

Micro-macro Modeling of Particle Crushing Based on Branch Lengths

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ABSTRACT: A micro-macro model of particle crushing is proposed. Microstructure changes are tracked with the density and size distribution of branch lengths. At the scale of a Representative Elementary Volume (REV), the free energy density of a set of branches of same length is written as the product of the total deformation energy stored in the REV by an energy split function, assumed to follow a power law. The distribution of deformation energy stored by the branches of a granular assembly subjected to isotropic compression is calculated with *PFC3D* Discrete Element Method (DEM) program. It is shown that this distribution varies indeed with branch lengths, and that the power-law provides a good fit for an exponent of 3. A macroscopic crushing parameter is defined to follow the progress of particle comminution (and therefore, dissipation). Constraints on the expression of the dissipation potential associated to particle crushing are explained, in order to ensure the convexity of the elastic domain. The proposed framework is expected to improve current thermodynamic models of particle crushing based on Grain Size Distributions (GSDs), especially to predict “shielding effects”. Better energy estimates could be used to optimize processes to make powders in the pharmaceutical and food industry.

INTRODUCTION

Breakage mechanics is of interest to many research disciplines including medicine and powder technology. Particle crushing occurs when high contact forces are produced within a granular medium, implies the division of particles into smaller parts, and may involve a change in particle shape and size. Discrete Element Methods (DEM) are appropriate to capture the loss of compression and shear strength with particle crushing. In DEM, a Representative Elementary Volume (REV) typically contains several thousands of particles, within “walls” representing boundary conditions. As a result, DEM-based models designed with realistic grain sizes cannot be used to simulate large-scale particle assemblies involved in faults, railways, embankments, or powder engineering. The objective of this study is to propose an alternative approach to the modeling of grain crushing, more descriptive than a purely

phenomenological model, but less computation-intensive than particulate mechanics. Historically, theoretical studies of particle comminution related the energy stored in a particle to the size of that particle. For instance, Rittinger (1867) assumed that the energy required to reduce particle size should be proportional to the area of new surface created. Kick (1885) and Bond (1952) proposed that the energy required in any comminution process should be proportional to the ratio of the volume of the input particle to the output particle. In the theoretical framework of breakage mechanics presented by Einav (2007), the free energy of the REV is related to the Grain Size Distribution (GSD). The crushing process is tracked by a weight coefficient, defined as the difference between the current GSD and the initial GSD, and normalized by the difference between the ultimate and initial GSD. We hypothesize that a better prediction of the energy dissipated during crushing should rather account for the relative size of two particles in contact, because shielding effects are known to occur when there are large differences of sizes between two particles in contact (Bakhtiary and Arson, 2013). Oda (1982) established a strong framework to determine the fabric tensor of granular materials. The same approach is used herein to find the fundamental microscopic descriptors of a granular assembly during crushing. In the first section of the paper, an alternative microstructure description, based on branch lengths, is explained. The bases of the associated thermodynamic framework are presented in the second section. The density and size distribution of branch lengths are related to the GSD, the number of contacts, and to a macroscopic crushing parameter. In the third section, DEM simulations in elastic compression are used to calibrate the energy split function introduced in the thermodynamic framework to relate the branch length distribution to the free energy of the REV.

MICROSCOPIC DESCRIPTORS

Introduction of Branch Lengths

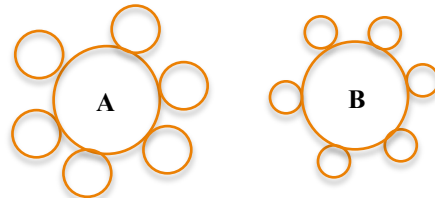


FIG 1. Two particles (A and B) in the granular assembly, with the same size and the same number of contacts, but with different sets of neighboring particles.

Within the assembly, particles with a larger radius have a larger specific surface and can potentially have more contacts with other particles. On the other hand, tiny grains almost float between the other particles and store no energy. Thinking of the mechanical energy stored in the assembly as the summation of thermodynamic potentials defined at the particle level, the number of contacts of a particle shall increase the portion of energy stored by that particle in the assembly. However, the number of contacts per particle is not sufficient to characterize the energy split: two particles can have the same size and the same number of contacts with different sets

of neighbors. In Fig. 1 for instance, particle A is in contact with particles larger than particle B. Although particles A and B have the same size and number of contacts, particle A can potentially be subjected to higher contact forces and therefore receive more mechanical energy during the evolution of the granular assembly. Therefore, instead of only describing a particle by its size and number of contacts, we propose to account for the size of the neighboring particles.

