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HERAUSGEGEBEN VON PROF. DR.-ING. H. RUMPF
UND PROF. DR.-ING. K. SCHÖNERT

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Herausgegeben von Prof. Dr.-Ing. H. Rumpf und Prof. Dr.-Ing. K. Schönert,
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Inhaltsverzeichnis

Autorenverzeichnis

Asai, N.,	M.Eng., Nagoya University, Furo-cho, Chikusa-Ku, Nagoya, Japan (s. S. 559)
Austin, L.G.,	Ph.D., Pennsylvania State University, Mineral Processing Section, Dept. of Mat. Sci.,University Park, USA (s. S. 519)
Callcott, T.G.,	Prof., B.Sc., D.Appl.Sc., B.H.P. Central Research Laboratories, Shortland, Australien (s. S. 587)
Frühwein, P.,	Dipl.-Math., Institut für Mechanische Verfahrenstechnik, Karlsruhe, Universität, Bundesrepublik Deutschland (s. S. 505)
Fuerstenau, D.W.,	Prof. Sc.D., Dept. of Materials Science and Engineering, University of California, Berkeley, USA (s. S. 613)
Gardner, R.P.,	Professor, North Carolina State University, Raleigh, USA (s. S. 489)
Gupta, V.K.,	M. Techn. Ph.D., Indian Institute of Technology, Dept. of Metallurgical Engineering, Kanpur, Indien (s. S. 447)
Heiskanen, K.,	Dipl.-Ing., Helsinki, University of Technology, Dept. of Mining and Metallurgy, Otanfemi, Finnland (s. S. 631)
Herbst, J.A.,	D.Eng., Associate Professor, Dept. of Mining, Metallurgical Fuels Engg., University of Utah, Salt Lake City, USA (s. S. 467)
Jaspan, R.K.,	Ph.D., M.Sc. (Eng.), Johannesburg Consolidated Investment Co. Johannesburg, Südafrika (s. S. 539)
Jimbo, G.,	Prof. D.Eng., Nagoya, University, Furo-cho, Chikusa-Ku, Nagoya, Japan (s. S. 559)
Kapur, P.C.,	M.Sc., M.S., Ph.D., Indian Institute of Technology, Dept. of Metallurgical Engineering, Kanpur, Indien (s. S. 447)
Kropholler, H.W.,	Dept. of Polymer and Fibre-Science, University of Manchester, England (s. S. 539)
Luckie, P.T.,	Ph.D., Kennedy van Saun Corporation, Danville, PA, USA (s. S. 519)
Malghan, S.G.,	Dr. D., Minerals Research Laboratory, North Carolina State University, Asheville, USA (s. S. 613)
Mika, T.,	D.Eng., Assistant Professor, Dept. of Materials Sci. Engg., University of California, Berkeley, USA (s. S. 467 u. S. 539)
Onuma, E.,	B.Engg., Onoda Cement Manufacturing Co, Tahara-cho, Atsumigun, Aichi, Japan (s. S. 559)

A Critical Appraisal of the Discrete Size Models of Grinding Kinetics

V.K. Gupta and P.C. Kapur

Summary

We consider a mathematical model of linear and time invariant grinding system in continuous size and time variables and derive the exact relationships between the continuous size selection and breakage functions and the apparent selection and breakage parameters in the corresponding size discretized model. We show that the selection parameters and the breakage parameters are not independent of each other. The inner breakage parameter is not vanishingly small even when the sieve size ratio is $\sqrt[4]{2}$ and, in general, the discretization step introduces a gross nonlinearity which is implicitly reflected in time dependence of the discrete size grinding parameters. Next we derive a number of specialized discrete size grinding models and establish sharply defined mathematical conditions for time independence of the selection parameters and the breakage parameters, the normalizability of breakage parameters, the first order disappearance kinetics and the zero order appearance of fines.

Zusammenfassung

Wir betrachten ein mathematisches Modell eines linearen und zeitunabhängigen Zerkleinerungsprozesses bei kontinuierlichen Zeit- und Korngrößenvariablen und leiten die exakten Beziehungen zwischen der zu diesem Modell gehörenden Auswahl- und Bereichfunktion und den scheinbaren Auswahl- und Bruchparametern für ein in der Korngröße diskretisiertes Modell ab. Es zeigt sich, daß Auswahlparameter und Bruchparameter voneinander nicht unabhängig sind. Die Zerkleinerung innerhalb einer Klasse ist nicht verschwindend klein, auch bei einer Klassenstufung von $\sqrt[4]{2}$.

