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Microstructural Modeling Approach Applied to Rock Material

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The importance of the microstructural parameters in rock mechanical behavior has been investigated by several authors. Moreover, the Weibull statistical model has been used to characterize the heterogeneity of several materials on the basis of the concept that the microscopic defects within the material determine their mechanical strength. The modeling of different rocks is a topic that is fundamental for the prediction of rock fragmentation. In this article, the analysis of rock microstructure is performed using the microstructural modeling approach, which consists of the simplification, quantification, and modeling of the main properties of rock microstructure. The grain size, grain shape, and microcracks are modeled by means of statistical density functions, namely, Cauchy, chi-squared, exponential, extreme value, gamma, Laplace, normal, uniform, and Weibull. It is found that the Weibull distribution is the most appropriate statistical model of the grain size and grain shape, when compared with the other eight statistical models. Regarding microcracks, the results show that the gamma distribution is the most appropriate model. The Weibull and gamma distributions are then used to analyze the heterogeneity of the microstructure. This is done by comparison of the statistical models of each microstructural property evaluated in several thin sections of the same rock. It is found that with respect to grain size and grain shape, the rock is homogeneous, while the size distribution of the microcracks shows a clear trend toward less homogeneity. The microstructural modeling approach is important for modeling, characterizing, and analyzing the microstructure of rock material. Among other applications, it can be used to explain differences in the mechanical behavior obtained in testing several specimens.

Keywords heterogeneity, image analysis, microstructure, statistical models

1. Introduction

In the current study, the term *microstructure* is used to refer to the morphological features observed in thin sections (TSs) with a microscope on the millimeter scale, whereas the term *texture* refers to morphological features observed in specimens without magnification, usually on the centimeter scale. However, some authors use texture and microstructure as synonyms.

Several properties of rock microstructure are known to influence the mechanical properties of rock, and analysis of their relationship has been performed previously (Ref 1-4). Microstructural properties, such as grain size (Ref 5, 6), microcracks (Ref 5, 7-9), porosity (Ref 10, 11), mineral composition (Ref 12), and the overall microstructure (Ref 13-15), have been considered by several authors to be important microstructural parameters for determining rock mechanical behavior.

Geological materials are highly heterogeneous if compared with man-made materials. However, the analysis of the microstructures of man-made materials is accepted as an essential control factor concerning their mechanical properties, and microstructure characterization is becoming more systematic (Ref 16).

Even though the importance of quantitative microscopic studies is not new (Ref 12), this area of study has received additional attention recently due to the emergence in the geological sciences of image analysis techniques (Ref 17). Quantitative image analysis of the microstructure as a way to estimate mechanical properties has been applied by Vales et al. (Ref 18) in rocklike material with satisfactory results. Andriani and Walsh (Ref 11) have used quantitative image analysis of sedimentary rocks to determine their physical properties.

Liu et al. (Ref 19) have used a microscopic image to simulate a specific rock, as well as a statistical model for the distribution of the mechanical properties. The future trend, based on recent positive research results, some of which are mentioned above, indicates that the modeling of the microstructure of rock material is a promising way to explain and predict its mechanical behavior. Moreover, a microstructure-modeling approach is important for investigating and understanding more deeply the intrinsic properties of rock material, such as their heterogeneity. Rocks with a similar mineral composition have different mechanical behavior due to differences in their texture. Moreover, rock specimens with a similar texture and mineralogical composition react to mechanical forces differently, due to the heterogeneous distribution of their microstructural properties.

In this article, a microstructure-modeling approach, which, in short, consists of simplifying, quantifying, and modeling microscopic images, was adopted. Considering the microstructure as a network of defects made of mineral grain boundaries and microcracks and establishing some assumptions constitute

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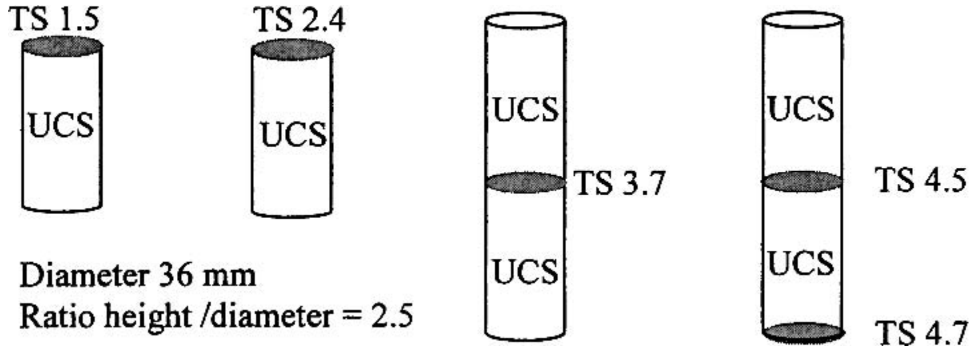