Former micro-macro crushing models described microstructure with particle sizes (e.g. Einav, 2007). In this paper, granular microstructure is described with “branches” instead (Fig. 2). “Branches” are defined as lines linking the centroids of two particles in contact with each other (Satake, 1978; Oda, et al., 1980). We propose to select statistical branch descriptors and to introduce associated moments of probability in the expression of the free energy of the assembly (at the scale of the Representative Elementary Volume, REV). The REV is therefore described as an assembly of branches, assumed to be representative of the geometrical properties and arrangement of the particles (Fig. 2).

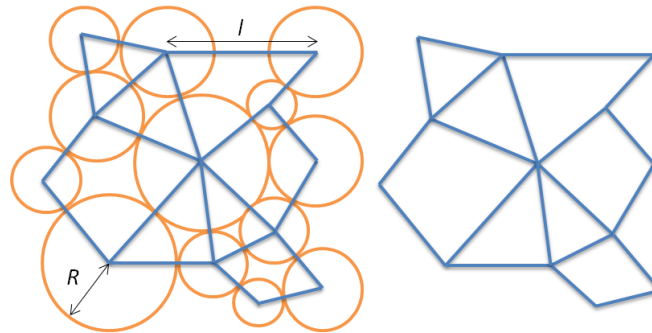


FIG 2. Concept of “branch”: Definition of braches in an assembly of particles (left). Transformed microstructure by using branches instead of particles (right).

For simplicity, each particle is idealized as a sphere with the same volume (more general shapes will be considered in a future study). With this simplifying assumption, the evolution of particle sizes during crushing can be expressed by a probability density function $P(R)$, which is equivalent to the grain size distribution (GSD) obtainable from laboratory sieve experiment. Thus, $P(R)dR$ is the fraction of the number of spheres with a radius ranging from R to $R+dR$. In order to uniquely define the fabric of an assembly of particles with branches, the density of branches and the probability density function of branch dimensions and orientations must be identified. Another simplifying assumption is made herein, by ignoring the effect of anisotropy on the arrangement of particles. Intuitively, anisotropy must be an important factor in the behavior of particulate materials during the crushing process. However, this study is focused on the construction of a thermodynamic framework for particle crushing, based on alternative descriptors of the GSD: at this point, anisotropy is not accounted for; only the density and distribution of branch lengths will be defined.

Branch Length Descriptors

Density. The solid volume V_s occupied by all spheres (particles) can be estimated by:

$$V_s = N \int_{R_m}^{R_M} \frac{4}{3} \pi R^3 p(R) dR = \frac{4}{3} \pi N \langle R^3 \rangle \quad (1)$$

where R_m and R_M are the radius of smallest and largest particles in the assembly, respectively, and N is the total number of particles in the assembly. The total volume of the granular assembly V (solid volume + void volume) equals to $(1+e)V_s$. Using this fact and rearranging Eq. 1, the total number of particles can be expressed as:

$$N = \frac{3V}{4\pi(1+e)\langle R^3 \rangle} \quad (2)$$

where e is the void ratio of the assembly, which can be calculated as $(V - V_s)/V_s$. Now having the total number of particles we can calculate the total number of branches in the assembly. Each contact point in the volume V involves two spherical particles. Therefore, the total number of contact points in V (which is equal to the total number of branches) is equal to $\kappa N/2$, in which κ is the mean number of contact points per particle known as ‘‘Mean Co-ordination Number’’ in the literature. Dividing the total number of contacts by the total volume of the assembly V , the volume density of contacts ρ can be calculated (Oda, 1982), as:

$$\rho = \frac{\kappa N}{2V} = \frac{3\kappa}{8\pi(1+e)\langle R^3 \rangle} \quad (3)$$

Smith et al. (1929), Field (1963), Gray (1968) and Oda (1977) found the relationship between the mean coordination number κ and the corresponding void ratio e ; this relationship is independent of the GSD.

