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A SIMULATION STUDY OF MIXING GRANULAR MATERIALS

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Abstract

Mixing the granular materials is a critical process in many industries, especially in pharmaceutical one, where homogeneous blends of ingredients are required. The homogenisation process is time and energy consuming, thus this article is focused on the process. The mixing process has been simulated with the discrete element method – DEM, which gives an opportunity to study the granular flow of mixed ingredients. Following stages of the mixing process have been presented for various shapes of blenders and analysed, which gives an opportunity to understand the process and mechanisms of homogenisation. Apart from the three basic mechanisms of homogenisation: diffusion, convection and shear, one more has been found.

Key words*: discrete element methods, blender, mixing*

1. Introduction

Blenders are applied in: pharmaceutical [4, 15, 27], cosmetic, food [32] and detergent industries, to name a few. The mixing process influences both quality of products and their cost, thus there is a need to describe the process. The mixing process is a result of diffusion, convection and shear, which are the main mechanisms of the homogenisation described in the literature [1, 4, 27]. The mechanisms can be observed during simulation of the granular flow with DEM. The mixing process has been described in two books [1, 27], which are basic ones for this subject. Apart from the theoretical analysis, and experimental results the authors presented there some practical advice. Nevertheless recommended parameters of the mixing process, and results of simulation obtained with DEM have not been presented [1, 27].

The discrete element method (DEM) is a numerical method dedicated for computing motion of a large number of particles. The discrete element method is closely related to molecular dynamics (MD), particle method (PM), multibody systems (MBS) and smooth particle method (SPM). The fundamental assumption in the discrete element method is that material consists of large assembles of separate particles. The number of the discrete particles can be a few millions [29] and even billions [2, 18, 24]. The basic idea of modelling bodies, as large assemblages of separate-discrete elements, makes the method very universal; because each body can be modelled as an assemblage of separate atoms, or groups of atoms. Materials like gases, liquids, solids (powder, sand or rock) can be simulated with the method. The particles may have different shapes and properties. Complex non-linear interactions between bodies, and within bodies, are simulated with a numerical method. Next, the motion of particles, which is described by differential non-linear equations, is computed. Finally, the motion of a large number of particles, like molecules or grains of sand, is presented as a movie and analysed [8, 11, 17, 19, 28, 29]. The discrete element methods are applied to solve a wide range of engineering and scientific problems in: mineral processing, rock blasting, crushing, powder technology, laser processing, granular flow of stones, blow up of building and many more areas [23].

Particles in DEM can be modelled with: points, polygons, circles, ellipses, polyhedral [19] or with spheres [10]. A discrete element can represent: a stone, a grain of sand, a seed, a grain of powder, or a molecule. In the case of modelling solid bodies the elements can represent rigid of deformable bodies (primitives). If bodies are modelled with FEM primitives, then both elasto-plastic distortion of bodies and their fragmentation (cracking) can be simulated. The phenomena can be simulated with so cold combined finite-discrete element method [23]. More details about DEM have been published in literature [5, 6, 22, 23, 25, 33].

The considered problem of mixing granular materials is studied with rigid discrete elements. Three forces act on particles: terrestrial gravity force Q, normal contact force F_n and friction force F_t (Fig. 1). The normal force is usually described by simple models, which reflects restitution phenomena [16, 20, 23], while the friction force is described with Coulomb's model. Motion of each element is described by three differential equations:

$$\ddot{x} = m^{-1} \sum F_x \,, \tag{1}$$

$$\ddot{y} = m^{-1} \sum F_y \,, \tag{2}$$

$$\ddot{\alpha} = I^{-1} \sum M \,, \tag{3}$$

where:

x denotes x-component of displacement,
y y-component of displacement,
F_x x-component of acting force,
F_y y-component of acting force, m mass of element,
α angular displacement of element,
I moment of inertia,
M moment of acting force.

