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Surface Morphology: Theoretical Model and Correlation with Experimental Results

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Abstract*: In this work, we propose a model for the description of the surface morphogenesis of a dispersed system of the solid-solid type. To obtain the model, stochastic formalism based on the master equation and the principles of fractal geometry was applied, so that the surface morphology is characterized by the fractal dimension and the roughness exponent, which are expressed as a function of the composition of the dispersed system and the dynamic parameters associated with surface formation. Theoretical results obtained were compared with experimental results, finding that the variable that shows a significant effect on the morphology of the surface of the solid-solid dispersed system is the specific surface area of the particles of the dispersed phase found in the surface, as predict theoretically.

***Keywords* : surface morphology, earth construction.**

I. INTRODUCTION

The solid surfaces, unlike the mobile interfaces present in the liquid - liquid, and liquid - gas systems, are characterized by presenting a constant surface area[1], which exhibits a rough character whose manifestation depends on the size of the observed system [2]. This roughness, which is related to the fact that the height of the solid interface changes randomly with the observed area, is the result of two fundamental factors: one is associated with the possibility of action of external forces that cause deposition or detachment of particles [3,4], which in turn influences the value of the specific surface area and the other that relates to the processes of solid formation that take place on the microscopic scale.
The roughness causes that the real surface area of the solid cannot be determined by Euclidean geometry [5,6], and the use of experimental methods is necessary for its determination. Traditional methods are based on the measurement of some chemical-physical property that depends on the surface area [7], the observed value of this property, in turn, depends on the selected method, so in principle, it is practically impossible to determine the surface area of the solid with accuracy.

With the rise and development of the theory of complexity in the second half of the twentieth century, different works have been carried out to theoretically describe the formation of solid surfaces [8] through the use of stochastic formalism,

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which explicitly takes into account the irregularities that occur in the systems, as well as the use of fractal geometry as a means to experimentally estimate the surface area value. This work presents the results of a theoretical and experimental study related to the surface morphogenesis of a solid-solid dispersed system, proposing a model to describe the relationship between the fractal dimension of the solid interface and the composition of the dispersed system.

OBTAINING THE THEORETICAL MODEL

In order to obtain the theoretical model, it is assumed that the surface roughness constitutes an expression of the microscopic processes that take place during the solid formation process, where the roughness is associated with the internal fluctuations that take place around the average height of the solid interface. From this initial assumption, mesoscopic formalism based on the Master Equation (ME) is applied to describe the interface formation process.

Obtaining the ME

To obtain the ME, it is taken into account that the solid is formed by introducing solid particles (dispersed phase) into a liquid dispersion medium which solidifies resulting in the formation of a solid-solid dispersed system, where it will be assumed that all particles have equal size. In this system, the interface is considered equal to a volume $V = HA$ (Figure 1) adjacent to the surface of the solid, where H is the thickness of the interface and A is the area of the corresponding flat surface.

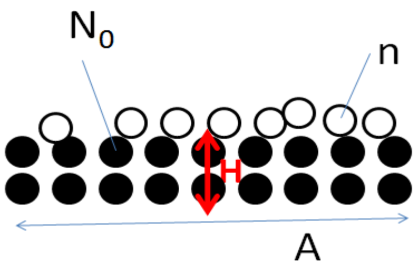

Figure 1. Visualization of the dynamic behavior of the particles of the dispersed phase that are on the surface during the solid formation process.

