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ENERGETIC APPROACH FOR THE CHARACTERIZATION OF TAPS IN GRANULAR COMPACTION

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ABSTRACT

We report numerical investigations for the compaction dynamics of dense granular assemblies. The studies are based on the non-smooth contact dynamics model. Our work suggests that the dimensionless acceleration parameter Γ, used by a large majority of authors, is not appropriate for rescaling the data. We prove that the dimensionless energy Ξ, injected in the granular system at lift-off, is more appropriate and leads to robust interpretations of the compaction dynamics. Indeed, the injected energy allows to pass energy barriers that separate local equilibrium states. Using the Eyring picture of relaxation dynamics, we show that the consideration of Ξ leads to a new law for compaction.

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Introduction

When a pile of grains is submitted to a series of identical taps, the packing fraction of the pile η, defined as the ratio of the volume occupied by all grains divided by the volume of the assembly, slowly increases [1]. This phenomenon is called granular compaction. Despite numerous studies devoted to granular compaction dynamics and associated quasi-static properties of granular packing [2,3], the physical understanding of those phenomena is a serious challenge for physicists. Indeed, the complexity comes from the fact that the system visits a large number of states despite the slow macroscopic dynamics. Moreover, it is known that the compaction dynamics may be influenced by many parameters. The boundary conditions, the way of shaking (taps or sinusoidal excitation) and the aspect ratio of the container are probably the most crucial parameter. Recent works show that the memory effect can be observed [4-6] and also the sudden motion of some grains, so-called rare events [7]. The compaction process may be considered as a trajectory of the system from one minimum to another one of the potential energy which is characterized by a large number of local equilibrium states. From that basic observation, we propose, that, the energy injected by one tap or sinusoidal cycle is the key parameter for describing the compaction dynamics.

In most compaction experiments [8-10] and numerical studies [11-13], the granular assembly is kept in a container which is submitted to a series of identical taps. Each tap is defined by a sinusoidal motion of the container: $z = A[1 + \sin(\omega t - \pi/2)]$ with $0 < t < T = 2\pi/\omega$. The amplitude A and the frequency f (or an angular frequency $\omega = 2\pi f$) characterize the motion of the system boundaries. A typical trajectory of the container is illustrated in figure 1. Two successive taps are separated by a time delay in order to allow the total relaxation of the granular assembly. When the delay is too short, one expects to observe a fluidized granular bed. It may be assumed that the dimensionless maximum acceleration experienced by the container $\Gamma = \frac{A\omega^2}{g}$ should be larger than 1 in order to allow the granular assembly to take off from the container. Nevertheless, recent experiments have shown that granular compaction could be also observed when $\Gamma < 1$ [2] since internal rearrangements of the grains are able to slightly increase η. The flight condition ($\Gamma > 1$) defines, however, a lift-off time

$$\tau = \frac{\arcsin(1/\Gamma)+\pi/2}{\omega}, \tag{1}$$

after which the assembly starts to dissipate energy. In a recent work [14], it has been shown that a free fall is not observed for a large value of the tap number n. Indeed, friction plays an important role when the packing densifies such that the granular packing follows an exponential decay motion, instead of a parabolic flight (see also figure 1). The exponential decay reveals the dissipation kinetics to be associated to many frictional contacts and many inelastic collisions. Therefore, the time τ separates energy injection and dissipation.

In long compaction experiments, the packing fraction η of the granular system is monitored. Even if the question is still debated [8], the dynamics of compaction can be considered as well described by an inverse logarithmic law:

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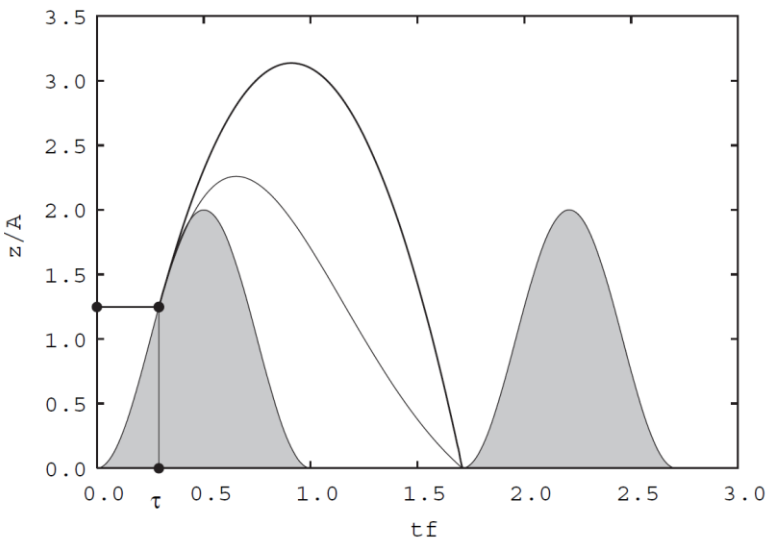
$$\eta = \eta_0 + \frac{\eta_\infty - \eta_0}{1+\log(n/\Upsilon)}, \tag{2}$$