Prinzipiell führt die Diskretisierung zu einer merkbaren Nichtlinearität, die sich implizit in der Zeitabhängigkeit der diskretisierten Zerkleinerungsparameter äußert. Wir leiten eine Reihe von speziellen diskretisierten Zerkleinerungsmodellen ab und stellen scharf definierte mathematische Bedingungen auf für die Zeitunabhängigkeit der Auswahlparameter, die Normalisierbarkeit der Bruchparameter, die erste Ordnung der Zerkleinerungskinetik sowie die nullte Ordnung der Feingutentstehung.

Résumé

Nous considérons un modéle mathématique d'un systéme de pulvérisation linéaire et indépendant de temps avec des variables continues de temps et de grandeur et nous dérivons les relations exactes entre les fonctions continues de choix de grandeur et de pulvérisation et les paramètres apparents de choix et de pulvérisation dans le modèle à grandeurs discrétisées correspondant. Nous montrons que les paramèteres de choix et les paramêtres de pulvérisation ne sont pas indépendants entre eux. Le paramètre de pulvérisation interne n'est pas infiniment petit, même quand le rapport de diamètres de passage de tamis est $\sqrt[4]{2}$ et l'étape de discrétisation introduit en général une non-linéarite grossière, qui se traduit implicitement dans la dépandance du temps des paramètes de pulvèrisation à grandeurs discrètes. Nous dérivons ensuite un nombre de modèles particuliers de pulvérisation à grandeurs discrètes et nous établissons des conditions mathematiques bien définies pour l'indépendance du temps des paramètres de choix, la normalisabilité des paramètres de pulvérisation, la cinétique de disparition en premier ordre et l'apparition de fines à ordre zéro.

1. Introduction

We shall first focus our attention on size reduction phenomena in a batch mill containing a large population of particles which can be described, to a high degree of accuracy, by the following spatially homogeneous, continuous size and time variables mathematical model of the time invariant grinding system /1-8/

$$\frac{\partial M(x,t)}{\partial t} = -S(x)\, M(x,t) + \int_{x}^{x_0} S(v)\, B(v,x)\, M(v,t)\,dv \quad , \quad 0 < x \le x_0 \qquad (1)$$

where $M(x,t)dx$ is the mass fraction of particulate solids in size range x to $x + dx$ at grinding time t, the selection function $S(x)$ is the statistical expectation of the mass fraction of particles of size x selected for breakage per unit time, and $B(v,x)$, the breakage function, is normalized frequency function in size over the range $0 < x \leq v$ resulting from an average event of breakage of particles of size v. The model in eqn.(1) does not admit of any agglomeration of particles. Equation (1) may be formulated in terms of the cumulative distribution also; the resulting expressions are

$$\frac{\partial F(x,t)}{\partial t} = \int_x^{x_0} S(v)\, \bar{B}(v,x)\, \frac{\partial F(v,t)}{\partial v}\, dv \qquad (2)$$

$$\frac{\partial R(x,t)}{\partial t} = -\, S(x)\, R(x,t) + \int_x^{x_0} \frac{\partial (S(v)\, \bar{B}(v,x))}{\partial v}\, R(v,t)\, dv \qquad (3)$$

where the cumulative fraction passing $F(x,t)$ is

$$F(x,t) = \int_0^x M(v,t)\, dv \qquad (4)$$

the fraction retained $R(x,t)$ is

$$R(x,t) = 1 - F(x,t) \qquad (5)$$

and the cumulative breakage distribution

$$\bar{B}(v,x) = \int_0^x B(v,w)\, dw \qquad (6)$$

is the normalized product cumulative distribution over the range $0 < x \leq v$ resulting from an average event of breakage of particles of size v.

For engineering analysis of grinding operation, there has existed a valid motivation for an appropriate size discretized grinding model. For i-th size interval $x_i \leq x \leq x_{i-1}$ and the sieve size ratio $\delta = x_{i-1}/x_i$ is usually a constant, typically 2, $\sqrt{2}$ and $\sqrt[4]{2}$.

