ON THE METHOD OF CALCULATING THE CORRELATION BETWEEN THE PARAMETERS THAT DESCRIBE THE ULTRA FINE GRIDING PROCESS SIMULATION AND THE REAL PROCESS TIME

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Abstract

To simulate the ultra fine grinding process of solid matter composed of crystals, agglomerates or aggregates – a random process that bears the features of a physical chemistry collective process – we can use algorithms based on probability methods, as was proved in earlier publications [9, 10, 13]. These publications also discuss grinding simulations for uniform and non-uniform size distributions. In this paper, we describe the method of determining a correlation factor between the parameters that describe a simulation (the energy factor) and the real process time. This correlation is the most important piece of information required to define the kinetics of the process, as it allows to judge the real process by examining the simulation results.

Key words: soft computing, simulation of physical chemistry processes, Monte Carlo method, size distribution of particles, grinding

1   Introduction

Non-quantum collective processes are such processes that take place in large sets of grains (or generally speaking – elements) and change the distribution of a certain attribute of these sets [10, 11]. Collective processes are strongly affected by the internal interactions between the elements of a large set. These interactions have a significant impact on the result of the process. In the case of a grinding process, it is the grain size distribution that changes $p(l)$.

The ultra fine solid matter grinding process changes the grain size distribution in a sample. Disperse dyes, which were being measured in the experiments and whose models will be tested, contain molecular crystals, which range between a few manometers and a dozen micrometers in size. The number of grains per fraction is between 1 and 20 million. Naturally, the size distributions of these crystals $p(l)$ are discrete distributions. Because of the large number of fractions and the very narrow fraction width, it is possible in this case to approximate the size distributions with continuous functions. The crystal forming process in turn (mass crystallization from solutions) lets us use continuous probability distributions for approximations. The size densities are then approximated by two-parameter probability density functions [6]. The log-normal distribution density is the best approximation (which is absolutely natural and was proved as the Edgeworth-Kapteyn theorem [7, 8]):

$$p(l) = \begin{cases} 0 \quad for \quad l = 0 \\ \dfrac{1}{\sqrt{2\pi}\sigma l} e^{-\frac{1}{2}\left(\frac{\ln l - m}{\sigma}\right)^2} \end{cases},$$
(1)

where: l is the grain diameter, m and σ are the density function parameters. An example of a log-normal distribution is illustrated in Figure 1.
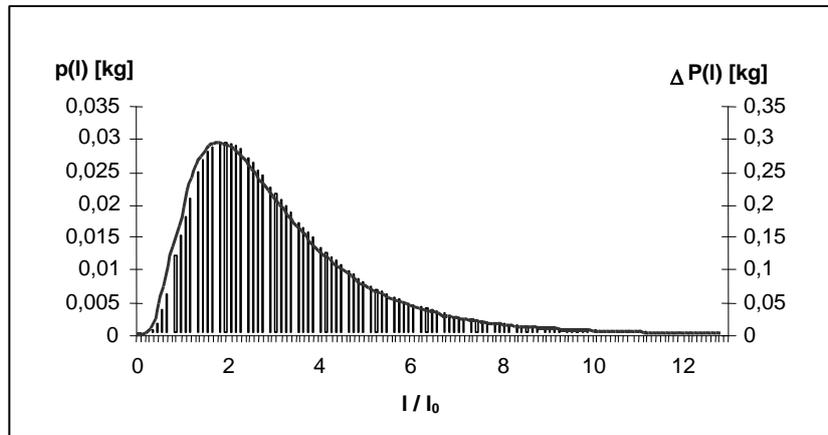
Figure 1. An example of approximating the size distribution (bar graph) p(l) by a log-normal density function p(l), where ΔP(l) is the share of each fraction in the entire sample

Two forms of the size density functions can be used for the calculations: the mass density or the amount density function $p_i(l)$. Because the Edgeworth-

Kapteyn theorem is applicable, we used the mass size density function for calculating the model.

The aim of a process simulation is to determine the changes in size distribution in time.

Random and empirical models based on approximating functionals defined on size distribution densities [9- 14] are used to simulate the grinding process kinetics *p(l,t)*.