where Υ is a characteristic tap number which is directly linked [15] to the flow properties of a dense granular system. The characteristic tap number, Υ, is considered to depend unambigously on the reduced acceleration Γ [16]. However, recent reports [6] have underlined that multiple situations could be reached from a unique value of Γ. Actually, hysteretic behaviors are observed in some cases when varying Γ [4]. Most of the time, the packing is lift-off when the container reaches the maximum acceleration which defines the reduced acceleration Γ. These considerations underline that Γ is commonly used but is not an appropriate parameter for studying the compaction of granular materials.

The aim of this work is to develop the energetical point of view for describing the compaction phenomenon. More precisely, our main motivation is to characterize the compaction of a vibrated granular packing with respect to experimental parameters such as A and f. The tapping process will be described as a function of the energy that the tap injects in the system. The dissipation processes and the ability of the system to densify depend on the history and on the geometrical constraint of the packing. Our work is based on a 3D numerical model which has been developed on Non-Smooth Contact Dynamics (NSCD) [17]. This numerical approach has been chosen because the NSCD built a realistic force network instead of a group of independent local forces. The details of the model are presented in [13].

***Figure 1**. Two successive taps in grey. The position of the container z/A is shown as a function of dimensionless time tf where A and f are, respectively, the amplitude and the frequency of the sinusoidal motion. The position of the grains in the container is also shown (continuous curves) in order to illustrate the lift-off time τ. Two cases are shown: parabolic flight (free fall) and the typical motion when friction and elasticity dominate.*



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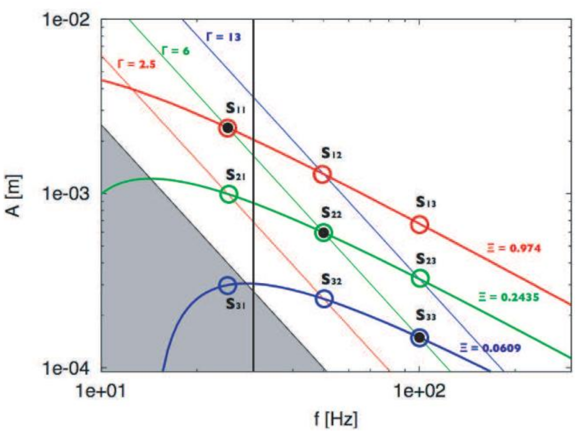
Reduced energy

Each value of compacity η corresponds to a stable state among the multiple minima of the potential energy. During the compaction process, the pile jumps from a minimum to another one. In order to reach the next minimum, some energy must be injected in the system. Moreover, a set of minima are accessible at each tap and some of them have a lower or higher energy than the initial state. The value of the injected energy influences the movement of the system in the space of states. From this point of view, an original dimensionless parameter is proposed for describing the dependency of the compaction dynamics with the intensity of taps. This parameter is based on the mechanical energy injected in the granular system when the assembly lifts off (at time $t = \tau$) normalized by some characteristic energy mgd of the grain. Since the mechanical energy is given by the sum of the kinetic energy $mv^2/2$ and potential energy mgz, the new parameter Ξ is defined as

$$\Xi = \frac{1}{2d}\left(\frac{A^2\omega^2}{g} + \frac{g}{\omega^2} + 2A\right) \tag{3}$$