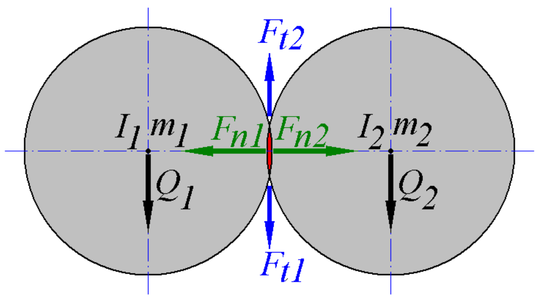

Fig. 1. Forces acting on two discrete elements during their collision

The discrete element method (DEM) gives an opportunity to model mixing the granular materials [21, 23] and consider various: shapes of blenders, values of speeds and fill levels, which are the key factors. An analysis of the factors can be done at a very early stage, at the stage of conception and designing. This gives an opportunity to improve construction of blenders, and to make them more efficient. Moreover, DEM makes an easier understanding of the mixing process.

Thus this article presents results of simulation obtained with DEM and their interpretation. The simulations have been done with Algodoo [12].

2. Simulation of the mixing process

One of the most common technique of mixing the granular ingredients is to rotate a container with the ingredients [15]. This type of blenders are: double cone, IBC and drum blender, which are widely used in the pharmaceutical industry [1, 9, 15, 27]. The ingredients are well mixed after making - from 200 to 700 rotations [1], or after fifteen minutes [27]. The mixing process takes place in the space near the surface, where following layers of particles slide down. Deep under the surface the mixing process does not exist [21]. The layers near the surface move quicker, than the ones deeper under the surface, which in turn introduce the shear. The diffusion process is coupled with collisions between particles, chaotic behaviour [7, 26], and the butterfly effect. The butterfly effect is a part of chaotic dynamics, which are result of non-linear interactions. The collisions are particularly intensive in the space, where the sliding particles reach a wall of a container (Fig. 4b). The convection is coupled with shear, and is observed when particles of one ingredient are displaced by particles of a second ingredient (Fig. 2e). Summarising the mixing process, we can say that, the grains of ingredients are periodically brought into the mixing zone, near the surface, where chaotic dynamics appear, and next after sliding down, they are covered by the following layers of particles. That makes the blend more homogenous.

This section presents results of the simulation. The computations have been done for three blenders: double cone, IBC and drum blender, the two dimensional models of which are presented in the Figs. 2-3. The simulation has been computed for 2400 particles, and the following values of parameters: radius of particles r=0,01m, the restitution coefficient C_R=0,05 and coefficient of Coulomb friction μ=0,5. The polygons (Figs. 2-4) are inscribed in a circle, the centre of which defines the centre of rotation. The circle determines the radius R=1m, which has been adopted to calculate the dimensionless Froude number. The Frode number is relationship between centrifugal and gravitational acceleration, it can be treated as a dimensionless rotating frequency [30]. It is dimensionless number of mixing, which reflects flow condition. The Frode number is expressed by the following formula [1]:

$$Fr=\omega^2 R g^{-1}, \tag{4}$$

where:

Fr - denotes the Frode number,
ω - angular speed [rad/s],
R – radius of the circle [m], and
g - acceleration of gravity [m/s^2].

The Frode number equals one, when the angular speed ω reaches the critical value ω_{kr}. The presented calculations (Figs. 2-4) have been done for Fr = 0,3025 and fill level close to 50%, which are typical for industrial blenders (e.g. [9, 13,14]).

The obtained results show that the border between red and blue ingredients becomes longer and more sophisticated (Figs. 2b, 3b, 4b) after one rotation. Next rotations make the border more and more sophisticated. The process, which can be observed, is baker's transformation. The ingredient is stretched and folded, which leads to a spiral shape -"vortex" (Figs. 2ef, 3f, 4d). The spiral structures have been observed previously in cylindrical blenders [3, 26, 31]. The spiral structures, which are a result of baker's transformation, are finally destroyed by diffusion, which is a result of chaotic dynamics. The two processes - baker's transformation and diffusion lead to a mixed state

(Figs. 2a-o, 3a-o, 4a-o). The spiral structures are sensitive to the speed of blenders, that is an interesting problem.