The empirical models are based on approximating functionals, which are defined on a set of size distribution densities. Selected moments of approximating the size density distributions by density functions are most commonly used. For example, the distribution average μ or the grain size l_w, for which the cumulated size distribution approximation assumes the defined value $w(l_w)$, is used in [1, 3, 4] and [6]. The $\mu(t)$ or $l_w(t)$ dependencies approximate the process kinetics. Although the approximation functions are used at the core of optimisation algorithms and process automatics [8, 11], they do not allow to simulate the process in a virtual environment.

2   Simulation model of ultra fine grinding

The starting point for the model used for the simulation is the assumption that a single grain may shatter into a collection of smaller grains and the probability of creating a collection of grains of a given size depends on the enthalpy of each element of the collection [2, 5, 14].

As the grain is shattered, the volume enthalpy remains constant (i.e. the volume enthalpy of the initial grain is equal to the sum of volume enthalpies of all grains in the collection, because we assume that the set does not lose mass.

Let the energy ΔE_0 (calculated for a single grain) be delivered to the set and $\{K_i\}_N$ be the set of grain collections with smaller grain sizes, created from the initial grain.

The collection K_N is a set of grains with the same sizes, equal to the crystallisation nucleus size.

For each collection K_i we can determine the energy required to create a new surface ΔE_i:

$$\Delta E_i = \Delta E_0 - \sum_{j=1}^{J}\left(\sum_{l=1}^{L} G_{Slji}\right), \tag{2}$$

where: $\underline{l}$ is the number of same-size grains in the collection K_i , G_{Slji} is the surface enthalpy of a single grain whose size corresponds to the index l in the collection K_i, and j is the fraction index in the collection.

By adding up all ΔE_i for $i \in< 1; N >$ we obtain:

$$E_K = \sum_{i=1}^{N} \left(\Delta E_i \right), \tag{3}$$

which is the probability space normalising factor.

The probability of the initial grain shattering into the given collection $K_i(p_i)$ is:

$$p_i = \frac{\Delta E_i}{E_K}, \tag{4}$$

In the simulations that we conducted we assumed the energy E_0 (E_0 − energy required to shatter a grain into nuclei) to be the standard energy delivered during one instance of grinding a single grain. It turned out that this assumption allowed us to normalise the calculations. In life, this means that regardless of the initial grain size, the process will always be identical for an energy defined by the factor k that is delivered to the grain ΔE_0:

$$\Delta E_0 = k \cdot E_0, \tag{5}$$

We assumed that the grains shatter homogeneously, which means that the shapes of the resulting grains are the same as the shape of the initial grain. Of course, this assumption is a gross simplification, but it is possible (and unfortunately necessary) in the initial research testing phase. It is also an assumption that should not lead to major errors in the simulation results if there are grains created from numerous nuclei and in the case of molecular crystals.

3 Simulation results

For the simulation, we assumed an initial crystal sample with a log-normal mass distribution described by formula (1) with the parameter values $m = 1.742$ and $\sigma = 0.8$. It was assumed that a crystal of size $R_{max} = L$ (the largest in the sample) consists of 10,000 nuclei. The sample was divided into 10,000 fractions, corresponding to the various crystal sizes (i.e. different numbers of nuclei that they are composed of). The number of crystals for each fraction was calculated from the distribution function.