using eq. (1). The procedure to test whether the Ξ-parameter is able to scale the compaction dynamics is given in the following. The compaction curves are compared when Γ is constant and when Ξ is constant, for three different values of the frequency ($f = 25$, 50 and 100 Hz). Nine sets of parameters have been considered. Figure 2 allows to locate the compaction studies presented in this paper on the diagram amplitude/frequency (A, f). Both iso-Γ (lines) and iso-Ξ (thick curves) are represented. The sets of parameters are located by circles (full for conservation of Γ and empty for Ξ) and two numbers, the second number is for the frequency (1, 2 and 3 mean 25, 50 and 100 Hz). Note that s_{11}, s_{22} and s_{33} have the same reduced acceleration Γ equal to 6. Sets (s_{21}, s_{32}) and (s_{12}, s_{23}) are thus characterized by $\Gamma = 2.5$ and 13 respectively. On the other hand, (s_{11}, s_{12}, s_{13}), (s_{21}, s_{22}, s_{23}) and (s_{31}, s_{32}, s_{33}) are sets for which Ξ is constant and equal to 0.974, 0.2435 and 0.0609, respectively. The compaction curves are simulated for all these sets and compared in order to evidence scaling.

***Figure 2**. The log-log plot of the amplitude-frequency diagram emphasizing the no-flight region $\Gamma < 1$ (grey area) and the situations numerically investigated in this paper. Curves and lines indicate constant Ξ and Γ values, respectively. The vertical black line represent the zone of the diagram which is studied by experimental groups from Chicago [1] and Rennes [9].*



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Numerical simulations

Our numerical simulations consider $N = 512$ identical spheres of diameter $d = 5 \cdot 10^{-3}$ in a rectangular container (base width $D = 5d$) with vertical borders. The static friction μ between the beads and the resitution coefficient ε are fixed to 0.6 and 0.9, respectively. The compacity η is evaluated via the measurement of the packing's height. Different values of these parameters do not affect the results presented in this paper. The slight effect of those physical parameters on compaction can be found in [13,17]. The initial packing has been built on a 3D lattice for which all grains have a velocity randomly oriented with a constant magnitude. The initial pile corresponds to a compactity of $\eta = 0.53$, as illustrated in figure 3. Afterwards, the pile is submitted to a serie of taps. Each tap is described in figure 1 as a sinusoidal motion of the container. The time between two succesive taps is called relaxation, which ends when no grain moves anymore.

In figure 4, the compacity η is plotted as a function of the number of n taps for three different frequencies: $f = 25$, 50, 100 Hz. All compaction dynamics presented in figure 4 are fitted using eq. (2): the obtained Υ could be found in table 1. The amplitude A has been selected in order to obtain a similar dimensionless reduced acceleration Γ equal to 6 (figure 4a) and for three different values of the reduced energy (figs. 4b, c and d). Compaction curves exhibit quite different behaviours when the maximal acceleration Γ is constant. Fitted values of the dynamical parameter Υ are summarized in table 1. They are significantly different. The reduced acceleration Γ cannot describe the link between compaction dynamics and the tap intensity. In particular, the low-frequency curve exhibits huge fluctuations and seems to reach a saturation value of compacity around 0.58, while the high-frequency curve is still growing after $n = 1000$ taps.

Figure 4 (b, c and d) presents the compaction dynamics for a constant value of the reduced energy Ξ corresponding to the three simulations realized at a constant value of reduced acceleration Γ: $\Xi(\Gamma = 6,\ f = 25\ \mathrm{Hz}) = 0.974$, $\Xi\,(\Gamma = 6,\ f = 50\ \mathrm{Hz}) = 0.2485$ and $\Xi\,(\Gamma = 6,\ f = 100\ \mathrm{Hz}) = 0.0609$. For each value of Ξ, the compaction behaviours collapse on a single curve except for the compaction computed at $\Xi = 0.0609$ and $f = 25$ Hz for which $\Gamma = 0\,.75 < 1$. This set of parameters is out of the studied domain and will not be discussed below. The fits give closer values of Υ for a constant value of Ξ than for a constant value of Γ (table 1). Fluctuations have also been studied. The deviation $\delta\eta$ around the logarithmic law, for $n > \Upsilon$ is taken into account:

$$\delta\eta(n) = \eta(n) - \left(\eta_0 + \frac{\eta_\infty - \eta_0}{1 + \log(n/\Upsilon)}\right). \qquad (4)$$

A large $\delta\eta$ value means that the system explores a wide set of configurations from loose to dense packing. In so doing, $\delta\eta$ is related to the number of accessible states in the potential energy. In figure 5, the distribution of fluctuations is plotted relatively to the curves of figure 4. All the distributions are Gaussian-like centered on zero. If one considers a constant acceleration Γ, the dispersion decreases when the frequency increases which corresponds to an increasing value of the reduced energy Ξ. On the other hand, when Ξ is kept constant, a single normalized distribution is recovered for the three values of frequencies. This is confirmed on the measurements of the standard deviation σ of $\delta\eta$'s listed in table 1.