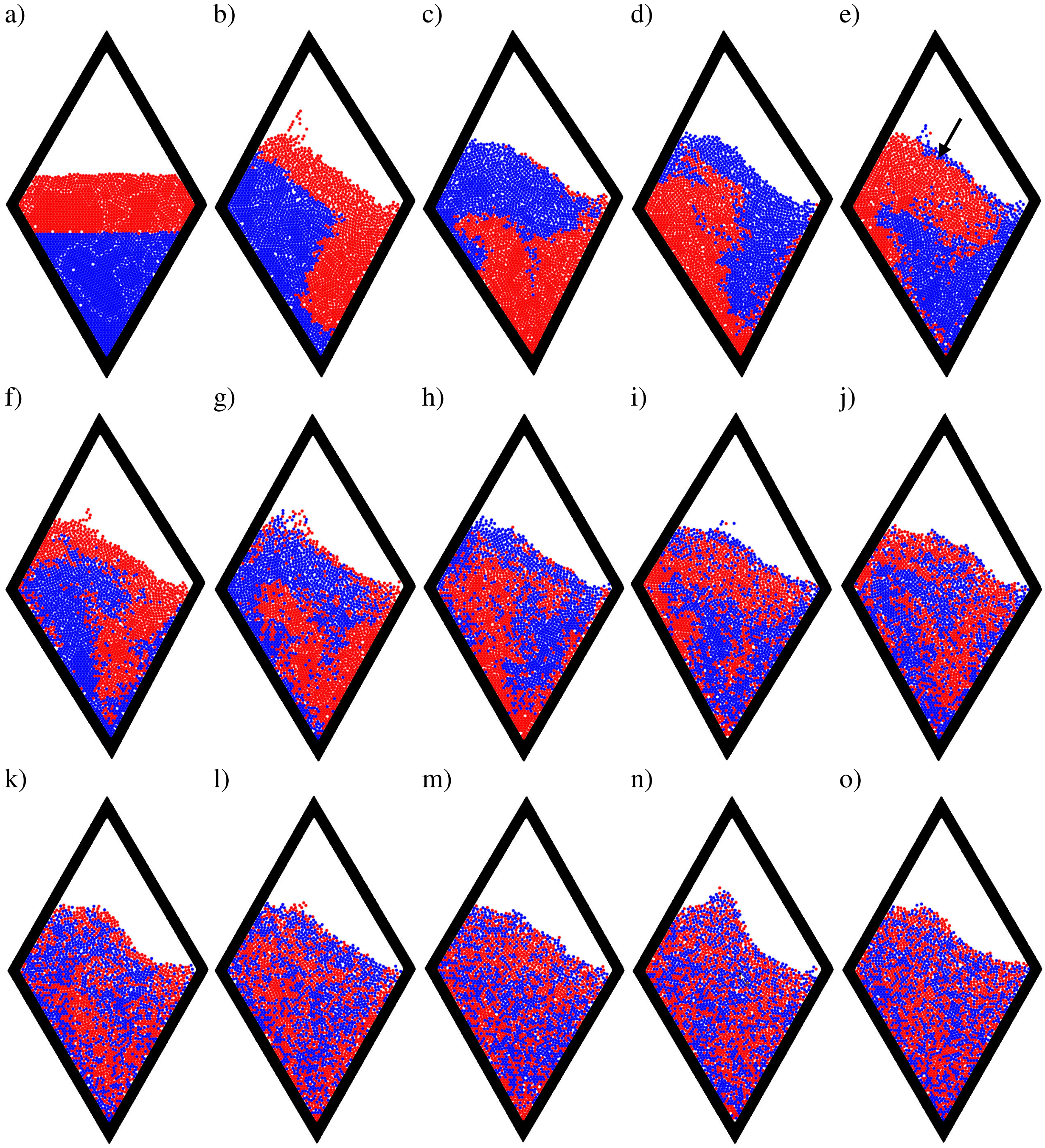

Fig. 2. The consecutive stages of the mixing process calculated for the double cone blender, the pictures present particles after: 0 a), 1 b), 2 c), 3 d), 4 e), 5 f), 6 g), 7 h), 8 i), 9 j), 10 k), 11 l), 12 m), 13 n) and 14 o) rotations