Distribution of Lengths. Noting l the branch length, the branch length probability distribution $B(l)$ can be expressed in terms of the grain size distribution $P(R)$ available from laboratory experiments (Oda, 1980):

$$B(l) = \int_{l-R_M}^{l-R_m} P(R)P(l-R)dR / \int_{2R_m}^{2R_M} \int_{l-R_M}^{l-R_m} P(R)P(l-R)dRdl \quad (4)$$

CONSTRUCTION OF A THERMODYNAMICS FRAMEWORK

As explained above, the mechanical energy stored in the REV by a particle depends on the number of contacts and on the size of the neighbors of that particle. The density of branch lengths and the distribution of branch lengths are two independent mathematical variables that depend on the sizes and numbers of contacts of particles, and that are used herein to track the energy stored in particles. For given initial and ultimate grain size distributions ($P_0(R)$ and $P_u(R)$), the initial and ultimate branch length distributions $B_0(l)$ and $B_u(l)$ can be determined from Eq. 4. The initial and

ultimate n th moments of l , $\langle l^n \rangle_0$ and $\langle l^n \rangle_u$, are defined as:

$$\langle l^n \rangle_0 = \int_{2R_m}^{2R_M} l^n B_0(l) dl \quad (5)$$

$$\langle l^n \rangle_u = \int_{2R_m}^{2R_M} l^n B_u(l) dl \quad (6)$$

The crushing parameter C is introduced to relate the initial $B_0(l)$ and ultimate $B_u(l)$ branch length distributions to the current distribution $B(l)$:

$$C = \frac{B_0(l) - B(l)}{B_0(l) - B_u(l)} \quad (7)$$

During crushing, C varies from zero to one. To write the above equation, we assumed that the evolution of crushing (and the associated reduction of branch lengths) is uniform in the REV, i.e., for a given state of crushing, the crushing parameter C does not depend on the branch length variable l . At the beginning of crushing, C is zero (no crushing) and when the evolution of crushing is complete, C becomes equal to one (end of crushing). The free energy density of a set of branches with the same length l is written in the following form:

$$\hat{\psi}_l = \hat{\psi}_l(l, \varepsilon) = f(l) \psi_r(\varepsilon) \quad (8)$$

where ε is the bulk deformation of the REV, and $f(l)$ is an ‘‘energy split function’’, which controls the distribution of energy between fractions of branches with different lengths l . $\psi_r(\varepsilon)$ is the normalized reference deformation energy defined as:

$$\psi_r(\varepsilon) = \frac{\Psi_0}{\langle f(l) \rangle_0} \quad (9)$$

where:

$$\langle f(l) \rangle_0 = \int_{2R_m}^{2R_M} f(l) B_0(l) dl \quad (10)$$

In which Ψ_0 is the total free energy of the granular assembly (REV) before any crushing happens. This normalization ensures that the actual total stored free energy Ψ can be computed from integrals defined at the REV scale. A reference branch length l_r is defined so as to have $\hat{\psi}_l = \psi_r(\varepsilon^e)$, and therefore $f(l_r)$ equals to one for the reference branch length. In soils, the fractal representation of porous networks is attractive, since it provides a theoretical foundation to the power-law constitutive relationships established empirically for permeability and retention properties (Tyler and Wheatcraft, 1990). Einav (2007) naturally assumed that the ultimate GSD after crushing was fractal. Entropy maximization then imposes that $f(l)$ should be a power function of l :

$$f(l) = \left(\frac{l}{l_r} \right)^n \quad (11)$$

where l_r is a reference length to normalize l . The value of the exponent n has to be

determined based on experimental data. A methodology based on numerical simulation is proposed in the following section. The energy stored in a branch is related to the length of the branch l . The total free energy of the REV is obtained by integration over the full span of branch lengths in the assembly:

$$\Psi = \int_{l_m=2R_m}^{l_M=2R_M} \hat{\psi}_l B(l) dl = \int_{2R_m}^{2R_M} \psi_r(\varepsilon^e) f(l) B(l) dl \quad (12)$$

$$\Psi = \psi_r(\varepsilon) \int_{2R_m}^{2R_M} f(l) B(l) dl = \psi_r(\varepsilon) \int_{2R_m}^{2R_M} \left(\frac{l}{l_r}\right)^n B(l) dl = \frac{\psi_r(\varepsilon)}{l_r^n} \int_{2R_m}^{2R_M} l^n B(l) dl \quad (13)$$

$$\Psi = \frac{\psi_r(\varepsilon)}{l_r^n} \langle l^n \rangle \quad (14)$$

Using Eq. (7), $\langle l^n \rangle$ can be written as:

$$\langle l^n \rangle = (1-C) \langle l^n \rangle_0 + C \langle l^n \rangle_u \quad (15)$$