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Both the aspect ratio and the friction coefficient influence the presence of convection during the compaction process. In this work, the convection plays an important role which is revealed by the geometrical structure of the packing [17]. The grains are organized in vertical layers from border to center of the container. Figure 6 illustrates the evolution of the compactivity wall to wall. At the beginning, the nucleation of layers close to the walls is observed. During the compaction process, additional layers appear from the wall towards the center of the pile. At the end, the pile is fully layered. This type of structure is however far from a perfect crystal. When the frequency increases (dashed curves in figure 6) and the reduced acceleration is conserved, the total energy injected in the pile decreases and the propagation of the layers is lower than in the initial simulation (solid curves in figure 6).

Figure 3. *Illustration of the simulated pile in the initial state (left) and in the final state (right), i.e. after $n = 1000$ taps.*

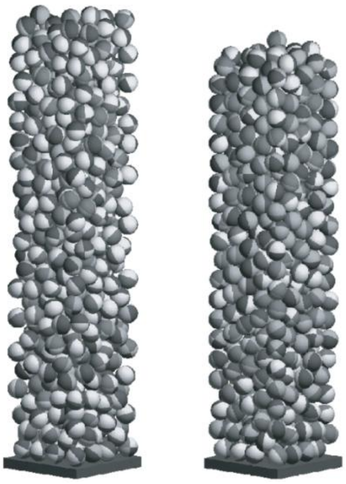

Figure 4. *Evolution of the packing fraction η as a function of the number of n taps. The curves correspond to different frequencies (25, 50 and 100 Hz, see the legend in graphic (b)) at the same reduced acceleration Γ (a) and for a constant value of the reduced energy Ξ (b), (c), (d) as indicated in the figure.*

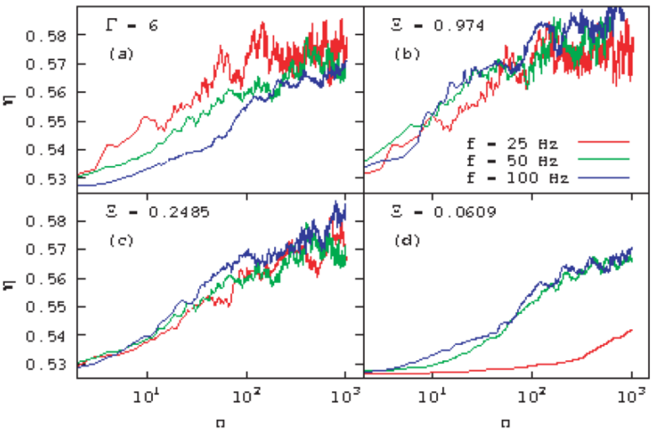

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Table 1*. Tap characteristics and the fitted* Υ*-parameter from the inverse logarithmic law (eq. (2)). The fourth column presents the values of the standard deviation of the normal distribution by an adjustment on the data presented in the first column. The two last columns denote the figures in which these results are illustrated.*

Tap	f [Hz]	Υ	$\sigma(10^{-5})$	Fig. 2	Figs. 4, 5
$\Gamma=6$	25	9.38	462	s_{11}	(a)
$\Gamma=6$	50	36.77	398	s_{22}	(a)
$\Gamma=6$	100	67.16	187	s_{33}	(a)
$\Xi=0.9741$	25	9.38	462	s_{11}	(b)
$\Xi=0.9741$	50	12.39	442	s_{12}	(b)
$\Xi=0.9741$	100	15.99	385	s_{13}	(b)
$\Xi=0.2485$	25	44.82	424	s_{21}	(c)
$\Xi=0.2485$	50	36.77	398	s_{22}	(c)
$\Xi=0.2485$	100	40.91	380	s_{23}	(c)
$\Xi=0.0609$	50	84.72	182	s_{32}	(d)
$\Xi=0.0609$	100	67.16	187	s_{33}	(d)