In the microscopic scale, it is considered that the extensive variable is the total number n of solid particles present in the surface of the interface. During the interface formation process, it is assumed a priori that the microscopic processes that occur and their associated transition probabilities are as follows:

i) the increase in 1 of n due to the movement of the particles from the bulk dispersion medium to the surface of the solid, where the probability of transition per unit of time is:

$$W_{n+1/n} = k_1 N_0 \qquad (1)$$

where N_0 is the total number of solid particles present in the interface.

ii) the decrease in 1 of n due to the passage of solid particles from the surface to the bulk interface, whose probability of transition per unit of time is:

$$W_{n-1/n} = k_2 n \qquad (2)$$

so that the ME, which describes the behavior of the probability $P(n;t)$ that there are n particles on the surface at time t, is given by:

$$\frac{\partial P(n;t)}{\partial t} = (E^{-1}-1)k_1 N_0 P(n;t) + (E^{+1}-1)k_2 n P(n;t)$$
$$P(n_0;0) = 1 \qquad (3)$$

In equation (3) E^q is the step operator that acts on discrete variable functions such that $E^q[f(n)] = f(q+a)$, k_1 and k_2 (t^{-1}) are dynamic parameters associated with the microscopic processes that occurs during the surface formation The ME (3) is a differential equation in differences, where the partial derivative found on the left side involves the temporal changes observed in the macroscopic scale, while the microscopic time is intrinsic involved in the constant k_1 and k_2.

Obtaining the steady state mesoscopic model

If it is taken into account that n is high enough to be able to consider that when an individual microscopic process occurs, the change Δn is negligible compared to n, then n can be considered as a continuous variable, then the Fokker - Planck Equation (EFP) corresponding to ME (3) is:

$$\frac{\partial P(n;t)}{\partial t} = -\frac{\partial}{\partial n}(k_1 N_0 - k_2 n)P(n;t) + \frac{1}{2}\frac{\partial^2}{\partial n^2}(k_1 N_0 + k_2 n)P(n;t)$$
$$P(n_0;0) = 1 \qquad (4)$$

In order to obtain the mesoscopic model of the system According to Van Campen [9], the intensive variable that describes the behavior of the system is considered to be the excess surface area θ, defined as the ratio between the real area of the irregular surface and the area corresponding to a flat surface, ~~the~~ which is estimated through the relationship:

$$\theta = \frac{n\gamma}{\varphi_s A} \qquad (5)$$

where γ is the surface area of each individual particle, φ_s is the fraction of the area of the solid that is covered by the dispersed phase and A corresponds to the area of a flat surface. Taking into account that:

$$P(n;t)\partial n = P(\theta;t)\partial\theta \qquad (6)$$

is obtained:

$$P(n;t) = P(\theta;t)\frac{\gamma}{\varphi_s A} \qquad (7)$$

such that the EFP is then written as a function of θ:

$$\frac{\partial P(\theta;t)}{\partial t} = -\frac{\partial}{\partial\theta}(\alpha k_1 - \theta k_2)P(\theta;t) + \frac{1}{2}\frac{\partial^2}{\partial\theta^2}\frac{1}{\Omega}(\alpha k_1 + \theta k_2)P(\theta;t)$$
$$P(n_0;0) = 1 \qquad (8)$$

Where α and Ω are system parameter defined as:

$$\alpha = \frac{1}{A}\frac{\gamma}{\varphi_s}N_0 \qquad (9)$$

$$\Omega = \frac{A\varphi_s}{\gamma} \qquad (10)$$

The total number of particles N_0 in the interface is determined as:

$$N_0 = \frac{\varphi_w M}{\rho_0 v_0} = \frac{\varphi_w V\rho}{\rho_0 v_0} \qquad (11)$$

where M and ρ represent the mass of the interface and the total density of the solid-solid dispersed system, respectively, φ_w is the weight fraction of the dispersed phase, ρ_0 is the density of the dispersed phase and v_0 represents the volume of the particles that constitute the dispersed phase Substituting (11) in (9):

$$a = \frac{\gamma}{v_0} \qquad (12)$$

where a is the specific surface area of the particles that form the dispersed phase. In the vicinity of the steady state, the mesoscopic model that describes the behavior of the average value Φ of the excess surface θ and the variance σ of the internal fluctuations that occur around Φ are given by:

$$\frac{d\Phi}{dt} = k_1\alpha - k_2\Phi \qquad (13)$$

$$\frac{d\sigma}{dt} = -2k_2\sigma + \frac{1}{\Omega}(k_1\alpha + k_2\Phi) \qquad (14)$$

$$\Phi(0) = \Phi_0; \sigma(0) = \sigma_0 \qquad .(15)$$

In a steady state:

$$\Phi = \frac{k_1}{k_2}\alpha \qquad (16)$$

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$$\sigma = \frac{1}{2}\frac{1}{\Omega}(\beta + \Phi) = \frac{\Phi}{\Omega} \quad (17)$$