Fig. 1 Schematic representation of the rock sampling of the TSs. The first number refers to the drilling core, while the second number refers to the cut piece.

the simplification. Then the microstructure is quantified by means of image analysis of the grain size, grain shape, and microcracks. Thereafter, by means of statistical distributions, the microstructure is modeled. Moreover, a new approach to assessing the heterogeneity of the microstructure is suggested that consists of a comparison of the statistical models of the microstructural properties measured in several TSs of the same rock. Specifying different rocks with a similar mineralogical composition, by means of the parameters of the statistical distributions, and quantitatively analyzing their heterogeneity are the applications of the microstructural modeling approach presented in this article.

2. Sampling of Rock Material

The sampled rock is a granite ore from an aggregate quarry for road-building material located in Härno, in northwestern Sweden. Härno granite has a massive structure without a preferred orientation. It has fine and evenly distributed grains. It is unweathered and has a very low porosity. Thus, its defects are mainly microcracks and grain boundaries. The microcracks existing in the samples come from the geological processes, because the area for the production of aggregates where blasting occurs was avoided during sampling. The mineral composition of the Härno granite is 35% quartz, 60% feldspar, and 5% mica, as estimated by the point-counting method (Ref 20) in a polarizing microscope with about 200 points.

Four vertical drilling cores of 36 mm diameter were sampled from the surface of the quarry at random locations. Five TSs were prepared from the four drilling cores (Fig. 1). Two TSs are from the same drilling core with a vertical distance between them of 90 cm (TS 4.5 and TS 4.7), whereas the other TSs (TS 1.5, TS 2.4, and TS 3.5) came from three drilling cores with several meters between them.

3. Microstructure Modeling Approach

3.1 Simplification of the Microstructure

Using a digital camera and a computer installed in the polarizing microscope, polarized light microscopy was used to produce images from a regular grid in such a way that they neither matched nor overlapped. Four digital images of the simplified microstructure have been taken for each of the TSs (Fig. 2a, b). Four characteristics are primarily responsible for the complexity of the microstructure, which are associated with the optical properties of the minerals and its heterogeneity: (a) different tones and patterns can be observed for the same mineral type, depending on the orientation of the crystallographic axis relative to the cutting plane of the TS; (b) the boundaries of the small grains are seldom clearly observed due to the intergrowth of grains; (c) the minerals show a nonhomogeneous surface within the grain boundaries; and (d) dark minerals occur due to optical extinction, and it is not possible to identify them mineralogically. These characteristics of the microscopic image make automatic image analysis difficult, and assumptions for simplifying the procedure are necessary.

To reduce the complexity of the microstructural characterization, it is assumed that: (a) five TSs give representative information about the microstructure of the rock and (b) the grain minerals are homogeneous within their boundaries (i.e., the heterogeneity of the minerals is not considered). On the basis of assumption (a) the methodology used in the microstructural modeling approach consists of using the measurements of the grain size, grain shape, and microcrack size performed on the five TSs to select the appropriate statistical models. Thereafter, the model is used to analyze the heterogeneity. On the basis of assumption (b), only the grain boundaries are extracted from the microstructural network of the minerals.

It was observed in the optical microscope that the microcracks are intergranular and closed. The microcrack width is approximately 4.3 μm, which indicates that the microcracks are associated with mineral cleavage. Approximately 99% of the microcracks are well fitted to straight lines, and thus, simplification consists of ignoring the width of the microcrack. On the basis of these simplifications, the analyzed microstructure is considered to be representative of the rock microstructure.

3.2 Quantification of the Microstructure

Quantification of the microstructure is achieved by means of image analysis of the simplified microstructure. Presently available image analysis software is not appropriate for dealing with the microscopic images due to the complexity previously mentioned. Therefore, automatic image analysis requires the development of specific routines. Consequently, in the present research, the boundaries have been marked by hand in the

