1 Adjust the hydraulic radius of one phase

Following the filtering process, the surface area fractions of the filtered phases may not match those of the phases in the starting 2-D SEM images. These surface area fractions can be adjusted using a 3-D "sintering" algorithm to swap specific locations of the two phases in a manner that obtains the desired surface area fractions. Details of the 3-D sintering algorithm have been published previously [1, 2], with the specific application to cement particles described in the CEMHYD3D Version 2.0 User's Manual [3].

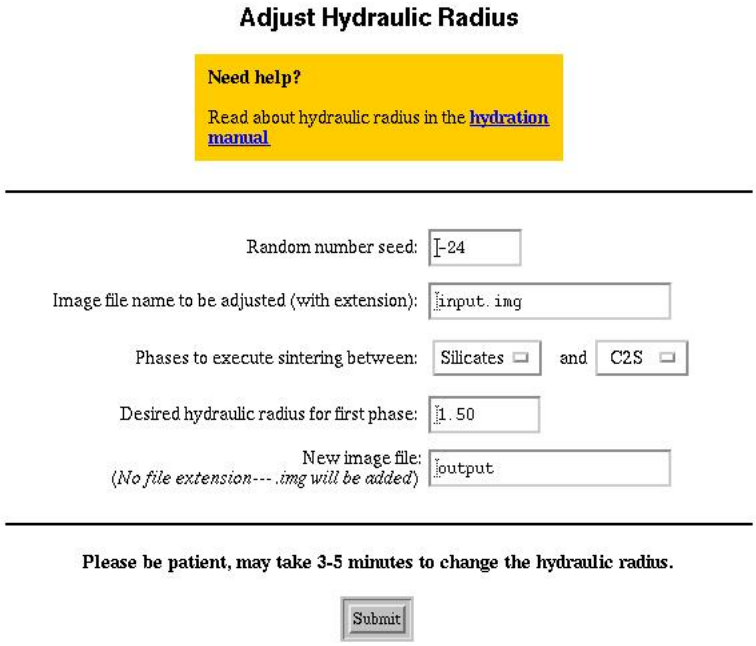

Figure 1: Form for adjusting the hydraulic radius of the surfaces of a single phase in a 3-D microstructure image.

The input form, shown in Figure 1, has the following entries:

1.1 Random number seed

The user must enter a *negative integer* (in the range [-32767,-1]) in this field.

1.2 Image file name to be adjusted

This must be the name of any 3-D microstructure image (extension `.img`) that contains at least the two phases defining the interface that is to be modified by this action. Files created using the **Generate initial microstructure** submenu or the **Distribute cement phases** submenu can be entered.

1.3 Phases to execute sintering between

The algorithm increases the hydraulic radius of the first phase by selecting n pixels of that phase that have the n highest values of mean curvature—using capillary porosity to determine the surface—and switching the identity of those pixels to that of a second phase. To conserve volume of each phase during the process, n pixels of the second phase having the n lowest values of mean curvature—using either capillary porosity **or** the second phase itself to determine the surface—have their identity switched to that of the first phase [1].

1.4 Desired hydraulic radius for first phase

If one already knows the desired surface area (in number of pixels) of the first phase, then the desired hydraulic radius R_h can be calculated using the following equation:

$$R_h = \frac{3V}{2S} \tag{1}$$

where V is the volume (in number of pixels) of the first phase. V for any phase can be found by computing the phase statistics as described in the **Phase Statistics** submenu. The factor 3/2 is included to correct for the difference between the approximate surface area of a digitized (pixel-based) sphere and a continuum sphere of the same diameter.

NOTE: The hydraulic radius of a phase can only be *increased* when applying the sintering algorithm to it. If it is necessary to decrease the hydraulic radius of a phase, the algorithm should be executed so as to increase the hydraulic radius of the secondary phase, thus decreasing that of the primary one [3].

1.5 New image file

Enter the name that you wish the processed microstructure to have after this phase separation has been accomplished. As in previous forms already described, only the file root name should be supplied here; the extension `.img` will be added automatically.

1.6 E-mail address

The program `sinter3d` that performs the adjustment to the hydraulic radius may take several minutes to complete. The VCCTL interface automatically sends a note to the e-mail address provided when execution completes. If no e-mail address is supplied, then a note will not be generated.

References

[1] D.P. Bentz, E.J. Garboczi, P.J.P. Pimienta, and W.C. Carter. Cellular automaton simulations of surface mass transport due to curvature gradients: Simulation of sintering. In *Synthesis and*

Processing of Ceramics: Scientific Issues, number 249 in MRS Proceedings, pages 413–418, 1992. Available at http://ciks.cbt.nist.gov/~garbocz/paper36/paper36.html.

[2] J.W. Bullard, E.J. Garboczi, W.C. Carter, and Jr. E.R. Fuller. Numerical methods for computing interfacial mean curvature. *Computational Materials Science*, 4:103–116, 1995.

[3] D.P. Bentz. Cemhyd3d: A three-dimensional cement hydration and microstructural development modelling package. version 2.0. NISTIR 6485, U.S. Department of Commerce, April 2000.