Figure 5*. Histogram of the compacity fluctuations* $\delta\eta$ *for the compaction curves presented in figure 2: 11, 22, 33 in (a); 11, 12, 13 in (b); 21, 22, 23 in (c) and 31, 32, 33 in (d). The fluctuations* $\delta\eta$ *of the packing fraction seems to be normalized when* Ξ *is a constant.*

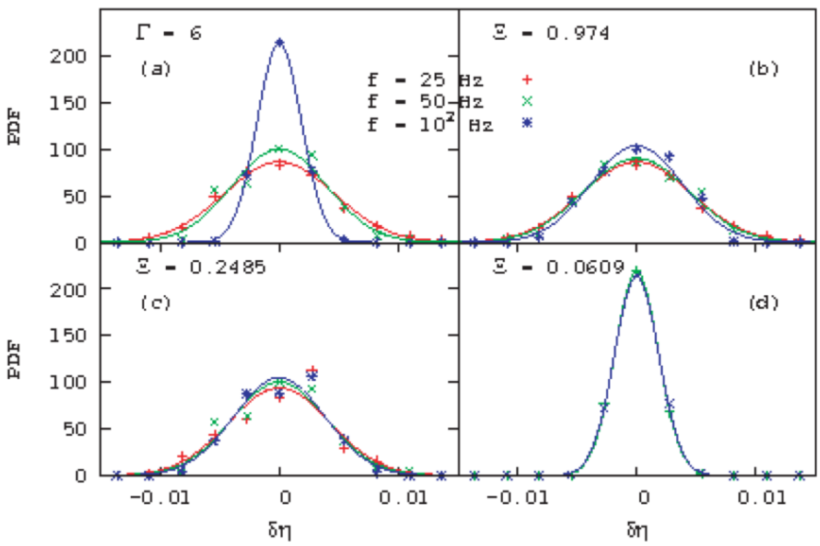

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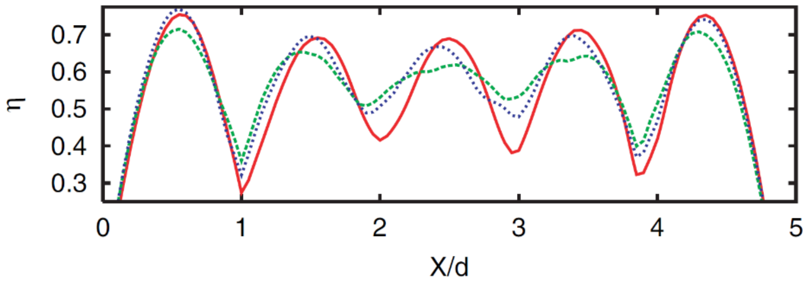
Figure 6. *Evolution of the 2D compactivity as function of the position along the X-axis normalized by the diameter of the grain. The curves correspond to studies at n = 1000 taps which have been realized at a constant value of Γ = 6 and for f = 25 Hz (solid curve, 11 in figure 2), f = 100 Hz (dashed curve, 33 in figure 2) and for a constant value of Ξ = 0.974 for the same value of frequency f = 100 Hz (dotted curve, 13 in figure 2).*



Discussion

From our different observations, it is clear that Ξ is a more relevant parameter than Γ for describing the strong link between the compaction phenomenon and the tap characteristics. The behaviour of the fluctuations indicates unambiguously that the injected energy during one cycle is driving the compaction dynamics. The higher the injected energy is, the more important the structural modifications are, in agreement with the fluctuations of compacity which reveal the amplitude of those structural changes. This energy allows to jump over a potential barrier to move the system from one equilibrium state to another one.

By considering Ξ instead of Γ as a relevant parameter for compaction, one gets the opportunity to bring some concepts of statistical physics into simple models. Various experiments and models underline that dense packings are described by the coexistence of local states exhibiting various structures [18]. For simplicity, we may consider only two antagonist local configurations: loose and close packing. We may assume that a fraction x of particles are in close-packed configurations while the remaining $1 - x$ particles are still in loose configurations.

