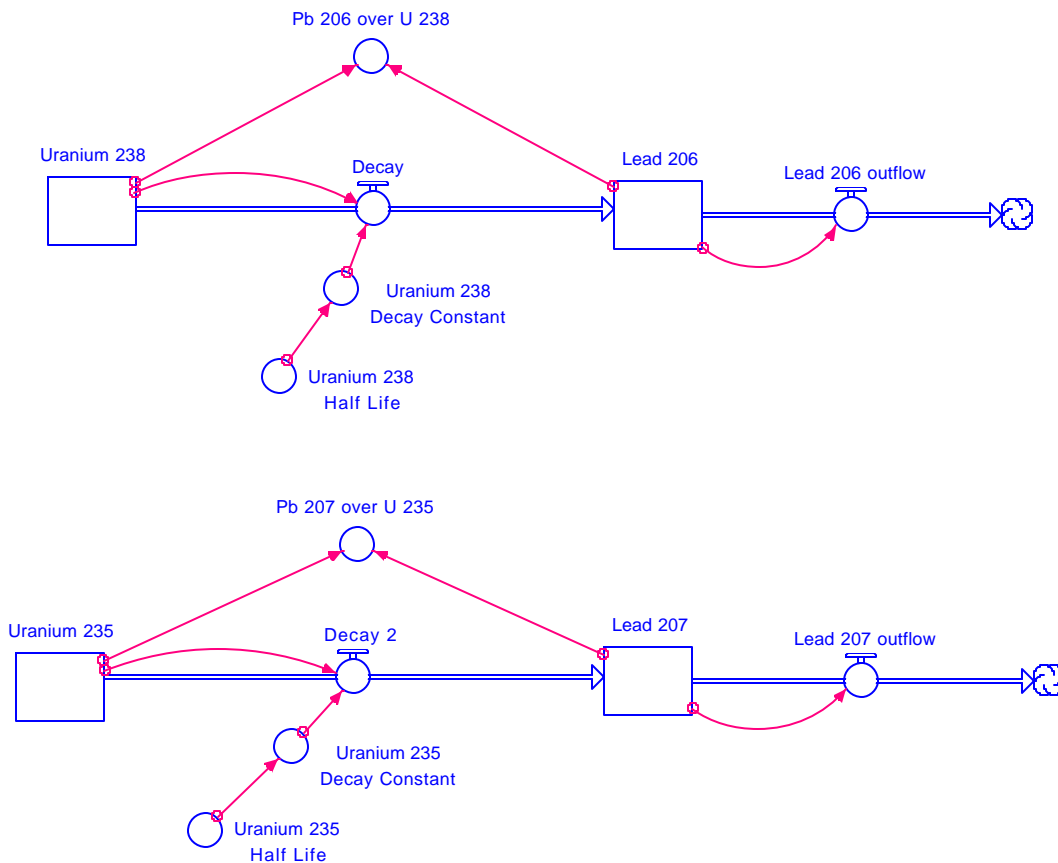
When you're done, export the data as text and open them in Kaleidagraph so you can create a new graph that we'll use in the next step.

- to export the data, open the table pad and go to File > Save as Text.

- 13) We're going to experiment with a loss of lead from the system now. Modify your model so that you can lose lead from each isotopic system at 1.5 billion years into the model run. Run the model for 3.5 billion years.

U – Pb Models with Lead Outflows

These models can be found in the file "Documented_UPb_Model.v.2.stm"



Pb Outflow code

$Lead_206_Outflow = IF(TIME=1500)THEN(0.1*Lead_206/DT)ELSE(0)$
 $Lead_207_Outflow = IF(TIME=1500)THEN(0.1*Lead_207/DT)ELSE(0)$

**The above equations are set for a 10% loss (0.1) of lead at 1.5 billion years (1500 million years). This variable may be changed to 0.2 for the 20% loss, 0.3 for the 30% loss, or 0 for no loss. Note that the THEN statement contains a division by DT. This is essential in order for the model to work correctly, because without this division, the flow values do not represent rates. STELLA automatically multiplies inflows and outflows by DT to determine how many atoms to add or remove from time-step to time-step, so if the division by DT is not included here, the outflows will be incorrect.*

Do multiple runs in which you lose 10% of the Pb you have accumulated at 1.5 billion years, and then 20% of the Pb, etc. Remember that you will have to subtract values from both the Pb-206 and Pb-207 reservoirs, and that the amounts subtracted will be different because the amounts that have built up in 1.5 billion years are different (due to the individual half-lives of the 2 systems).