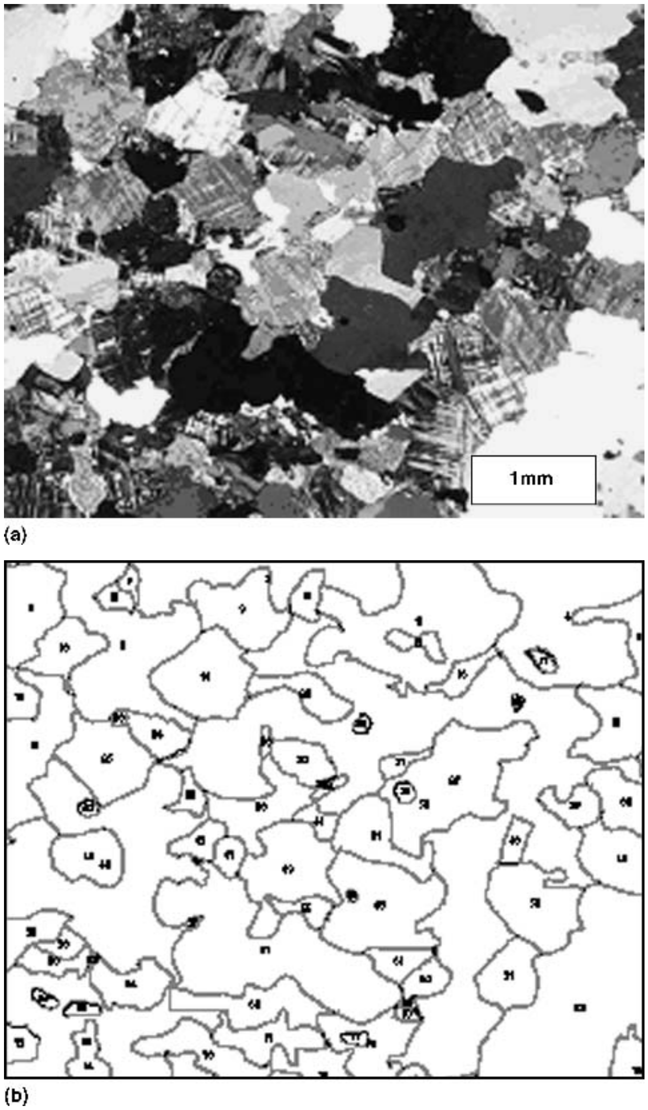

Fig. 2 (a) One microscopic images of the Härno granite taken from TS 1.5, and (b) one image of the simplified microstructure after image analysis of the microscopic images

original image and then saved as a new image. The descriptors can then be measured automatically. Figure 2(b) shows a digital file of the granite after manual segmentation of the network of minerals. Thereafter, four descriptors have been selected to quantify the properties of the networks of boundaries, and one descriptor has been used to describe the microcracks. The measurement of microcracks is accomplished by tracing straight lines along visible microcracks on the digital images. The microcracks have been numbered, and their size has been measured.

A descriptor of the microstructure is a parameter used to quantify a morphological property of the microstructure. A list of descriptors was summarized by Russ (Ref 21). Feret length (FL) and feret width are often used as measures of particle size (Ref 2, 22). For the study of Härno granite, FL is used as a measure of the grain size. It is defined as the length, in millimeters, of the best-fit rectangle (on the orientation) of a mineral

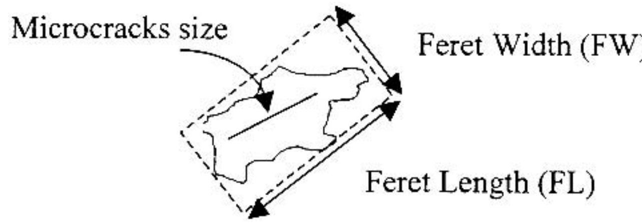

Fig. 3 Descriptor of grain size (FL), grain shape (FE = FL/FW), and microcracks size

grain. Feret elongation (FE) is the descriptor used for the grain shape and is defined as FL/FW (as a percentage), where FW is the feret width (i.e., the width of the best-fit rectangle of the particle). Concerning the microcracks, their length was considered to be the most important descriptor. Figure 3 shows the descriptors of the microstructure.

3.3 Modeling the Microstructure

Modeling the microstructure consists of choosing an appropriate statistical density function to model the quantitative evaluations of the microstructure descriptors. Ten density distribution functions are used. However, the Weibull distribution is by far the most interesting one, as its parameters have been used to model the heterogeneity of rock material for simulation purposes (Ref 19) and are related to the mechanical behavior of rock material (Ref 23, 24). The theory that underlies the foundation of the Weibull model is the concept that material defects constitute the factor that mostly influences the strength of materials (Ref 25, 26). Therefore, it is relevant to conclude that the Weibull distribution is a good model of the microstructure.

3.3.1 Kolmogorov-Smirnov Goodness-of-Fit Test. The variable x of the grain size, grain shape, and microcracks is modeled with the Cauchy, chi-squared, extreme value, exponential, γ, Laplace, normal, uniform, and Weibull density distribution functions $f(x)$, as defined in Eq 1 to 9 in the Appendix.

After the fitting operation, the question that emerges is which one of the distribution functions is best suited to model the data trend. A goodness-of-fit test is used to evaluate the quality of fit of the theoretical model to the data measurements. The Kolmogorov-Smirnov (K-S) goodness-of-fit test calculates the maximum distance between the cumulative distribution of the data and the cumulative statistical distribution function. For K-S values < 0.1, the model is statistically significant and is, therefore, an appropriate model of the population properties. Among models with K-S values < 0.1, the most appropriate model has the lowest K-S value.