A simulation using the algorithm shown in Figure 2 was performed for each fraction. The algorithm uses a modified Monte-Carlo method [13]. It anticipates that each crystal from a given fraction could initially have been shattered into two pieces and the probability of this happening depends on the change in the surface enthalpy, which is described by formula (4).
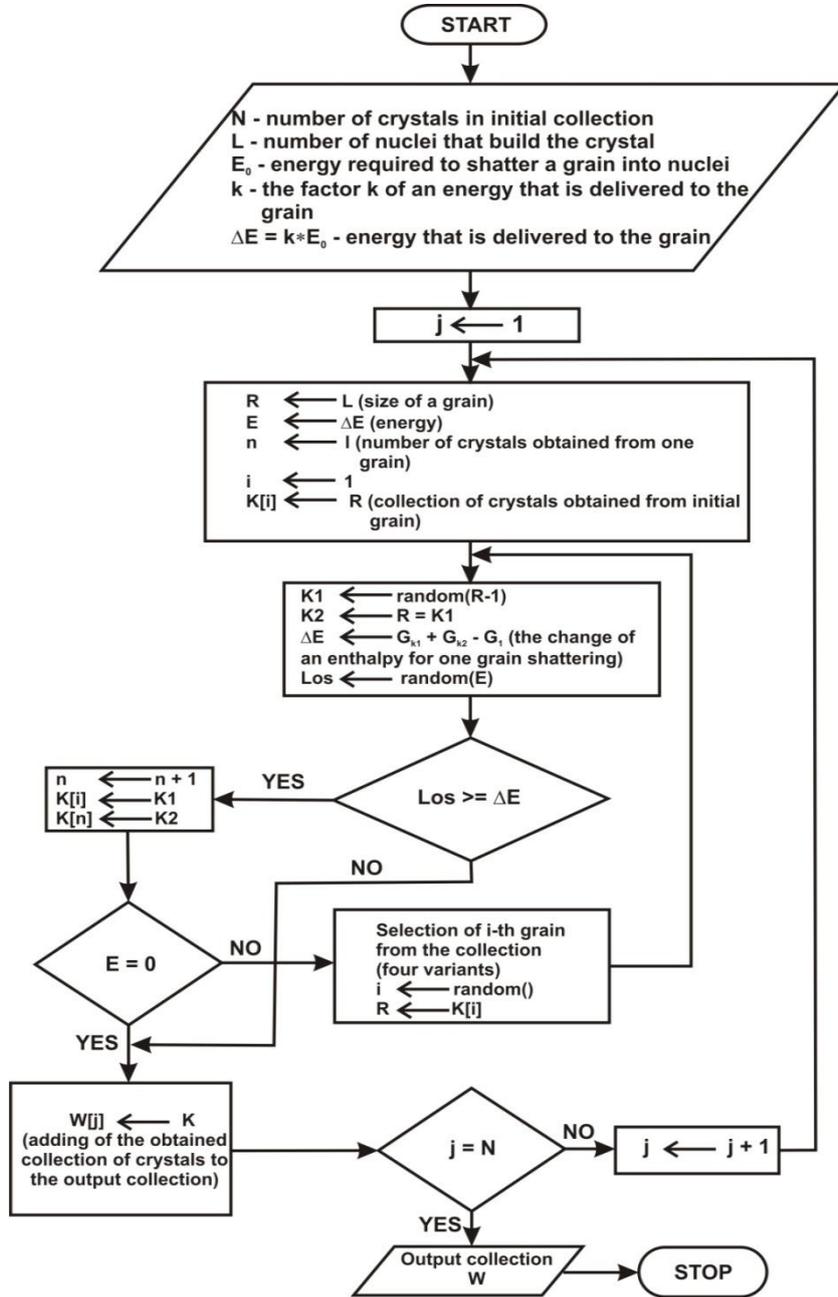
Figure 2. Algorithm used for the simulation

If this event took place, then the remaining shattering energy was diminished by the energy used to change the enthalpy in the process. The resulting grains formed a collection, from which new crystals were selected using the roulette-wheel method that could be further shattered. The process was stopped when the energy delivered to a single crystal became depleted or if a single crystal shattering event did not take place in the resulting collection thus formed.

All crystals from a given fraction were treated in the same way. A single crystal was shattered into a collection of grains and then the results obtained for all fractions were added up.

Selecting the grains for shattering using the roulette-wheel method introduced a certain dependence between the probability and the shattering medium. Several options for this dependence were checked in the simulation [9]:

- crystals selected with an equal probability,
- crystals selected depending on their radius,
- selection depending on the crystals' cross sections,
- grains selected depending on their volume.