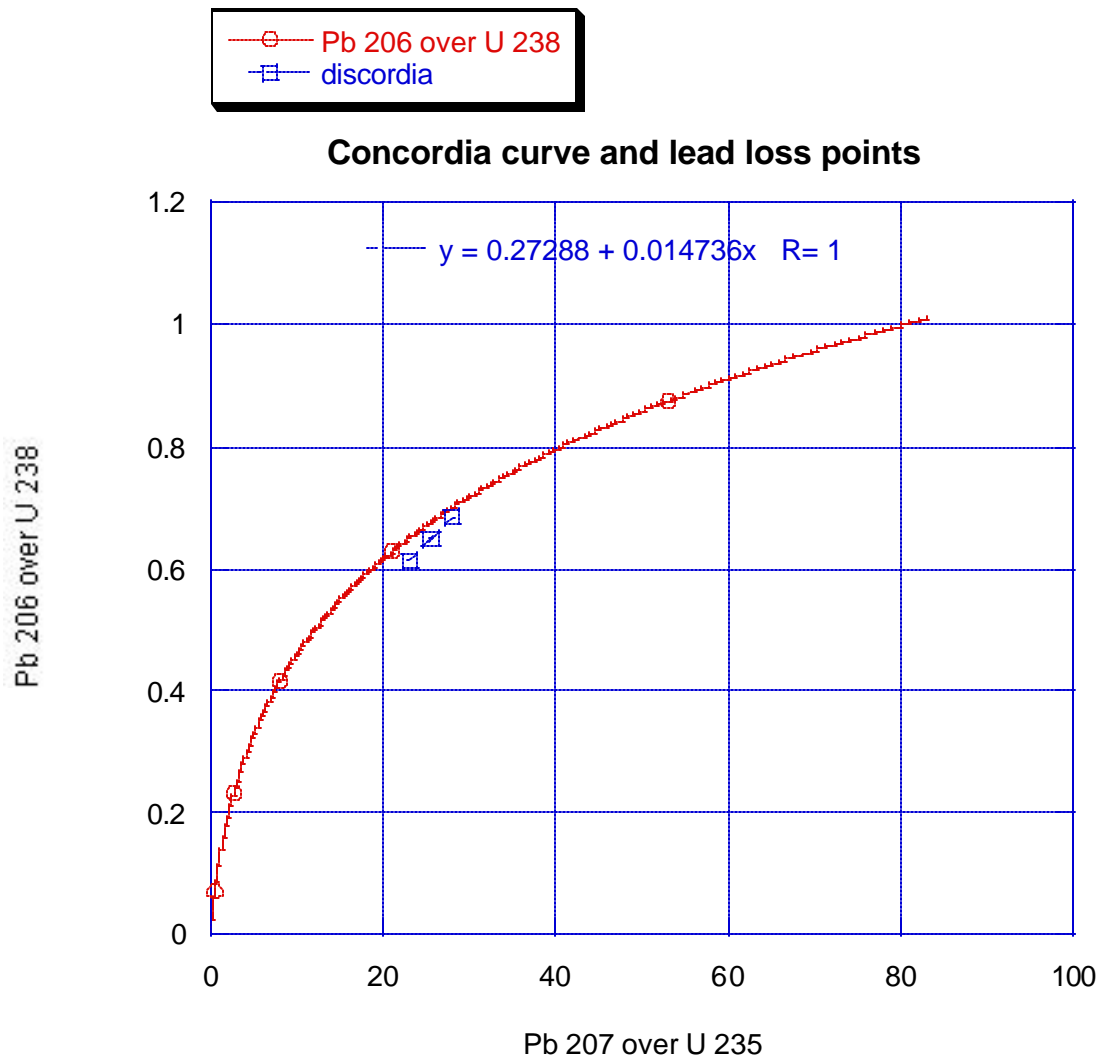
Each time you complete a run, go to the last values in your graph pad and make a note of the $^{206}\text{Pb}/^{238}\text{U}$ and $^{207}\text{Pb}/^{235}\text{U}$ ratios. Write these numbers into a new Kaleidagraph file.