The mechanical energy injected into the system is given by the dimensionless parameter Ξ. A part of this energy is dissipated by friction (for dense packing configurations) while the remaining induces the motion and collision of grains (for loose packing configurations). In so doing, only $(1 - x)\Xi$ participates to the compaction phenomenon. Similarly to the Eyring picture of relaxation into disordered structures, one may also assume that some dimensionless energy barrier B should be overcome in order to get a dense configuration from a loose one. Only a fraction x of grains are concerned by this process. The kinetic equation of compaction reads

$$\frac{\mathrm{d}x}{\mathrm{d}t} = \alpha(\Xi)(1 - x)\exp\left(-\frac{x}{1-x}\frac{B}{\Xi}\right), \tag{5}$$

where the exponential is an Arhenius-like factor taking into account the dimensionless energies for both barrier and grain agitation. The variable x represent the normalized compactivity: $x = \frac{\eta-\eta_0}{\eta_\infty-\eta_0}$.

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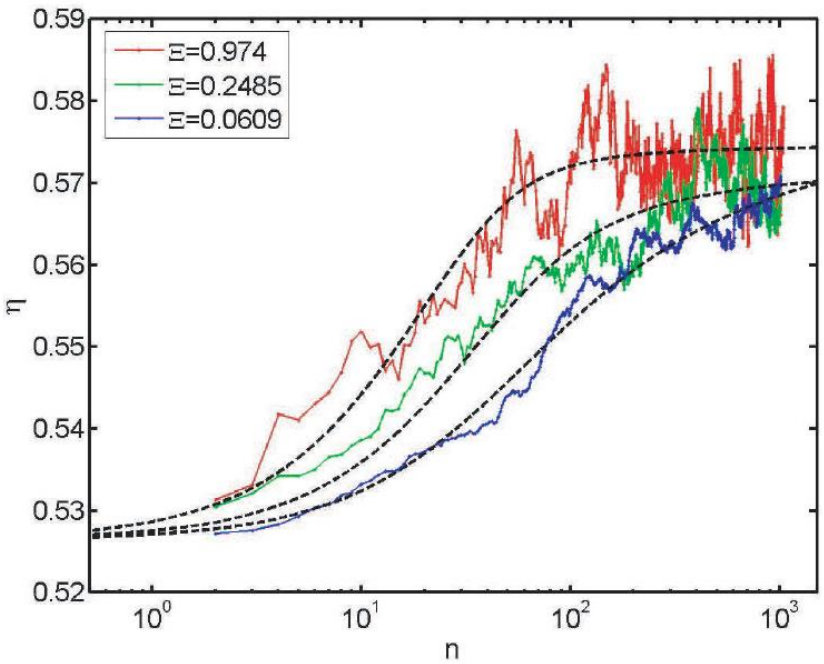
The factor $\alpha(\Xi)$ represents the dissipation of energy, in other words the energy that is not used for the reorganization of the heap. The observation of the data has shown that the factor α is well described by the phenomenological law $\alpha(\Xi) = \beta\sqrt{\Xi}$, β being a constant. The result of the eq. (5) is

$$t = \frac{e^{\frac{B}{\Xi}}}{\beta\sqrt{\Xi}}\left[E_i\left(\frac{B}{\Xi(1-x)}\right) - E_i\left(\frac{B}{\Xi}\right)\right], \tag{6}$$

where the integral exponential is defined by $E_i(x) = \int_{-\infty}^{x} \frac{e^y}{y} \mathrm{d}y$. Figure 7 presents the fits of the numerical data by the model in eq. (6). The B and β have been found to be equal to 0.0997 and 0.0473, respectively. These parameters are fixed the same for the three frequencies. The asymptotical values of the compaction η_∞ have been found to be 0.5752, 0.5737, and 0.5878 for $f =$ 25, 50 and 100 Hz, respectively.

***Figure 7**. Evolution of the compactivity predicted by the model for various reduced energies Ξ: 0.974, 0.2485 and 0.0609.*



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Conclusion

In summary, we underlined the wrong characterization of tapping during compaction dynamics by the reduced acceleration Γ. We propose a new dimensionless parameter Ξ for investigating the physical properties of dense granular systems. We prove that this parameter captures the entire dynamics of compaction. Indeed, the compaction dynamics is the same when the energy parameter Ξ is constant. The energy injected in the system allows to jump energy barriers that separate local energy states. The control of compactivity fluctuation has been shown. Finally, the apparition of structural layers reveal a better characterization of compaction taps by the new parameter Ξ. It allows experimentalists to compare their experiments even when setups are different. An original law for the compaction has been proposed. All the three compaction dynamics have been reproduced by the model as a function of the reduced energy Ξ.

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