4. Analysis of the Heterogeneity of the Microstructure

Generally, the concept of heterogeneity is close to that of variability. Heterogeneity refers to the variation in texture or pattern, whereas variability refers to the variation in values. Moreover, different levels of heterogeneity exist, according to the scale of observation.

The implications of the heterogeneity of rock material are many and cannot be neglected. Additionally, a rock model is a representation of reality, which can range from millimeters to kilometers. The capability of the model to represent rock material is limited by the heterogeneity of the rock (i.e., the greater the heterogeneity, the more difficult it is to model larger areas). The sampling required to produce good models depends on the heterogeneity of the rock material, which is the major cause of uncertainty in predicting rock mechanical response. Although heterogeneity is a key factor concerning modeling rock material, it is often assumed that the rock is homogeneous. This assumption is seldom investigated due to the lack of an effective assessment method besides visual evaluation and description of the rock structure or pattern.

On the basis of the qualitative evaluation performed by field observations of the rock mass and the samples, it is meaningful to assume that Härno granite is a homogeneous rock. However, when a TS is observed under the polarizing microscope at a magnification of 25×, the granite shows an imbricate and complex microstructure (Fig. 2a).

Analysis of the microstructural heterogeneity consists of the comparison of the statistical models obtained through the modeling of the same microstructural property in several TSs of the same rock.

Descriptive statistics and a histogram with 10 classes for the measurements of the grain size, grain shape, grain orientation, and microcracks of the microstructure of five TSs are shown in Fig. 4 to 6. The descriptive statistics for the microstructural measurements consists of the number of measurements (N), the