If the selection probability is equal for all crystals, their shattering depends solely on the change of the surface enthalpy. In this case the smallest possible changes to the grains' surface areas are accepted. This means that splitting the nucleus off the crystal is the most probable event. Consequently, the resulting mass distribution shows too many crystals with their sizes close to the nucleus size (Figure 3a), which is not confirmed by any experiment results.
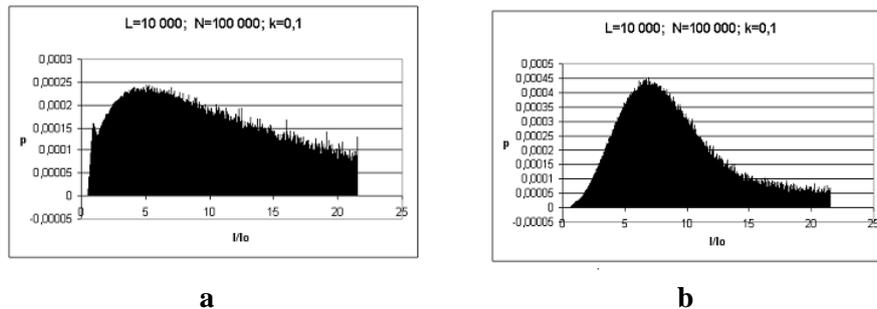
Figure 3. Mass histograms obtained from a simulation for a sample with an initial uniform size distribution where a) the crystal selection probability does not depend on the crystal size, and b) the probability depends on the crystal size (l/l_0 – crystal size compared to the nucleus radius)

This fault was corrected by introducing a relation where the crystals are selected depending on their size (Figure 3b) [9]. Further calculations use a de-

pendence based on the grain cross section. This choice was motivated by two factors. First, the distribution obtained from the simulation was the closest that it could be to empirical data in terms of quality; a log-normal function approximation resulted in the smallest error. Second, introducing this dependence reflects the real process, in which the crystals are shattered upon collision with the grinding medium, e.g. balls; and the probability of these collisions depends on the active cross section [9].

The simulations generated histograms of crystal quantity distribution throughout the fractions. These dependencies were changed into mass distribution histograms and then approximated by a log-normal function according to formula (1). The least square method based on the Levenberg-Marquardt algorithm was used for this approximation to determine the log-normal distribution parameters m and σ for selected histograms.

Empirical data is provided in the form of mass distributions for samples collected from the grinding machine at various points in time [14]. Figure 4 illustrates the change of the crystal size distribution over time during the grinding process.
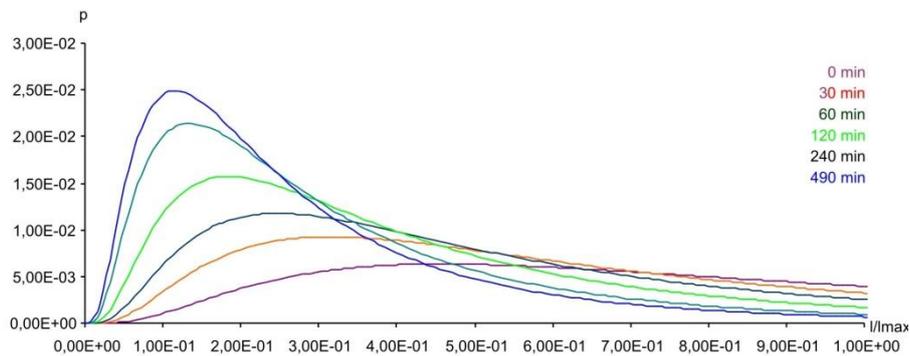
Figure 4. Changes in the distribution of crystal mass in the fractions over time in a real grinding process

As shown in [12], the parameter that controls the process in the simulation described above can be described by the amount of energy administered to a single crystal, represented by the coefficient k in formula (5). Increasing this parameter changes the crystal size distribution in a similar manner as the distribution changes over time in a real process, which only seems natural, because the energy delivered into the system increases with the elapsed grinding time.