The more significant digits recorded, the better this will work. Double click on the column headers in the table pad in STELLA to turn the numbers from 2 decimal place values to free float values.

*Pb loss points: 10% - (0.68541, 27.99514)
20% - (0.64967, 25.57018)
30% - (0.61394, 23.14521)*

14) In Kaleidagraph, plot both the concordia diagram and the runs in which Pb has been lost on the same graph. Where do the Pb loss points lie? Determine the slope of the line defined by the points using Kaleidagraph - I'll show you how to do this if you don't know how.

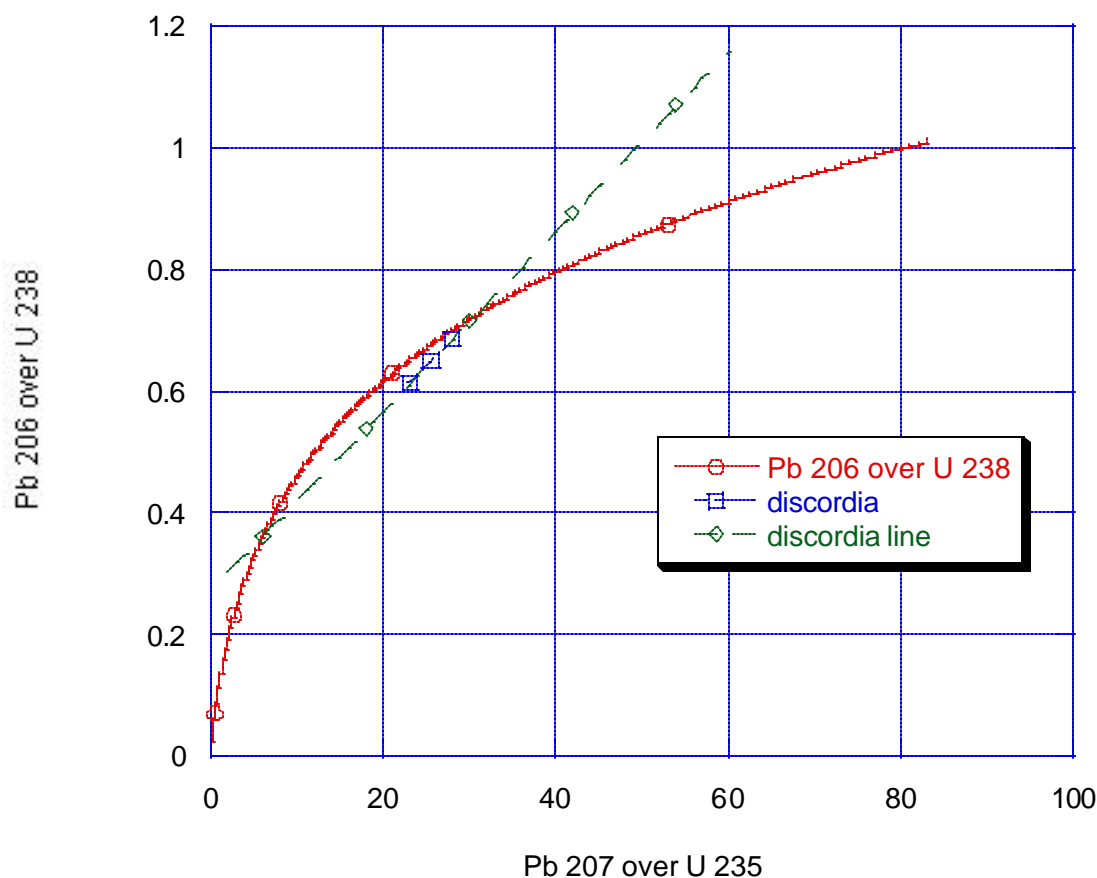
The Pb loss points lie beneath the Concordia graph in a line.