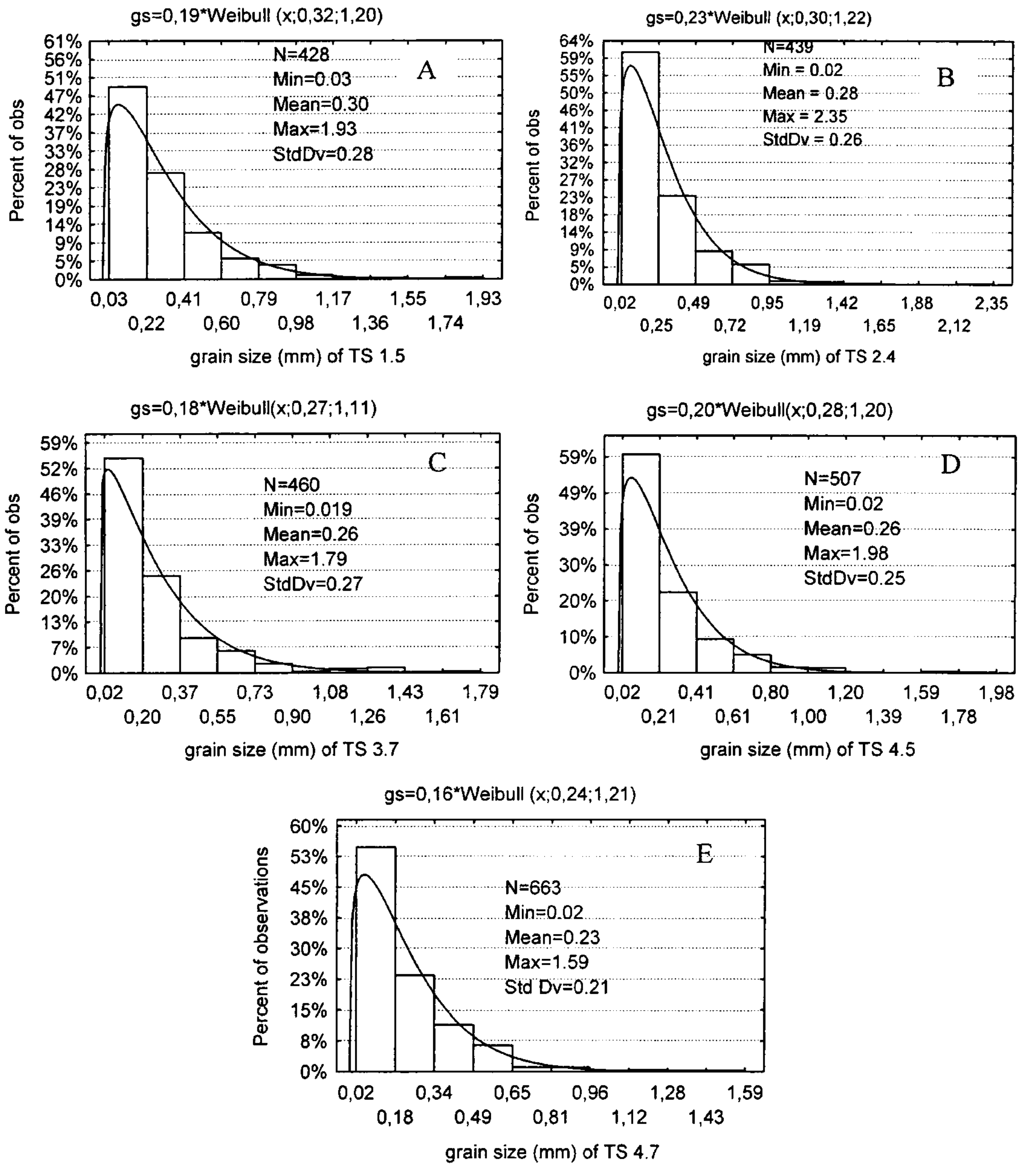

Fig. 4 Descriptive statistics, data histogram, and Weibull statistical model of grain size of the microstructure measured in five TSs

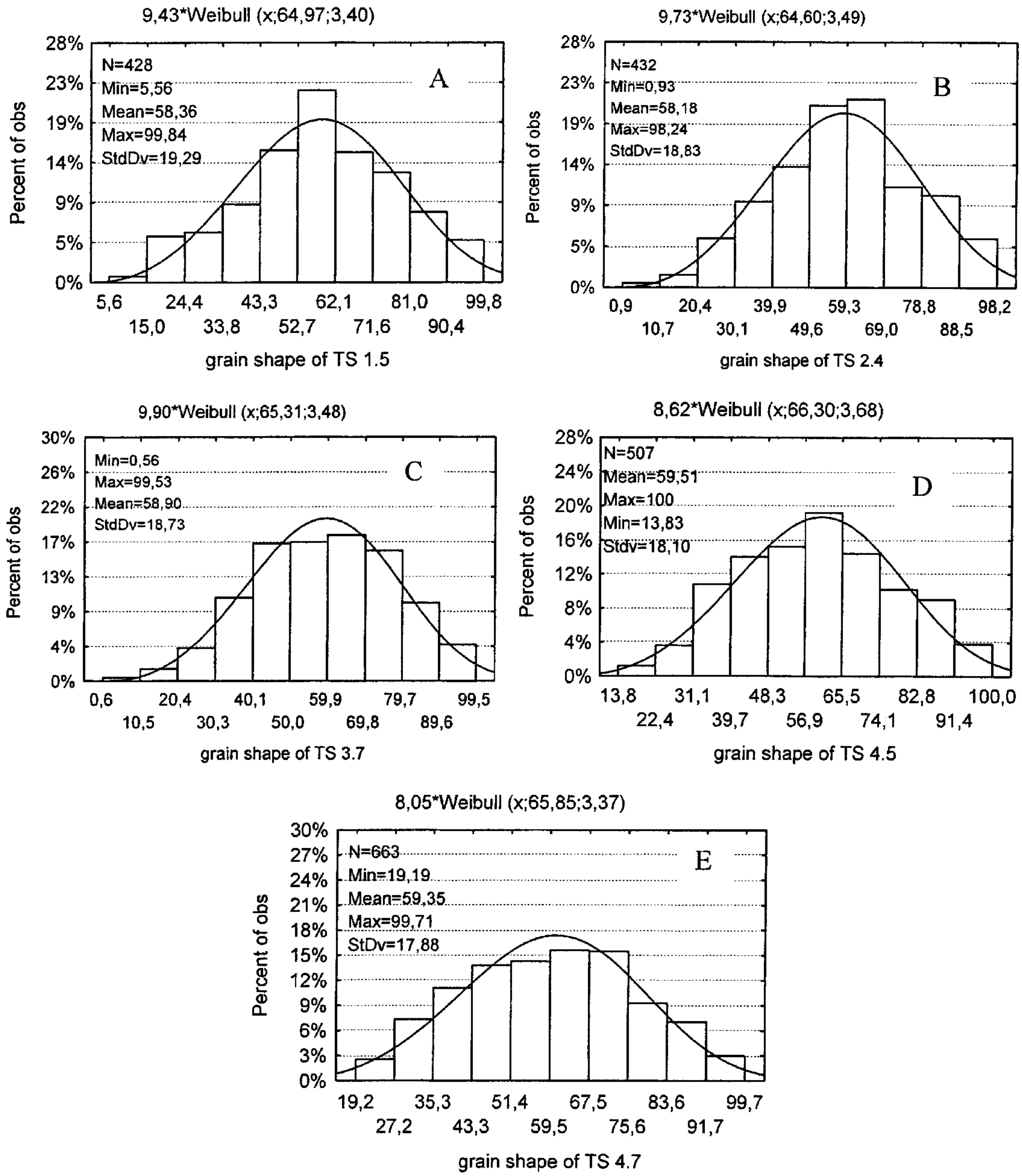

Fig. 5 Descriptive statistics, data histogram, and Weibull statistical model of the grain shape of the microstructure measured in the five TSs

minimum value (Min), the mean value (Mean), the maximum value (Max), and the standard deviation (SD).