Where:

$$\beta = \frac{k_1}{k_2}\alpha = \frac{k_1}{k_2}\frac{\rho}{\rho_0}\frac{\varphi_w}{\varphi_s}Ha \quad (18)$$

The probability function that describes the behavior of excess surface is normal or Gaussian and is given by:

$$P(\theta) = \frac{1}{\sqrt{2\pi\frac{\Phi}{\Omega}}}exp\left(-\frac{(\theta-\Phi)^2}{\frac{2\Phi}{\Omega}}\right) \quad (19)$$

Irregular surface morphology will be described based on the fractal dimension $\boldsymbol{f}$, such that the total surface area of the solid is expressed as:

$$A_t = g^{2-D_f}h^{D_f} \quad (20)$$

where h is the Euclidean distance between two extreme points on the surface and δ is a parameter related to the accuracy of the measurement of h and the observed magnification level. Applying logarithm to both sides of the equation (20) is obtained:

$$f = \lim_{h\to h_0}\frac{\ln A_t}{\ln h} \quad (21)$$

where h_0 is related to the smallest distance that can be observed in the system according to the level of magnification of the surface. The hypothesis that is established is that the fractal dimension $\boldsymbol{f}$ is related to the stochastic character of the excess surface area θ, which is described through the probability function $P(\theta)$ In steady state, the probability $P(\theta)$ can be visualized from the point of view of the ensemble [10] so that the probability that in a specific site the excess surface area θ is equal to b will be defined as:

$$P_{\theta=b} = \frac{S_{\theta=b}}{S_t} \quad (22)$$

where S_t is the number of total sites observed and $S_{\theta=b}$ is the number of sites in which the condition $\theta = b$ is observed. In this way, the average value of θ, which is identified with the fractal excess of the surface θ_f, is determined as:

$$\theta_f = \sum_{i=1}^{S_t} b_i P_{\theta=b_i} = \int [P(\theta)]P(\theta)\,d\theta = \int \frac{C}{\sqrt[2]{2\pi\sigma(\varepsilon)}}d\varepsilon \quad (23)$$

where ε is the length that characterizes the size of the sites observed in the mesoscopic scale, in which $\varphi_s \to 1$ and $\varphi_w \to 1$.

To determine the fractal dimension, it is necessary to express the variance σ as a function of powers of the non-dimensional parameter ε:

$$\sigma = \frac{1}{2}\frac{1}{\Omega}(\beta_0 + \varepsilon^2) = C_1\varepsilon^{\mu} \quad (24)$$

where:

$$\mu = \lim_{\varepsilon\to 1}\left(\frac{d\ ln\,\sigma(\varepsilon)}{d\varepsilon}\left(\frac{d\ ln\,\varepsilon}{d\varepsilon}\right)^{-1}\right) = \frac{2}{\beta_0 + 1} \quad (25)$$

$$\beta_0 = \lim_{\phi_s\to 1}\lim_{\phi_w\to 1}\beta = \frac{k_1}{k_2}\frac{\rho}{\rho_0}Ha \quad (26)$$

Substituting the ec (24) in the ec (23) is obtained:

$$\theta_f = \int \frac{C_2}{\sqrt[2]{\varepsilon^{\mu}}}d\varepsilon = C_3\varepsilon^{1-\frac{\mu}{2}} \quad (27)$$