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Figure 5 shows the histograms obtained for various different values of the coefficient *k*. The corresponding values of the parameters *m* and σ are shown in Table 1.
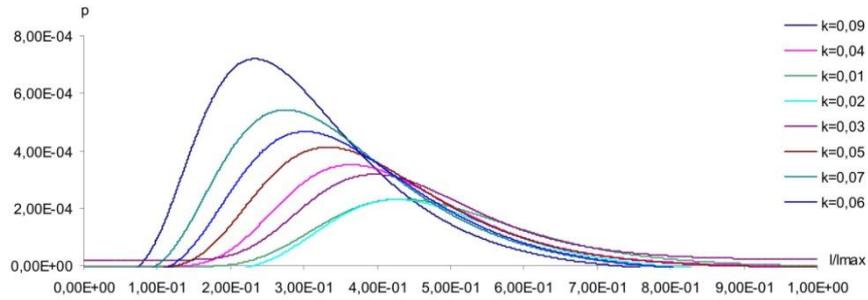
Figure 5. Mass distributions calculated in simulations for different values of the coefficient *k*

Table 1. Values of the parameters *m* and σ for different values of the coefficient *k* in the grinding process simulation

k	m	σ
0.01	2.489	0.296
0.02	2.461	0.272
0.03	2.392	0.284
0.04	2.327	0.314
0.05	2.262	0.354
0.06	2.196	0.394
0.07	2.125	0.421
0.08	2.052	0.437
0.09	1.982	0.446

Changes of the real distribution parameter *m* over time *t* were considered for further research [14], as illustrated in Figure 6.

The dependence *m(t)* from Figure 6 was approximated by a curve according to the following equation:

$$m(t) = p_1 - \frac{p_2}{(1 + p_3 t)^{\frac{1}{p_4}}}, \qquad (6)$$

The respective parameter values were calculated as follows: $p_1 = 0.28$ ($\Delta p_1 = \pm0.07$), $p_2 = -1.45$ ($\Delta p_2 = \pm0.07$), $p_3 = 0.0037$ ($\Delta p_3 = \pm0.0002$), $p_4 = 0.36$ ($\Delta p_4 = \pm0.11$).
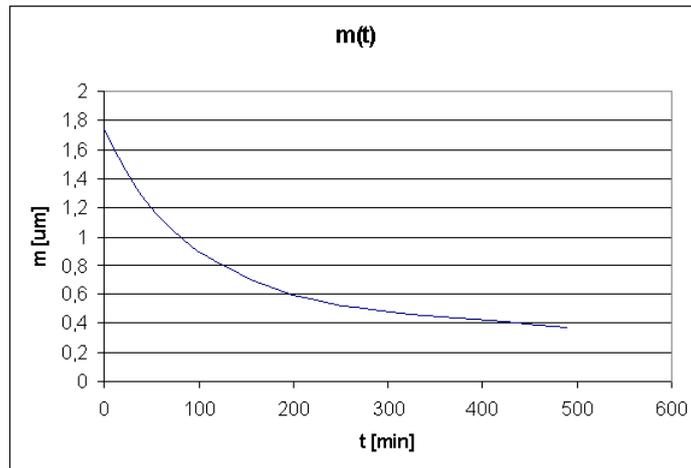
Figure 6. Changes of the parameter *m* over time in a real process

In order to obtain a linear dependence of *m* on the composite function *x(t)*, the function *x(t)* was determined. It turned out that the best match to a linear dependence was obtained by applying a transformation according to formula (7):

$$x(t) = -\frac{p_2}{\left(1 + p_3 t\right)^{\frac{1}{p_4}}},$$

(7)

After changing *m(t)* (6) to *m(x)* (7) we obtain the line:

$$m(k) = a \cdot k + b,$$

(8)

where: $a = 1$, $b = 0.28104$.

The results of the simulation $m_s(k)$ shown in Table 1 were approximated by the straight line:

$$m_s(k) = a_s \cdot k + b_s,$$

(9)

where: $a_s = -5.50$ ($\Delta a_s = \pm0.42$), $b_s = 2.50$ ($\Delta b_s = \pm0.02$).