5. Results from Microstructural Modeling Approach and Heterogeneity Analysis

5.1 Analysis of the Grain Size

From the results presented in Table 1, it was concluded that the Weibull distribution function is the most appropriate model of the grain size because it yields the lowest K-S value (section 3.3). The Weibull model (x; 1.178; 0.279) describes the overall trend of the grain size of the microstructure of Härno granite based on 2478 measurements of grain size.

From Fig. 4 it was observed that the five TSs have a similar distribution concerning the grain size, with a nonsignificant difference in their models. Even though TS 4.5 and TS 4.7 are TSs obtained a distance of 90 mm apart (Fig. 1), there is not a remarkable similarity between them. This is a strong indication that the rock has very low heterogeneity. Therefore, it can be stated that from the point of view of the grain size, this rock is homogeneous on the microscale, as most of the TSs show low variability.

5.2 Analysis of the Grain Shape

From results presented in Table 2 it was concluded that the Weibull and normal distribution functions are equally good

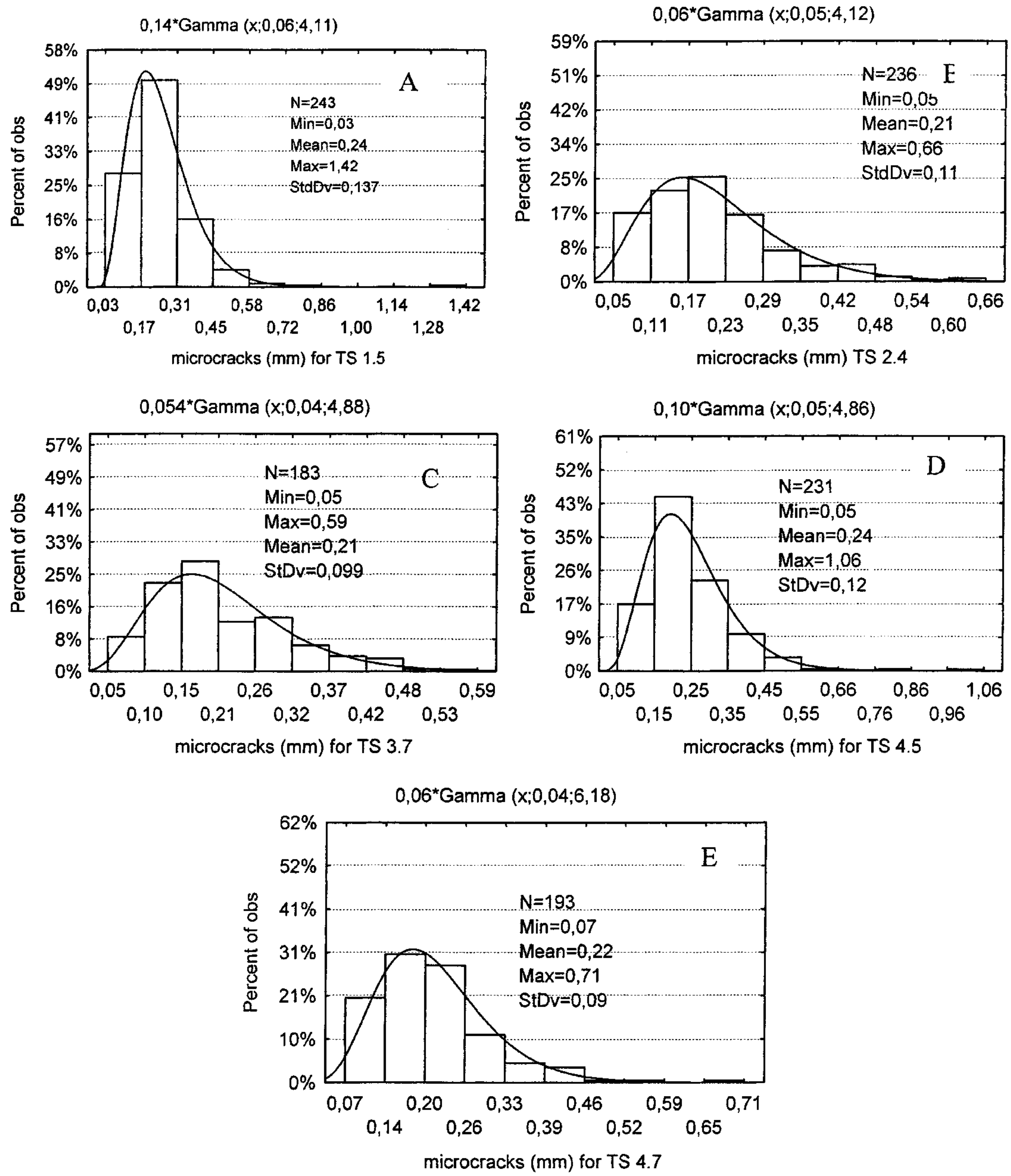

Fig. 6 Descriptive statistics, data histogram, and γ statistical model of the microcracks measured in the five TSs

models of the grain shape of the microstructure because they have the same K-S value. Based on the relation of the Weibull model with the strength of materials (section 3.3), the Weibull model (x; 3.550; 65.410) was selected as the most appropriate one. In this analysis, 2497 measurements of grain shape have been used to draw this conclusion.

Similar to what was seen for grain size, it was observed from Fig. 5 that the five TSs have a similar distribution in grain shape. Though TS 4.5 and TS 4.7 are TSs obtained a distance of 90 mm apart (Fig. 1), there is also no remarkable similarity between them. This supports the initial conclusion that the rock has very low heterogeneity. Therefore, from the point of view of the grain shape, this rock is homogeneous on the microscale.

5.3 Analysis of the Microcracks

From the results presented in Table 3, it was concluded that the γ distribution function is the most appropriate model to describe the microcracks because it had the lowest K-S value (section 3.3). The γ model (x; 4.620; 20.420) described the overall trend of the grain size of the microstructure of Härno granite based on 1086 measurements of microcracks size.

Unlike the situation with grain size and grain shape, the distribution of microcracks differs obviously from TS to TS.

