Some Quick Tips About Using SIZE EXTRACTOR v. 1.10 28 March, 2009

Typical analysis sequence:

1. Launch Size Extractor. Choose data file from dialog box that appears. If you cancel this, the program will remain up, but have no windows open. In this case, quit and relaunch the program.

2. Choose a diffusion geometry from Options menu (default is slab)
(can be changed at any time, but this restarts rgw analysis sequence)

3. Select the data that you wish to regress--do this in the 'Kinetic Data' window. Shift-click to select contiguous lines, command-click to add or deselect isolated lines to/from your selection.

4. Choose Regression > Regress. Line and stats appear on Arrhenius Plot, and two other windows appear: for domain-size entry, and log(R/Ro) plot)

5. Click in Domains window

6. Choose number of diffusion domains from pop-up

7. Enter size and volume for each domain. Activation energy can be changed but usually you won't do this.

8. Click "Update" button to see model results

9. Repeat steps 7 and 8 until satisfied

10. Keep a record of your modeling—the program doesn't print, and it's easy to lose your work (see below)! You can choose File > Save Results repeatedly if you like.

11. When done, you can choose to save your data, in the form of several files. The domain-entry window must be selected to use this option. The files will inherit the file-name prefix of your .size file.

(a) For the first file, which saves domain information in a format suitable for the arvert inversion program, you are prompted to choose a save location (and a change in name if you want – arvert wants a file called domains.in). The other files are simply saved with the file-name prefix and are placed in your working directory.

(b) The file [prefix]_domain-summary.out preserves are record of your modeling – use this to restart and continue modeling, or to store intermediate values as you model.

(c) The file [prefix]_size_out saves the fractional loss values, observed logRRo, modeled LogRRo, 10 000/K, observed $\ln D/a^2$, and modeled $\ln D/a^2$. You can use this file to make

plots of the logRRo and Arhenius data (but note that you need to plot the logRRo data as an age spectrum, not a series of x-y points).

(d) The file [prefix]_corr.smp outputs the logRRo data in a format suitable for use with the Lehigh version of Lovera's correlation program for age and logRRo spectra.

12. Sorry, you can't print from this program, but you can use the 'Grab' application that is bundled with OS X to get a screen shot of a window or part of a screen. Grab is located in Applications/Utilities.

Program Notes:

1. Often, the program will not load new data after you've loaded your first sample. The best workaround is to quit and relaunch.

2. Data files (usually suffixed by .size) are tab-delimited files with three entries per row

Temp (C)	fractional loss	duration (minutes)

If you have n heating steps you want a file with n-1 lines: do NOT include the final step with f = 1.0000: this can't be modeled!

3. Each time you run the program, you can set preferences as to the number of preselected Arrhenius data (default is 5), and activation energy to use when forcing a line through a single point (default is 50 kcal/mol)

4. To force a regression through a single point, just select the single point, and choose 'Regress.' A line will be forced through your chosen point, using the activation energy entered in 'Preferences.'

5. Although you can enter relative volumes in any units, the program will then normalize them to fractional losses that sum to 1.00. So, in the end it is easier to enter fractional losses from the start, and be careful to always have the volumes add up to 1.0

Modeling Tips

• Because of the reference frame (apparent size of 1 corresponds to the chosen regression line), the largest apparent size on the Log(R/Ro) plot will be correct, whereas the smaller apparent sizes depicted on the Log(R/Ro) plot will be too large. To model the smaller domains, you need to enter sizes smaller than they are depicted, some definitely less than one, possibly at times below 0.1.

• It's advisable to jot down your domain structure or repeatedly save your data as you model because there are some...

...Program Uglies (puglies):

> When you are doing domain modeling, if you change the number of domains, everything is reset.

> More commonly, you will find that if you enter domain volumes that do not sum to 1.00, the program will renormalize. The degree to which this ruins your work depends on how far the sum differs from 1.00 (if you make a gross typo, say omitting a decimal point, it's sayonara to your efforts). So keep track of your entries!