The change of the parameter m over time t (increase of $m(x(t))$ in formula (8)) corresponds to the same change of this parameter in the simulation (increase of $m_s(k)$ – formula (10)). On this basis and by comparing the curves obtained it is possible to calculate the value of coefficient k for any given point in time t:

$$k = \frac{m_s[x(t)] - m_s[x(0)]}{a_s},$$

(10)

Figure 7 illustrates the relation between the simulation coefficient k and the real process time t. By comparing these two parameters it is possible to calculate the energy required to shatter single crystals in the simulation in order to obtain a distribution that corresponds to the given moment in time, which defines the kinetics of the modelled process.
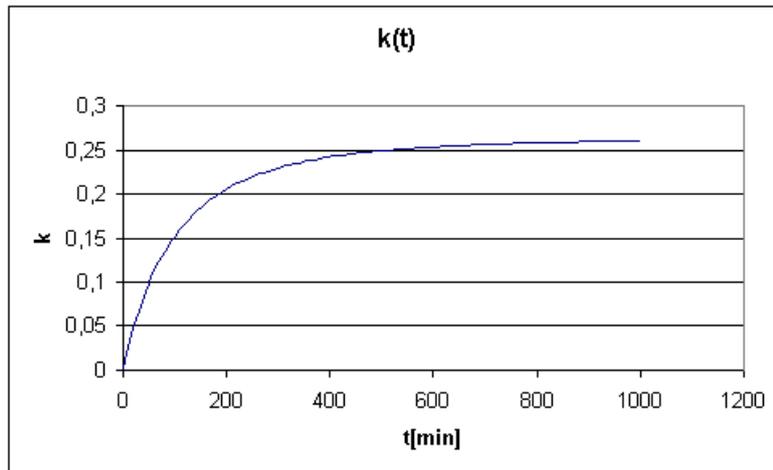
Figure 7. Coefficient k of the energy delivered in a simulation in relation to the time in a real process

When comparing the values of the size distributions in Figures 4 and 5 it is clearly apparent that the adopted range for the coefficient k ($0 \le k \le 0.9$) is too narrow and should be enlarged. Even for such small possibilities of comparing the size distributions obtained from simulations and the real experiment, one can see that the graphic distribution representations corresponding to $k = 0$, $k = 0.05$ and $k = 0.09$, respectively, are almost identical with the distributions corresponding to grinding times $t = 0$ min, $t = 30$ min and $t = 60$ min.

4 Conclusions

As was demonstrated in previous publications [9, 10, 13] algorithms based on probability methods may be used to simulate the ultra fine grinding process of solid matter composed of crystals, agglomerates or aggregates—a random process that bears the features of a physical chemistry collective process. Using the process simulation method for non-uniform size distributions as described above [13], we have performed simulations for various different values of the energy coefficient k, which describes the process in the simulation conditions. The results obtained were compared to the results of real process tests, which were conducted by one of the Authors [14].

A qualitative comparison clearly indicates a similarity between the size distributions that were determined using those two methods; in the real process it is possible to determine the dependence of a selected parameter that describes the size distribution on time ($p(l,t)$), whereas in the simulation experiment it is possible to determine the same parameter from the energy coefficient ($p(l,k)$).

The quantitative analysis of the results obtained allows to determine the relation between the energy coefficient k and the real process elapsed time t, which means that the simulation results can be scaled to the real process. The publication describes such a scaling method based on calculations for the parameter m, which describes the log-normal grain size distributions. The results of applying this method are illustrated in a graph, which is shown in Figure 7.

During our research we concluded that the simulation range (as described by the energy coefficient k) is too narrow, which means that the space of the size distributions obtained from the simulations does not fully match the space obtained from the real experiment. A comparison could only be performed for a time period from the process start ($t = 0$ and $k = 0$) to the time corresponding to 60 minutes of real grinding ($k = 0.09$). Yet even such a small range of the compared size distribution values seems to confirm the capabilities of the proposed method.

The choice of the log-normal distribution parameter m as the figure upon which a correlation between the simulation and the real experiment was determined also seems unfortunate. A different parameter should be taken for further research; the most reasonable of which seems to be the grain size, for which the size distribution achieves the maximum value (l_{pmax}), or a quotient of this value and the size distribution value $p(l_{pmax})$.

Subsequent research on the above topic will be conducted to widen the space covered by the simulation experiment results (performing simulations for k values greater than 0.09) and to optimise the parameter choice for which the correlation between the real process time and the energy coefficient describing the simulation process will be determined.

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