Table 1 Results of Komologorov-Smirnov goodness-of-fit test for modeling the grain size of Härno granite

Probability distribution	Parameters		K-S test
Cauchy	0.190	0.126	0.208
Chi-squared	0.262	0.262	0.600
Exponential	0.262	0.262	0.099
Extreme value	0.376	0.197	0.228
Gamma	1.480	5.639	0.061
Laplace	0.181	6.132	0.190
Normal	0.262	0.253	0.172
Uniform	0.019	2.351	0.670
Weibull	1.178	0.279	0.059

Table 2 Results of Komologorov-Smirnov goodness-of-fit test for modeling the grain shape of Härno granite

Probability distribution	Parameters		K-S test
Cauchy	58.820	14.548	0.109
Chi-squared	58.928	58.928	0.148
Exponential	58.928	58.928	0.340
Extreme value	67.245	14.418	0.079
Gamma	8.272	0.140	0.050
Laplace	59.310	0.066	0.060
Normal	58.928	18.491	0.020
Uniform	0.560	100.000	0.240
Weibull	3.550	65.410	0.020

Table 3 Results of Komologorov-Smirnov goodness-of-fit test for modeling the microcracks of Härno granite

Probability distribution	Parameters		K-S test
Cauchy	0.205	0.006	0.131
Chi-squared	0.226	0.226	0.711
Exponential	0.226	0.226	0.308
Extreme value	0.278	0.090	0.189
Gamma	4.620	20.420	0.057
Laplace	0.200	12.373	0.099
Normal	0.226	0.115	0.119
Uniform	0.030	1.420	0.666
Weibull	2.061	0.256	0.084

The microcrack size is different with respect to the number of small microcracks. Moreover, the TSs that are most alike in microcrack size distribution are not the TSs for samples taken in the smallest proximity (TS 4.5 and TS 4.7). This shows that microcrack size may vary in the rock mass and, therefore, may be responsible for the variation of mechanical behavior observed in the different samples of this granite. Therefore, from the point of view of the microcracks, this granite is less homogeneous on the microscale.

6. Discussion

It was found that the Weibull statistical model and γ distribution function were the most appropriate statistical functions for modeling the grain size and the grain shape, respectively. In this article, the microstructural modeling approach is focused on choosing the most appropriate statistical model for the entire set of TSs rather than having a different model for each TS. However, if the goal is to model the rock samples from the TSs they were taken from, then different statistical models for each analyzed TS can be used.

The present analysis was performed on a 1 cm^2 area per TS provided that a significant number of mineral grains could be analyzed. The number of TSs analyzed was five, and this was based on the low heterogeneity observed in the field of view and on the number of test specimens necessary to evaluate the mechanical properties.