By applying Eq. (15) into Eq. (14), it can be rewritten as:

$$\Psi = \frac{\psi_r(\varepsilon)}{l_r^n} (1-C) \langle l^n \rangle_0 + C \langle l^n \rangle_u \quad (16)$$

The above equation relates the current Helmholtz free energy to the initial and ultimate branch length distributions, which are functions of initial and ultimate GSDs available from laboratory sieve analysis. By taking the derivative of Eq. (16) with respect to strain ε , the increment of the average of the free energy can be written as:

$$\delta \Psi \equiv \frac{d\psi_r(\varepsilon)}{d\varepsilon} \frac{1}{l_r^n} \left[(1-C) \langle l^n \rangle_0 + C \langle l^n \rangle_u \right] \delta \varepsilon + \psi_r(\varepsilon) \left(\langle l^n \rangle_u - \langle l^n \rangle_0 \right) \delta C \quad (17)$$

The general expression of the dissipation inequality is:

$$\tilde{W} = \delta \Psi + \tilde{\Phi}, \quad \tilde{\Phi} \geq 0 \quad (18)$$

where Ψ and $\delta \Psi$ are the Helmholtz free energy and its increment, respectively; $\tilde{\Phi}$ is the non-negative increment of energy dissipation; \tilde{W} is the increment of mechanical work done on the boundaries of the system. The work input is equal to the strain energy (Principle of Virtual Work):

$$\tilde{W} = \sigma : \delta \varepsilon \quad (19)$$

where σ and ε are the stress and strain tensors defined at the REV scale (and $\delta \varepsilon$ is an imposed increment of strain). Using Euler's theorem, the non-negative increment of energy dissipation $\tilde{\Phi}_C$ can be written as a function of the crushing parameter C :

$$\tilde{\Phi} \equiv \tilde{\Phi}_C(C, \delta C) = E_c \delta C \geq 0 \quad (20)$$

where:

$$E_c = \frac{\partial \tilde{\Phi}_C(C, \delta C)}{\partial (\delta C)} \quad (21)$$

This choice (homogeneous function of degree one for dissipation) is to ensure the convexity of the elastic domain (Collins and Houlsby, 1997). Considering Eq. (20) and for the breakage to grow ($\delta C \geq 0$), it is essential to have:

$$E_c \geq 0 \quad (22)$$

Now using Eqs. (17), (18), (19), and (20) we can write:

$$\left(\sigma - \frac{d\psi_r(\varepsilon)}{d\varepsilon} \left[(1-C)\langle l^n \rangle_0 + C\langle l^n \rangle_u \right] \right) \delta\varepsilon + \left(\psi_r(\varepsilon) (\langle l^n \rangle_0 - \langle l^n \rangle_u) - E_c \right) \delta C = 0 \quad (23)$$

SIMULATIONS AND RESULTS

In this section, we want to check our hypothesis that the energy stored in each branch is related to the length of the branch and increases with the branch length. As mentioned earlier, the exponent in the expression of the energy split function (Eq. 11) has yet to be determined. In this paper, numerical experiments are conducted with the Discrete Element Method (DEM) to calculate the energy stored in each branch of an assembly subjected to a given stress gradient. The exponent n is then obtained by curve-fitting, for an assembly of spherical particles with a large span of particle sizes represented (in order to model crushing and comminution). A three dimensional granular assembly consisting of 1,000 particles (with the maximum particle size two hundred times larger than the minimum particle size) has been generated with *PFC3D* software. The grain size distribution is plotted in Fig. 3: the soil sample considered is relatively well-graded. Shear forces at contacts are ignored and only normal forces are considered in the simulation. As it is shown in Fig. 4a, particles with different sizes are located randomly in a cubic space surrounded by walls. Then the sample size is reduced by 40% through a slow dynamic strain controlled compressive loading. The resulted compacted assembly with linear elastic deformation is shown in Fig. 4b.