Considering that the fractal surface area is the product of the excess of the fractal surface by the area of a flat surface:

$$A_t = C_3\varepsilon^{1-\frac{\mu}{2}}\varepsilon^2 = C_3\varepsilon^f \quad (28)$$

in such a way that by properly combining the equations is obtained the relation between f and a :

$$f = \frac{3\psi a + 2}{\psi a + 1} \quad (29)$$

where ψ is a parameter that is determined experimentally and is given by:

$$\psi = \frac{k_1}{k_2}\frac{\rho}{\rho_0}H \quad (30)$$

The value of ψ takes into account the relationship between the velocity constants associated with the solid formation process, as well as the relationship of densities between the density of the dispersed system and the density of the dispersed particles, which can be approximately constant.

II. RESULTS AND DISCUSSION

To analyze the correspondence between the predicted theoretical behavior and the observed experimental values, the morphology of a solid-solid dispersed system that is formed from the solidification of the dispersion medium of a suspension as a result of a chemical reaction was analyzed. To carry out the experiment, common products were used that are used to manufacture the building materials, specifically sand (dispersed phase) and cement (dispersion medium).

To carry out the experimental procedure, a sieve was used to separate the dust particles into different average particle diameters, using those having an average diameter of 0.071, 0.2, 0.25 and 0.35 mm, respectively. The mixtures were prepared varying the proportion of cement from 15 to 25% in dry mass. After the dried samples were prepared, they were mixed with water, and these were allowed to stand for 72 hours on slide sheets.

During the resting process, a chemical reaction of crystallization of the cement takes place resulting in the formation of a solid-solid dispersed system in which it is considered that the sand particles form the dispersed phase and the crystallized cement the dispersion medium. The surfaces images of the solids were taken using a NOVEL brand microscope with X20 magnification and an HDCE-10 camera connected to a computer. The images were obtained with a format of 1024 × 768 pixels. The computational work of the edition of the images was carried out with the ImageJ version 1.51J8 program which can be downloaded for free from the page http://imagen.nih.gov/ij.

The design of experiments was constituted by 12 experiments, with the fractal dimension f as a dependent variable, and with the surface area and the composition of the samples as independent variables with 4 and 3 levels, respectively. This design, as well as the results obtained after its execution, is shown in Table 1.

Table 1. Results of the experimental design

Sample	Superficial area (mm2)	Composition (c)	Fractal dimension (f)
1	84.507	0.15	2.5561
2	30	0.15	2.538
3	24	0.15	2.5169
4	17.1428	0.15	2.4769
5	84.507	0.2	2.5842
6	30	0.2	2.5073
7	24	0.2	2.4835
8	17.1428	0.2	2.3477
9	84.507	0.25	2.5431
10	30	0.25	2.5011
11	24	0.25	2.4363
12	17.1428	0.25	2.4268

The experimental design analysis was carried out using the Stat graphics obtaining the results showed in Table 2:

Table 2. Analysis of experimental design results

Estimated effects for f			
Effect	Dear	Error Dear	V.I.F
average	2.27181	0.0443188	
A:d	0.0193715	0.00473136	108.672
B:c	-0.0474321	0.026237	3.12175
AA	-0.00015426	4.4427E-05	108.672
AB	0.00064672	0.00055587	3.12175
BB	0.0395	0.0257203	1
Standard errors based on the total error with 6 g.l.			

Analysis of variance for f				
Source	sc	Gl	CM	Reason -f
A:d	0.00739291	1	0.00739291	16.76
B:c	0.00144138	1	0.11144138	3.27
AA	0.00531709	1	0.00531709	12.06
AB	0.00059696	1	0.00059696	1.35
BB	0.00104017	1	0.00104017	2.36
Total error	0.00264614	6	0.00044102	
Total correct	0.0301047	11		