2. An Equivalent Size Discretized Model

In order to derive a size discretized grinding model which is equivalent to the continuous size model in eqn.(1) we first note that the mass fraction of solids in size interval i is

$$M_i(t) = \int_{x_i}^{x_{i-1}} M(x,t)\, dx \quad , \qquad i = 1,2,3,... \qquad (7)$$

We integrate eqn.(1) throughout over the range x_i to x_{i-1} and substitute eqn.(7), hence

$$\frac{dM_i(t)}{dt} = - \int_{x_i}^{x_{i-1}} S(x)\ M(x,t)dx + \int_{x_i}^{x_{i-1}} \int_{x}^{x_o} S(v)\ B(v,x)\ M(v,t)dv\ dx \tag{8}$$

From eqn.(6) we have

$$B(v,x) = \frac{\partial \bar{B}(v,x)}{\partial x} \tag{9}$$

Therefore, after substitution of eqn.(9), eqn.(8) may be written as

$$\frac{dM_i(t)}{dt} = \int_{x_{i-1}}^{x_o} S(v)\ \bar{B}(v,x_{i-1})\ M(v,t)dv - \int_{x_i}^{x_o} S(v)\ \bar{B}(v,x_i)\ M(v,t)dv \tag{10}$$

Break up of the integrals over discrete size intervals and rearrangement of the resulting terms gives

$$\frac{dM_i(t)}{dt} = - \int_{x_i}^{x_{i-1}} S(v)\ \bar{B}(v,x_i)\ M(v,t)\ dv + \sum_{j=1}^{i-1} \int_{x_j}^{x_{j-1}} S(v)\ [\bar{B}(v,x_{i-1}) - \bar{B}(v,x_i)]\ M(v,t)dv \tag{11}$$

which is the desired exact size discretized representation of the continuous size model.

We note that in eqn.(11) the selection and breakage functions occur in association only. This product term $S\bar{B}$, which will appear repeatedly in the discrete size analysis, deserves a name of its own. We shall call it as the selekage function $L(v,x)$, that is

$$S(v)\ \bar{B}(v,x) = L(v,x) \tag{12}$$

Equation (11) in terms of the selekage function may be written as

$$\frac{dM_i(t)}{dt} = - \int_{x_i}^{x_{i-1}} L(v,x_i)\ M(v,t)dv + \sum_{j=1}^{i-1} \int_{x_j}^{x_{j-1}} [L(v,x_{i-1}) - L(v,x_i)]\ M(v,t)dv \tag{13}$$

We mention in passing that the differential form of the selekage function

$$\frac{\partial L(v,x)}{\partial x} = S(v)\ B(v,x) \tag{14}$$

first appeared in the integro differential equation of grinding formulated by Bass /3/ in 1954.

3. Exact Relationships Between Continuous Size Grinding Functions and Discrete Size Grinding Parameters

In order to extract these relationships we compare the size discretized model in eqn. (13) with the master discrete size grinding equation

$$\frac{dM_i(t)}{dt} = - S_i(t)\, M_i(t) + \sum_{j=1}^{i-1} S_j(t)\, B_{i,j}(t)\, M_j(t) \quad , \quad i = 1,2,\ldots \qquad (15)$$

where for the time being we shall simply call S as the selection parameter and B as the breakage parameter and refrain from any elaboration at this stage. When either B or both S and B are time-invariant, the mathematical structure of the grinding model in eqn. (15) is formally identical to the discrete models of Bass /3/, Reid /9/, Mika et al./10/, Klimpel and Austin /11/, Herbst and Fuerstenau /12/, Kelsall and Reid /13/ and many others. Term by term comparison of eqns. (13) and (15) shows that

$$S_i(t)\, M_i(t) = \int_{x_i}^{x_{i-1}} L(v,x_i)\, M(v,t)dv \qquad (16)$$

Hence, the instantaneous selection parameter is

$$S_i(t) = \frac{\int_{x_i}^{x_{i-1}} L(v,x_i)\, M(v,t)dv}{\int_{x_i}^{x_{i-1}} M(v,t)dv} \qquad (17)$$

Similarly, the instantaneous breakage parameter is

$$B_{i,j}(t) = \int_{x_j}^{x_{j-1}} \frac{\left[L(v,x_{i-1}) - L(v,x_i)\right]\, M(v,t)dv}{S_j(t)\, M_j(t)} \qquad (18)$$