15) Once you've determined the slope of the line, open a new Kaleidagraph data window (keeping all others open), and create a series of numbers in the first column that has the same values as the X-axis on your concordia diagram. Now, using the formula entry feature in Kaleidagraph, create a corresponding set of Y-values to give you the discordia line determined by your Pb loss points.

Slope of discordia line = 0.014736

Discordia line extrapolated from points



16) Plot the discordia and concordia lines on the same graph and look to see where they intersect. Did the STELLA model correctly predict the time since isotopic decay began as well as the time since Pb loss? Why or why not?

To answer this question, determine the Pb-207/U-235 and Pb-206/U-238 ratio values for the points of intersection. Then, look for these points in the table pad to determine what time they represent.

*Intersection Points: (0.363804, 6.180463) – 2000 million years
 (0.721139, 30.42010) – 3500 million years*

**Note - there will be some slop in picking these points.*

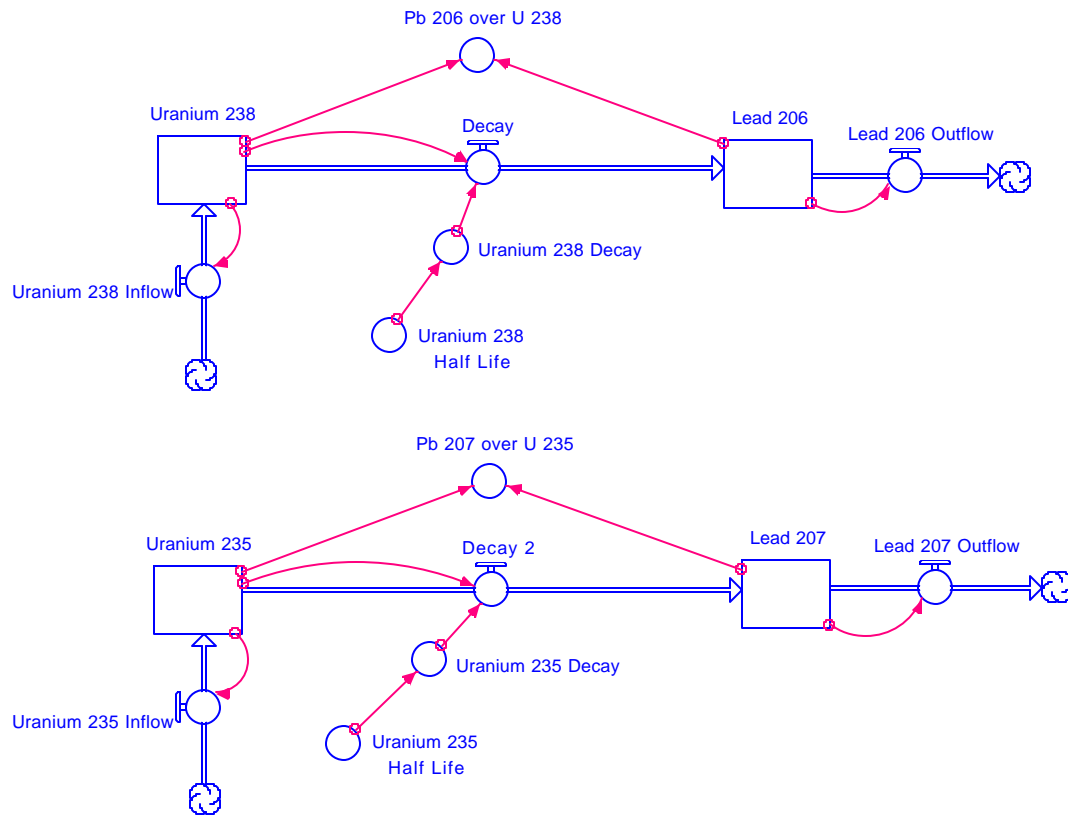
The STELLA model correctly predicted the time since the isotopic decay began (3.5 billion years), as well as the time since Pb loss occurred (2 billion years ago). The first point corresponds to the amount of time since Pb loss occurred (2 billion years). The second point represents the amount of time since the original crystallization of the minerals took place, or when isotopic decay began (3.5 billion years). The difference

between these points is 1.5 billion years, which is the time we asked STELLA to remove the lead (time of original crystallization - time of recrystallization = time since Pb loss occurred, 3.5 billion years - 1.5 billion years = 2 billion years).