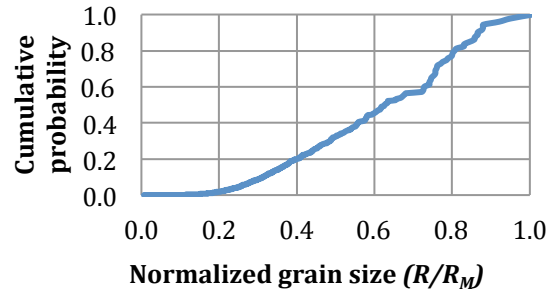


FIG 3. Grain size distribution of the particle assembly simulated with PFC3D.

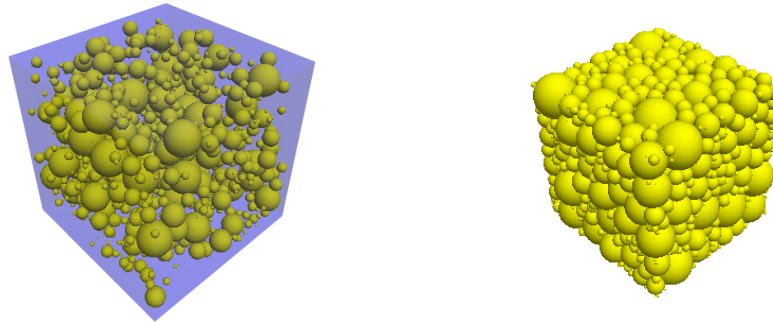


FIG 4. Granular Assembly simulated with PFC3D. Representation of the initial placement of particles in the numerical model (left). Compressed and compacted sample after loading (right).

As discussed in the previous section, particles could be replaced with branches and the total energy of the microstructure is distributed between the branches. First, we need to compute the elastic energy stored in each branch. *PFC3D* provides the force in each contact between two grains, and contacts are identified by the two particles involved, each of which being tractable by a label identification number (ID). Using the grains' ID, it is possible to relate the particles' radii to the contact forces. By adding the radii of two particles in a contact, it is possible to find the branch length for each contact. Therefore, we can have the force and branch length for each contact. Then the energy stored in a subset b including branches with the same length l can be obtained as:

$$\psi_b(l) = \sum_{i=1}^{N_b} \frac{|F_i^n|^2}{k^n} \quad (24)$$

where F^n is the normal force in a contact, k^n is the normal stiffness and N_b is the total number of branches with length l . In our numerical model, we included many different particle sizes and therefore many different branch lengths have been obtained. We know that the maximum branch length in a particle assembly is equal to $2R_M$ and the minimum branch length is equal to $2R_m$. To be able to compute Eq. 20, we divide the range of branch lengths into 20 different subsets with increments of $(2R_M - 2R_m)/20$ and for each subset with average branch length l , the average stored energy $\hat{\psi}(l, \varepsilon)$ is estimated over the REV, as:

$$\hat{\psi}_l(l, \varepsilon) = \psi_b(l) / N_b \quad (25)$$

Therefore, using Eq. 8, the energy split function $f(l)$ can be obtained for the numerical experiment as:

$$f(l) = \frac{\hat{\psi}_l(l, \varepsilon)}{\psi_r(\varepsilon)} = \frac{N_r \psi_b(l)}{N_b \psi_b(l_r)} \quad (26)$$

where l_r is the reference branch length, N_r is the number of branches in the reference subset with average branch length l_r , and $\psi_b(l_r)$ is the energy stored in the reference subset.

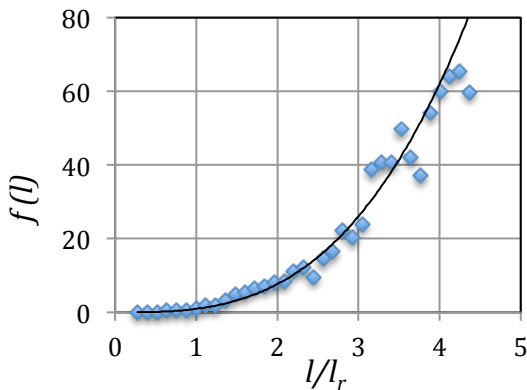


FIG 5. Representation of the relationship between branch length and the energy split function for that branch length.