Combining eqn.(18) with eqn. (16) gives

$$B_{i,j}(t) = \frac{\int_{x_j}^{x_{j-1}} \left[L(v,x_{i-1}) - L(v,x_i)\right]\, M(v,t)dv}{\int_{x_j}^{x_{j-1}} L(v,x_j)\, M(v,t)dv} \quad , \quad i \neq j \qquad (19)$$

Next, we formally define the cumulative breakage parameter $\bar{B}_{i,j}$ as

$$\bar{B}_{i,j} = \sum_{k \geq i+1} B_{k,j} \quad , \quad i \geq j \qquad (20)$$

Substitution of eqn.(19) gives the expression for instantaneous cumulative breakage parameter

$$\bar{B}_{i,j}(t) = \frac{\int_{x_j}^{x_{j-1}} L(v,x_i)\, M(v,t)\, dv}{\int_{x_j}^{x_{j-1}} L(v,x_j)\, M(v,t)\, dv} \qquad (21)$$

Note that

$$\bar{B}_{j,j} = 1 \qquad (22)$$

The correct definitions of the grinding parameters, consistent with the actual material transfer out of a size interval or from one size interval directly to another, follow immediately by inspection of eqns. (17) and (19). Thus, the selection parameter $S_i(t)$ is the fractional rate of exit of particles from the size interval i at time t. The breakage parameter $B_{i,j}(t)$ is the ratio of the rates at time t at which the particles of size interval j after breakage are reporting directly to size interval i and at which the particles are breaking out of the size interval j. Furthermore, by definition, the instantaneous inner breakage parameter, $IB_{j,j}(t)$ is simply the fraction of material broken and falling back into the original size interval; hence

$$IB_{j,j}(t) = \frac{\int_{x_j}^{x_{j-1}} S(v)\, M(v,t) dv - \int_{x_j}^{x_{j-1}} L(v,x_j)\, M(v,t) dv}{\int_{x_j}^{x_{j-1}} S(v)\, M(v,t)\, dv} \qquad (23)$$

Or

$$IB_{j,j}(t) = 1 - \frac{\int_{x_j}^{x_{j-1}} L(v,x_j)\, M(v,t)\, dv}{\int_{x_j}^{x_{j-1}} S(v)\, M(v,t)\, dv} \qquad (24)$$

4. Realizations of the Discrete Size Grinding Models

4.1 Bass Model

Bass /3/ had suggested that if the following criterion is satisfied

$$x_{i-1} - x_i << \frac{x_{i-1} + x_i}{2} \qquad (25)$$

then the continuous size model in eqn.(1) may be approximated to the size discretized model in the following equation:

$$\frac{dM_i(t)}{dt} = -\left(\sum_{k \geq i+1} \eta_{k,i}\right) M_i(t) + \sum_{j=1}^{i-1} \eta_{i,j}\, M_j(t) \quad , i = 1,2,... \qquad (26)$$

where the time-invariant parameters η are simply the specific rate constants for flow forward of material from one size interval to another size interval lower down. Moreover, the parameters are explicit functions of both the selection and breakage functions. We shall present an alternate derivation of this model using somewhat different arguments. Let us assume that we are justified in approximating the particle size distribution within the size interval by a uniform distribution. This implies

$$M(x,t) = f_i(t), \quad x_i \leq x \leq x_{i-1} \tag{27}$$

and

$$f_i(t) = \frac{M_i(t)}{x_{i-1}-x_i} \tag{28}$$

We substitute these equations in eqns. (7) and (19) and obtain the following results

$$S_i = \frac{\int_{x_i}^{x_{i-1}} L(v,x_i)dv}{x_{i-1}-x_i} \tag{29}$$

$$B_{i,j} = \frac{\int_{x_j}^{x_{j-1}} [L(v,x_{i-1}) - L(v,x_i)]dv}{\int_{x_j}^{x_{j-1}} L(v,x_j)dv} \tag{30}$$

Hence

$$S_j B_{i,j} = \frac{1}{x_{i-1}-x_i} \int_{x_j}^{x_{j-1}} [L(v,x_{i-1}) - L(v,x_i)]\, dv \tag{31}$$