17) Run an experiment in which, rather than losing Pb, the system gains U. Describe the discordia line created by different abundances of U gain, and then determine whether the STELLA model correctly predicted the time since U gain.

U-Pb Models with U Inflows

These models can be found in the file "Documented_UPb_Model.v.2.stm"



U Inflow code

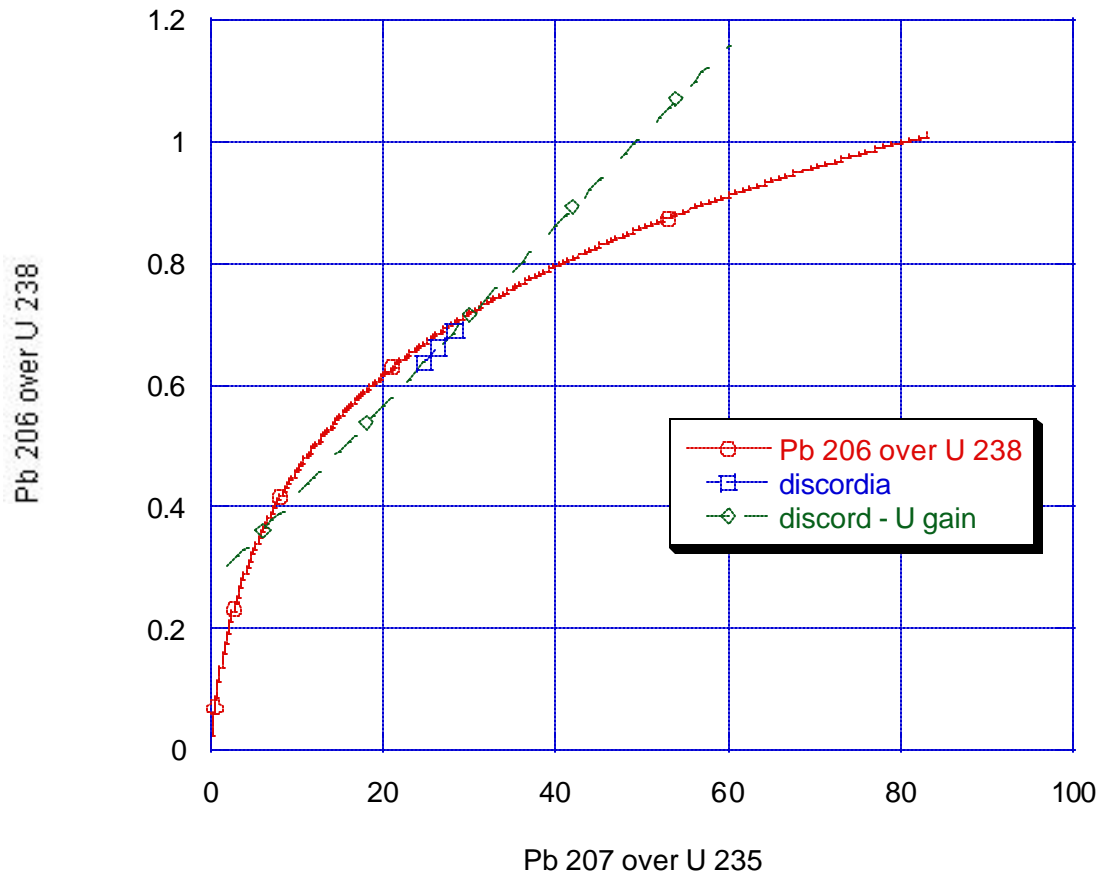
INFLOWS:

$Uranium_238_inflow = IF(TIME=1500)THEN(0.1*Uranium_238/DT)ELSE(0)$

$Uranium_235_inflow = IF(TIME=1500)THEN(0.1*Uranium_235/DT)ELSE(0)$

*In setting up the STELLA model for the U gain experiment, it is not necessary to delete Pb outflows in order to prevent Pb outflow. These flows may be stopped by changing the number multiplied by Pb in the outflows to 0.