SC: Sum of squares

CM: middle squares

R- square = 91,2102 percent

R- square (adjusted by g.l.) = 83,8854 percent

Standard error of the estimate = 0,0210005

Average absolute error = 0,0130938

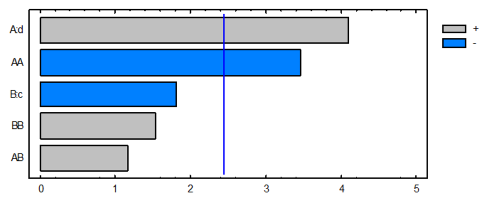
Statistician Durbin – Watson = 2,22493 (P=0,2402)

Residual autocorrelation of Lag 1 = 0,15571

d: specific surface area of the particles (mm^2 / mm^3), defined as the surface area divided by volume, calculated from considering the average particle size and that these are spherical**.**

Figure 2 shows the Pareto diagram that allows visualizing the effect of each of the independent variables considered on the fractal dimension. In this case it can be observed that the composition of the solid does not affect the value of the fractal dimension observed, at least for the composition intervals that were considered in this experiment, while the independent variable that does influence is the specific surface area, where The quadratic effect of this variable evidences a non-linear dependence between the fractal dimension and the specific surface area of the particle. This experimental results corresponding with the theoretic results given by ec. (29), which predicted that the fractal dimension depends on the specific superficial area of the particle, and it is independent of the system composition.

Standardized Pareto Diagram for f



Standardized effect

Figure 2. Pareto diagram showing the effects of the independent variables A (specific surface area of the particles) and B (the composition of the dispersed system) on the fractal dimension.

The experimental results was using to adjust the model given by the ec. (29) and to determine the value of parameter ψ. In tis case, was obtained the results showed in Table 3. This results are indicating that there is correspondence between the experimental and theoretical results.

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Table 3. Results of the adjusted experimental results to the proposed model given by ec. (29)

Estimation method: Marquardt			
Estimation results			
		standard error	Asymptotic
parameter	Dear	Asymptotic	LOWER
H	0.400368	0.0744884	0.234397
Q	0.153938	0.0299728	0.0871547
Variance analysis			
Source	SC	Gl	CM
Model	74.4279	2	37.2139
Residue	0.00590349	10	0.00059035
Total	74.4338	12	
Total (Corr.)	0.0301047	11	
R- SQUARE=80,3902 PERCENT			
R-SQUARE (ADJUSTED BY g.l.)=78,4292 percent			
standard error of est. =0,00242971			
absolute mean error = 0,0177525			
statistician Durbin – Watson = 1,59696			
residual delay autocorrelation 1 = 0,183999			
waste analysis			
	Estimate	Validation	
n	12		
CME	0.00059035		
MAE	0.719618		
MAPE	-5.5417E-05		
ME	-5.5417E-05		
MPE	-0.0108977		

The fitted model is:

$$f = \frac{0.400368 \times a + 2}{0.153938 \times a + 1}$$

In Figures 3 and 4, the graph of the adjusted model and the observed behavior is shown.