Recall that from eqn. (14)

$$L(v,x_i) = \int_0^{x_i} S(v)\, B(v,x)dx \tag{32}$$

Substitution in eqn. (29) gives

$$S_i = \frac{\sum_{k \geq i+1} \int_{x_k}^{x_{k-1}} \int_{x_i}^{x_{i-1}} S(v)\, B(v,x)dv\, dx}{x_{i-1} - x_i} \tag{33}$$

Following Bass, let

$$\eta_{k,i} = \frac{\int_{x_k}^{x_{k-1}} \int_{x_i}^{x_{i-1}} S(v)\, B(v,x)dv\, dx}{x_{i-1} - x_i} \tag{34}$$

then we have

$$S_i = \sum_{k \geq i+1} \eta_{k,i} \tag{35}$$

Similarly we can show that in eqn. (31)

$$S_j B_{i,j} = \frac{1}{x_{j-1}-x_j} \int_{x_i}^{x_{i-1}} \int_{x_j}^{x_{j-1}} S(v)\, B(v,x)\, dx \tag{36}$$

Hence

$$S_j B_{i,j} = \eta_{i,j} \tag{37}$$

Substitution of eqns. (35) and (37) into the master equation eqn.(15) immediately leads to size discretized time invariant parameter grinding model in eqn. (26), and the parameters can now be assigned physical interpretations as evident from eqns. (29), (30), (35) and (37), provided, of course, eqn. (27) is satisfied.

Bass had suggested that the inequality in eqn. (25) concurrently implies a vanishingly small inner breakage function $IB_{j,j}$. Substitution of eqn. (27) into eqn. (24) gives

$$IB_{j,j} = 1 - \frac{\int_{x_j}^{x_{j-1}} L(v,x_j)dv}{\int_{x_j}^{x_{j-1}} S(v)dv} \tag{38}$$

In order to obtain some numerical values of $IB_{j,j}$, let us assign — simply for the sake of convenience in computation — the following widely used forms for the selection and cumulative breakage functions

$$S(v) = Av^{\alpha} \tag{39}$$

$$\bar{B}(v,x) = (x/v)^{\beta} \tag{40}$$

Therefore, the selekage function is

$$L(v,x_j) = Av^{\alpha-\beta}x_j^{\beta} \tag{41}$$

Substitution of eqns. (39) and (41) into eqn. (38) gives

$$IB_{j,j} = 1 - [\frac{\alpha+1}{\alpha-\beta+1}][\frac{\delta^{\alpha-\beta+1}-1}{\delta^{\alpha+1}-1}] \text{ , } \alpha-\beta+1 \neq 0 \quad (42)a$$

$$= 1-[\frac{\alpha+1}{\delta^{\alpha+1}-1}]\ln \delta \text{ , } \alpha-\beta+1 = 0 \quad (42)b$$

which is independent of the size index.

Computations show that in general the inner breakage function is not insignificant and a substantial amount of material on breakage falls back into the original size interval even when the sieve size ratio is only $\sqrt[4]{2}$. For example, when $\alpha = 0.5$ and $\beta = 1$, $IB_{j,j}$=8.5%, and for $\alpha = 1$ and $\beta = 2$ its value is 16.3%.

However, as shown above, in order to generate the Bass model it is not necessary to stipulate that $IB_{j,j} = 0$. The sufficient condition is that the particles are uniformly distributed within a size interval. This condition of uniform distribution can be met by choosing sufficiently narrow size intervals.

The Bass model in eqn. (26) may also be written in the following manner

$$\frac{dM_i(t)}{dt} = - S_i M_i(t) + \sum_{j=1}^{i-1} S_j B_{i,j} M_j(t) \tag{43}$$

Equation (43) is formally identical to the most widely used discrete size grinding equation in the literature /9-14/. However, two important differences should be noted in respect of the model formulation. Firstly, unlike in the works of Mika et al. /10/, Herbst and Fuerstenau /12/, and Klimpel and Austin /11/, the derivation of eqn.(43) does not require the assumption of $IB_{j,j} = 0$. Secondly, parameters S and B, as given in eqn. (29) and (30), are not uncorrelated or independent of each other as regarded by most of the workers /9-14/. Both kinds of parameters are functions of the selekage function and, thus, are inter-related in a unique manner. It also follows that these parameters cannot be equated with mutually independent phenomena of selection for breakage and realization of breakage distribution function as originally proposed by Epstein /1,2/.