Uranium gain concordia-discordia



The discordia points again plot below the line. This makes sense since a gain of U is essentially the same as a loss of Pb.

Intersection Points: (0.363804, 6.180463) – 2000 million years
 (0.721139, 30.42010) – 3500 million years

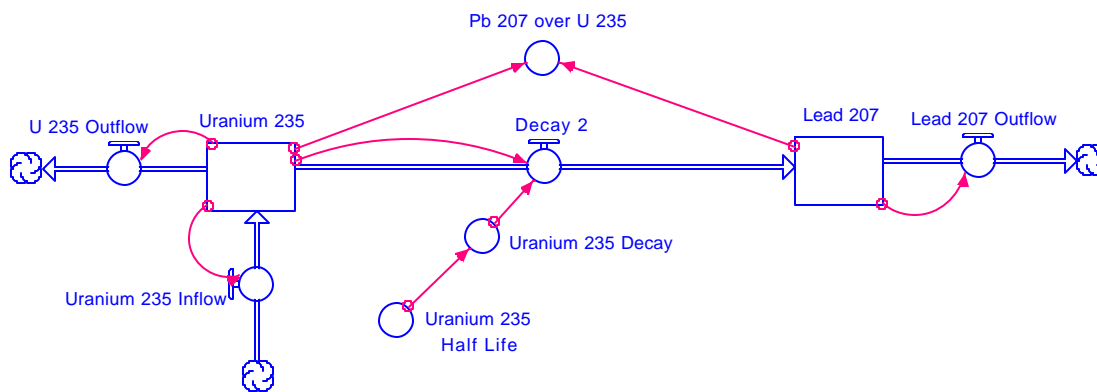
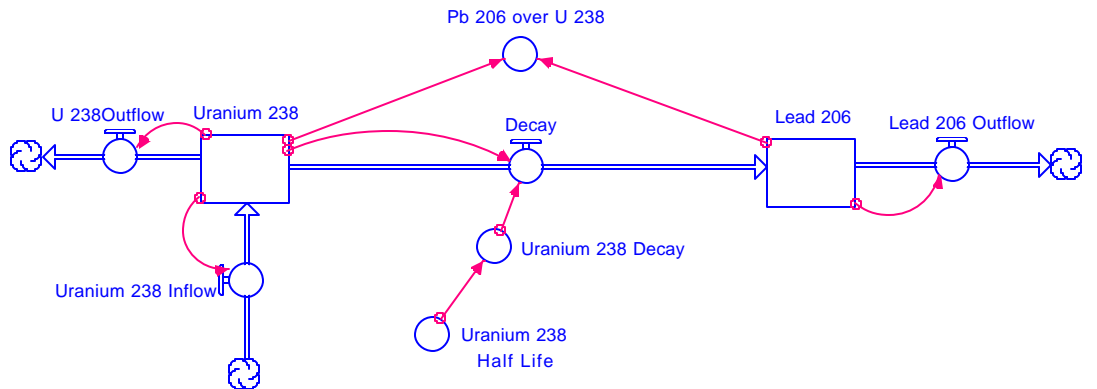
*Note - there will be some slop in picking these points.

The STELLA model correctly predicted the time since the isotopic decay began (3.5 billion years) as well as the time since U gain began (2 billion years).

18) Run an experiment in which the system loses U, but the Pb concentration remains the same throughout. Describe the discordia line created by different amounts of U loss, and then determine whether the STELLA model correctly predicted the time since U loss.

U-Pb Models with U Outflows

These models can be found in the file "Documented_UPb_Model.v.2.stm." Again, it is unnecessary to dynamite the Pb outflows and U inflows. Just make the multiplier in the if-then statement = 0 for these flows.