Interesting insight regarding the rock material is expected when the microstructural modeling approach is applied to different granites or other rock types. For granitic rock with a similar texture to Härno granite, the discontinuities of grain boundaries and microcracks are defects that determine rock failure. Thus, the size and the shape of the network of mineral grains and the microcracks are assessed using images taken with the optical microscope. However, microstructural modeling is an approach that is simultaneously rock-dependent and process-dependent (i.e., the model must be adapted to the specificities of the rock material, according to their importance for the failure process). In other words, the selection of the microstructural properties depends on the rock type and the goal of the rock-modeling approach. Other granites that are not fine-grained and/or even-grained might require the following changes:

- The stereological considerations for modeling the microstructural properties of the rock (i.e., stereology) are concerned with the interpretation of three-dimensional structures using two-dimensional sections or projections.
- The area per TS and the number of TSs under investigation should be selected to capture the overall microstructure.
- Modeling the grain orientation for nonisotropic rocks.

In this sense, microstructure modeling is simultaneously rock-dependent and process-dependent.

7. Conclusions

A microstructure-modeling approach was applied to Härno granite to model the microstructure and analyze its heterogeneity. A 1 cm^2 area was used to analyze each TS by means of optical microscopy image analysis. The grain size, grain shape, and microcrack distribution were modeled with various statistical models. The Weibull distribution, as well as the Cauchy, chi-squared, Erlang, exponential, extreme value, γ, Laplace, normal, triangular, and uniform distributions were evaluated. It was found that the Weibull distribution is the most appropriate model for the determining grain size and grain shape when compared with the nine other statistical models. Concerning microcrack characterization, it was concluded that the γ distribution is the most appropriate model, after a careful comparison with the Weibull model.

The grain size of the microstructure of Härno granite had values ranging from 0.03 to 1.93 mm and was modeled better with the Weibull distribution function (x; 1.78; 0.279). The measurements of grain shape had a range of 0.93 to 98.28 and are modeled well by the Weibull distribution function (x; 3.550; 65.410). The number of microcracks measured ranged from 183 to 243 in each TS, with a minimum size of 0.03 mm and a maximum size of 1.42 mm. The microcracks had a mean size of 0.25 mm. Microcracks were modeled well by the γ function (x; 4.620; 20.420).

Concerning microstructural heterogeneity, the microstructure of Härno granite is homogeneous with respect to grain size and grain shape. The statistical models are similar from TS to TS. However, microcracks show a clear variation in the statistical model among TSs, especially with respect to the number of small microcracks. Thus, Härno granite is less homogeneous when considering the size of the microcracks.

The microstructural modeling approach is important for overall modeling, microstructural characterization, and analysis of the heterogeneity of the microstructure of rock materials. Among other applications, it can be used to explain differences in the mechanical behavior of the rock ore obtained through mechanical testing of several specimens.

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Appendix

$$\text{Cauchy}\ (x;\alpha;\beta) = \left\{\pi\beta\left[1+\left(\frac{x-\alpha}{\beta}\right)^2\right]\right\}^{-1},\ \beta > 0 \qquad \text{(Eq 1)}$$

$$\text{chi-squared}\ (x;\upsilon) = \frac{x^{(v-2)/2}e^{(-x/2)}}{2^{(v/2)}\Gamma\left(\frac{v}{2}\right)},\ x > 0 \qquad \text{(Eq 2)}$$

$$\text{extreme value}\ (x;\alpha;\beta) = \left(\frac{1}{\beta}\right)\exp\left\{\left(\frac{1}{\beta}\right)(x-a) - \exp\left[\left(\frac{1}{\beta}\right)(x-\alpha)\right]\right\} \qquad \text{(Eq 3)}$$

$$\text{exponential}\ (x;\beta) = \frac{1}{\beta}e^{-x/\beta},\ x > 0 \qquad \text{(Eq 4)}$$

$$\text{gamma}\ (x;\alpha;\beta) = \frac{\beta^{-\alpha}x^{\alpha-1}e^{-x/\beta}}{\Gamma(\alpha)},\ x > 0 \qquad \text{(Eq 5)}$$

$$\text{Laplace}\ (x;\alpha;\beta) = \left(\frac{\beta}{2}\right)e^{(-\beta|x-\alpha|)} \qquad \text{(Eq 6)}$$

$$\text{normal}\ (x;\mu;\sigma) = \frac{1}{\sqrt{2\pi}}e^{-(x-\mu)^2/2\sigma^2} \qquad \text{(Eq 7)}$$

$$\text{uniform}\ f(x) = \frac{1}{(b-a)},\quad a \le x \le b \qquad \text{(Eq 8)}$$

$$\text{Weibull}\ (x;\alpha;\beta) = \alpha\beta^{-\alpha}x^{\alpha-1}e^{-(x/\beta)^{\alpha}},\ \text{with}\ x > 0 \qquad \text{(Eq 9)}$$

where $\Gamma(x)$ refers to the mathematical gamma function.

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