4.2 RSF Model

Inspection of eqns. (17) and (19) shows that it is not essential to assume a uniform distribution within a size interval, as done in the previous case, in order to generate a size discretized model with time-invariant parameters. Suppose there exist certain restrictive inter-relationships between the selection and breakage functions such that the selekage function L(v,x) becomes independent of variable v, that is

$$L(v,x) = L_2(x) \tag{44}$$

then, substitution of this reduced selekage function (RSF) into eqns. (17) and (19) gives

$$S_i = L_2(x_i) \tag{45}$$

and

$$B_{i,j} = \frac{L_2(x_{i-1}) - L_2(x_i)}{L_2(x_j)} \tag{46}$$

Substitution of these time-invariant parameters into eqn. (15), the master equation, leads to a size discretized RSF model as follows

$$\frac{dM_i(t)}{dt} = -L_2(x_i)\, M_i(t) + [\, L_2(x_{i-1}) - L_2(x_i)\,] \sum_{j=1}^{i-1} M_j \tag{47}$$

The inner breakage function for RSF model is

$$IB_{j,j}(t) = 1 - \frac{L_2(x_j)\, M_j(t)}{\int_{x_j}^{x_{j-1}} S(v)\, M(v,t)\,dv} \tag{48}$$

which is not time-invariant.

Let us consider the implication of the reduced selekage function for the continuous size model. Substitution of eqns. (44) and (45) into eqn.(3) gives the well known results /15,16/

$$\frac{dR(x,t)}{dt} = -L_2(x)\ R(x,t) \tag{49}$$

which is the expression for Rosin-Rammler type grinding kinetics.

4.3 SSF Model

In this model we formulate a separable selekage function (SSF) as follows

$$L(v,x) = L_1(v)\ L_2(x) \tag{50}$$

The discrete size grinding parameters in eqns. (17) and (19) become

$$S_i(t) = \frac{L_2(x_i)}{M_i(t)} \int_{x_i}^{x_{i-1}} L_1(v)\ M(v,t)dv \tag{51}$$

Or compactly

$$S_i(t) = L_2(x_i)\ P(x_i,t) \tag{52}$$

which is a function of time. And

$$B_{i,j} = \frac{L_2(x_{i-1}) - L_2(x_i)}{L_2(x_j)} \tag{53}$$

which is independent of time and similar to $B_{i,j}$ in the RSF model in eqn. (46). Substitutions in the master equation eqn. (15) generates the size discretized SSF model for grinding kinetics

$$\frac{dM_i(t)}{dt} = -L_2(x_i)\ P(x_i,t)\ M_i(t) + (L_2(x_{i-1}) - L_2(x_i)) \sum_{j=1}^{i-1} P(x_j,t)\ M_j(t) \tag{54}$$

Incidentally, this is first time that this model has been clearly delineated. The inner breakage parameter for the SSF model is obtained from eqn. (24)

$$IB_{j,j}(t) = 1 - \frac{L_2(x_j) \int_{x_j}^{x_{j-1}} L_1(v)\ M(v,t)dv}{\int_{x_j}^{x_{j-1}} S(v)\ M(v,t)dv} \tag{55}$$

An example of the separable selekage function was given in eqn. (41). Kapur /17/ has shown that when eqns. (39) and (40) are substituted into eqn. (1), a similarity solution to the resulting equation is

$$M(x,t) = \frac{C_o}{\mu_1(t)} \left[\frac{x}{\mu_1(t)}\right]^{\beta-1} \exp\left[-\frac{1}{\alpha k}\left(\frac{x}{\mu_1(t)}\right)^{\alpha}\right] \tag{56}$$

where

$$C_o = \frac{\alpha}{(\alpha k)^{\beta/\alpha}\,\Gamma(\beta/\alpha)} \tag{57}$$

$$k = \frac{1}{\alpha}\left[\frac{\Gamma(\beta/\alpha)}{\Gamma((\beta+1)/\alpha)}\right] \tag{58}$$

$$\mu_1(t) = (A\,\alpha k t + \mu_1(o)^{-\alpha})^{-1/\alpha} \tag{59}$$