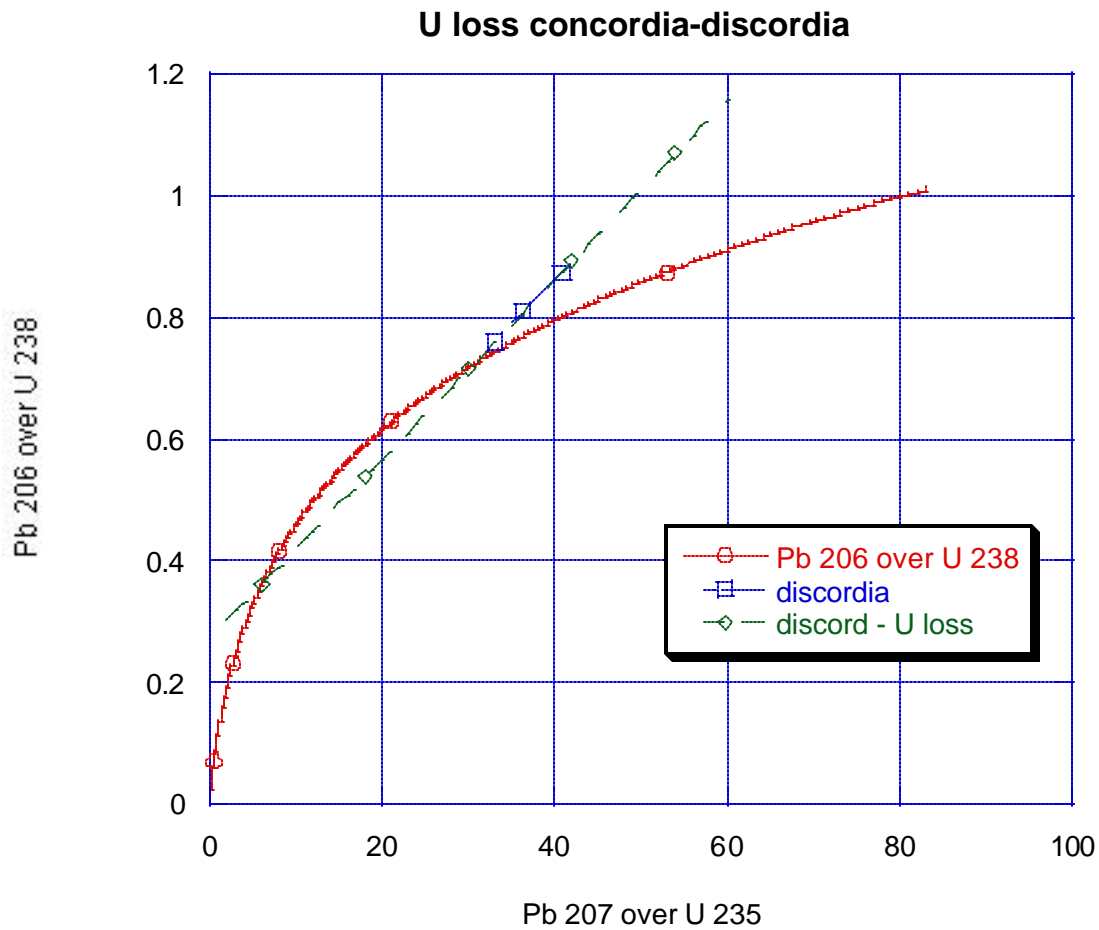


U Outflow code

OUTFLOWS:

$U_{238_Outflow} = IF(TIME=1500)THEN(0.1*Uranium_{238}/DT)ELSE(0)$

$U_{235_Outflow} = IF(TIME=1500)THEN(0.1*Uranium_{235}/DT)ELSE(0)$



*Intersection Points: (0.363804, 0.06180463) – 2000 million years
 (0.721139, 0.3042010) – 3500 million years*

**Note - there will be some slop in picking these points.*

It is important to recognize that U loss results in the discordia points plotting above the concordia line, as opposed to below it, but that the points of intersection of the discordia line with the concordia line remain the same. The STELLA model correctly predicts the time since the isotopic decay began (3.5 billion years), as well as the time since U loss began (2 billion years).