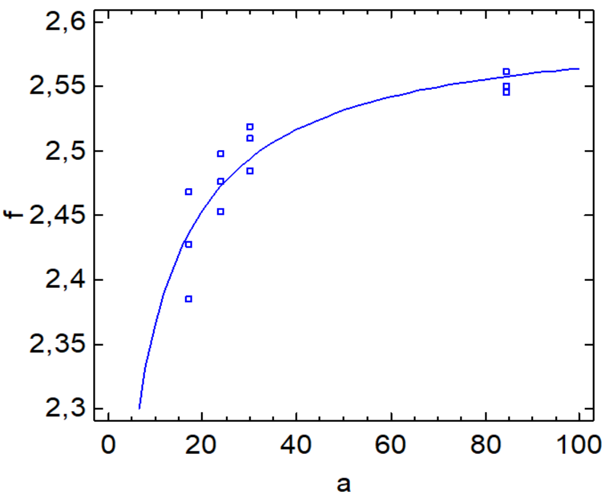

Figure 3 Graphic of the fitted model

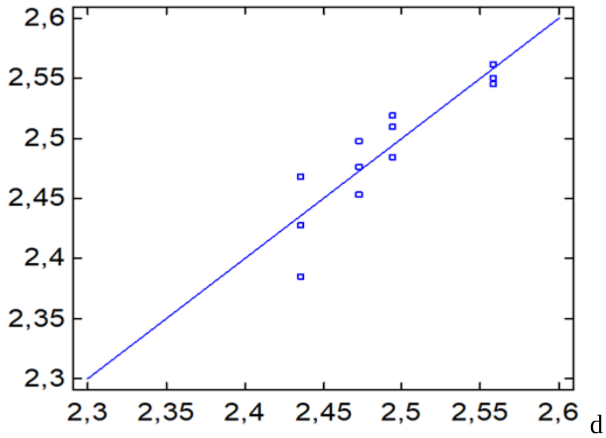

Figure 4. Graph of observed vs. predicted behavior

III. CONCLUSIONS

Due the supposition that rugosity exhibit by the Surface of diersed systems in solid-solid of random microscopic processes that occurs at level of dispersed particles during the the interfase formation it was obtained a model that relates the particles Surface área and the dyamic coefficient relation with fractal dimension of the interface. This model was obtained with an stochastic formalism based at a master equation and fractal dimension. This model was validated with experimental results obtaining an adequate correspondence between theoretical and observed results.

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REFERENCES

1. Schlüter, S., Berg, S., Rücker, M., Armstrong, R. T., Vogel, H. J., Hilfer, R., & Wildenschild, D. (2016). Pore-scale displacement mechanisms as a source of hysteresis for two-phase flow in porous media. Water Resources Research, 52(3), 2194-2205.
2. Geistlinger, H., Ataei-Dadavi, I., & Vogel, H. J. (2016). Impact of surface roughness on capillary trapping using 2D-micromodel visualization experiments. Transport in Porous Media, 112(1), 207-227.
3. Moreno, L., & Babadagli, T. (2015). Multilayer organic deposition on the rock surface with different wettabilities during solvent injection for heavy-oil recovery. The Canadian Journal of Chemical Engineering, 93(4), 664-677.
4. Kuang, J., Babu, N. R., Hu, J., Chen, A., Tavakkoli, M., & Vargas, F. M. (2018). Experimental Determination of Asphaltene Deposition. In Asphaltene Deposition (pp. 161-202). CRC Press.
5. Yang, H., Baudet, B. A., & Yao, T. (2016). Characterization of the surface roughness of sand particles using an advanced fractal approach. Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences, 472(2194), 20160524.
6. Feng, F., Liu, B., Zhang, X., Qian, X., Li, X., Huang, J., ... & Feng, P. (2018). Roughness scaling extraction method for fractal dimension evaluation based on a single morphological image. Applied Surface Science, 458, 489-494.
7. Watanabe, K., Sasaki, M., Mohri, M., & Yamashina, T. (1978). Quantitative measurement of surface roughness of graphite, silicon carbide and molybdenum irradiated with energetic deuterons. Journal of Nuclear Materials, 76, 235-239.
8. Pardo-Igúzquiza, E., Dowd, P. A., Durán, J. J., & Robledo-Ardila, P. (2018). A review of fractals in karst. International Journal of Speleology, 48(1), 2.

9. Benati, S., López-Blázquez, F., & Puerto, J. (2019). A stochastic approach to approximate values in cooperative games. *European Journal of Operational Research*, 279(1), 93-106.
10. Sanchez-Medrano, T. & Suarez-Dominguez, E.J. (2019) Microscopic Analysis of Bamboo Pieces and Its Relation to Compression Resistance IJRTE. 8[3] 3809-3812.
11. Abràmoff, M. D., Magalhães, P. J., & Ram, S. J. (2004). Image processing with ImageJ. Biophotonics international, 11(7), 36-42. http://imagen.nih.gov/ij

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