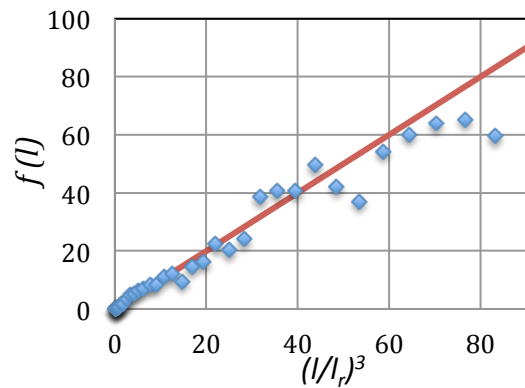


FIG 6. Curve-fitting: energy split function for a specific branch length against the third power of the normalized branch length.

$f(l)$ is calculated by introducing the numerical output into Eq. 26. In Fig. 5, $f(l)$ calculated from the numerical model is plotted versus the values of l/l_r . As it can be seen in the figure, longer branches store more energy than shorter branches and this relation seems to be exponential as assumed in Eq. 11. More numerical experiments are needed to find an appropriate general value for n in Eq. 11. However, for this specific experiment we suggest using n equal to 3 and the results for this assumption are shown in Fig. 6. Another interesting output from the numerical model is the probability distribution $B(l)$ of branch lengths l , presented in Fig. 7. As it is shown in this figure, it is more probable to have branches with the length equal to the maximum grain radius R_M (i.e., half of the maximum branch length) and the probability distribution seems to be a normal distribution. It means that it is more probable to have branches equal to an average length, and that the probability of having very long or very short branches is lower. This probability distribution changes by changing the grain size distribution $P(R)$, as explained in Eq. 4.

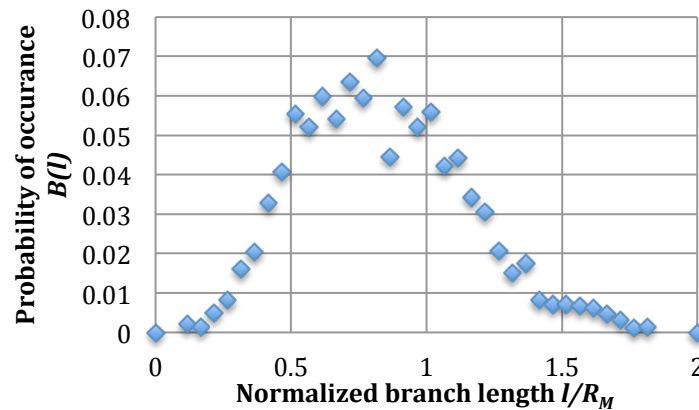


FIG 7. Probability distribution of branch length $B(l)$ for the numerical model.

CONCLUSIONS

A micro-macro model of the thermodynamic process of particle crushing is proposed in this paper. Microstructure changes are tracked with the density and size distribution of branch lengths (i.e., lengths relating the centroids of two particles in contact). At the scale of a Representative Elementary Volume (REV), the free energy density of a set of branches of same length is assumed to be a fraction of the total free energy of the REV, and is written as the product of the total deformation energy stored in the REV by an energy split function, assumed to follow a power law. The distribution of deformation energy stored by the branches of a granular assembly subjected to isotropic compression is calculated with *PFC3D* Discrete Element Method (DEM) program. It is shown that this distribution varies indeed with branch lengths, and that the power-law provides a good fit for an exponent of three. A macroscopic crushing parameter is defined to follow the progress of particle comminution (and therefore, dissipation). Constraints on the expression of the dissipation potential associated to particle crushing are explained, in order to ensure the convexity of the elastic domain. Further work will be devoted to the specific expression of the dissipation potential and yield functions necessary to model particle

crushing. The energy stored by a particle of given size and contact number varies with the size distribution of its neighbors. In particular, if the particle is in average more than one order of magnitude larger than its neighbors, the stored deformation energy at the contacts tends to vanish, and the particle tends to be protected against crushing. This phenomenon, known as “shielding effect”, is impossible to capture with previous micro-macro models of particle crushing, which represented the granular fabric by Grain Size Distributions (GSDs). Therefore, the proposed framework is expected to improve current thermodynamic models of particle crushing. In particular, better energy estimates could be used to optimize processes to make powders in the pharmaceutical and food industry.

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