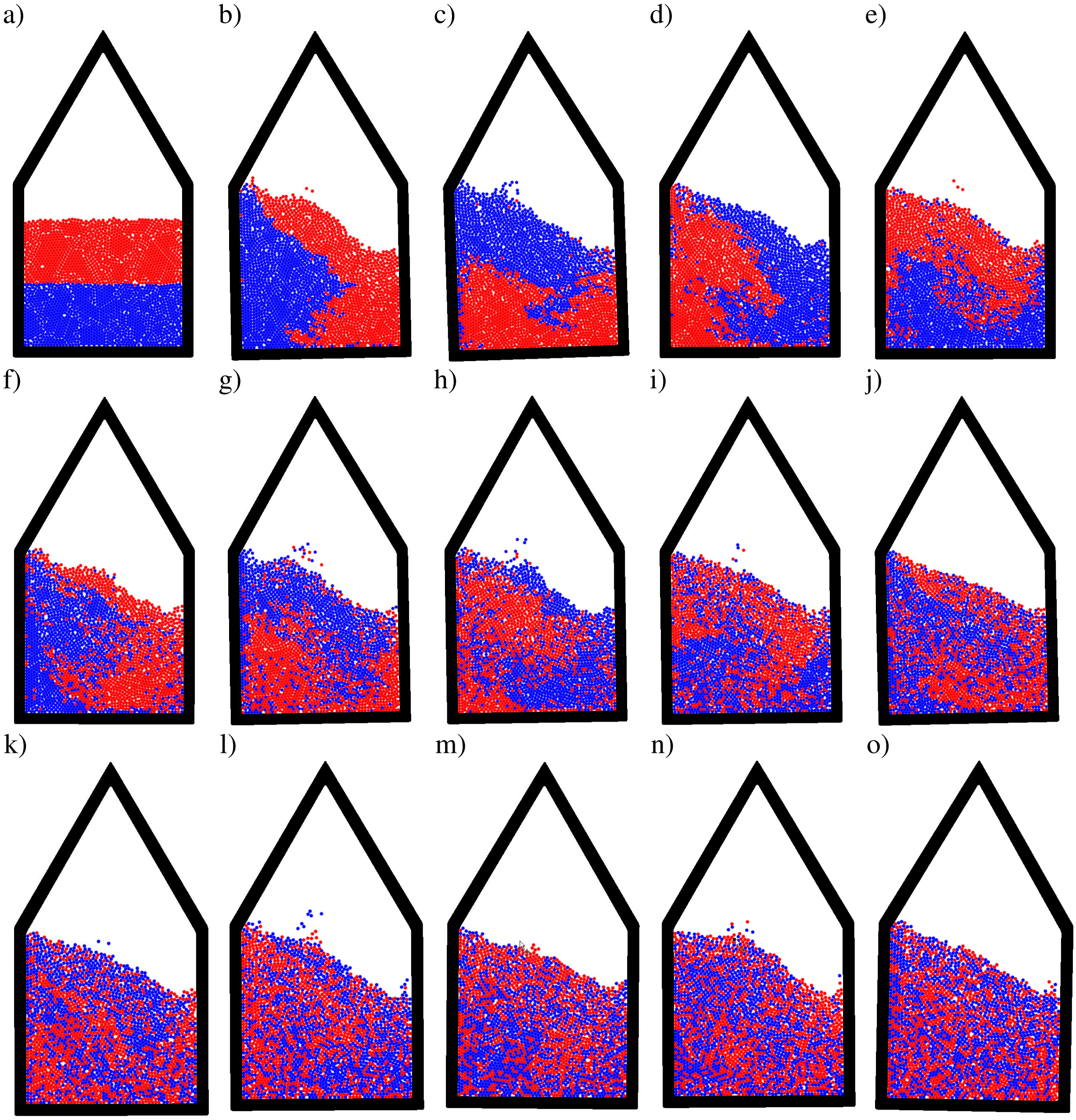

Fig. 3. The consecutive stages of the mixing process calculated for the IBC blender, the pictures present particles after: 0 a), 1 b), 2 c), 3 d), 4 e), 5 f), 6 g), 7 h), 8 i), 9 j), 10 k), 11 l), 12 m), 13 n) and 14 o) rotations

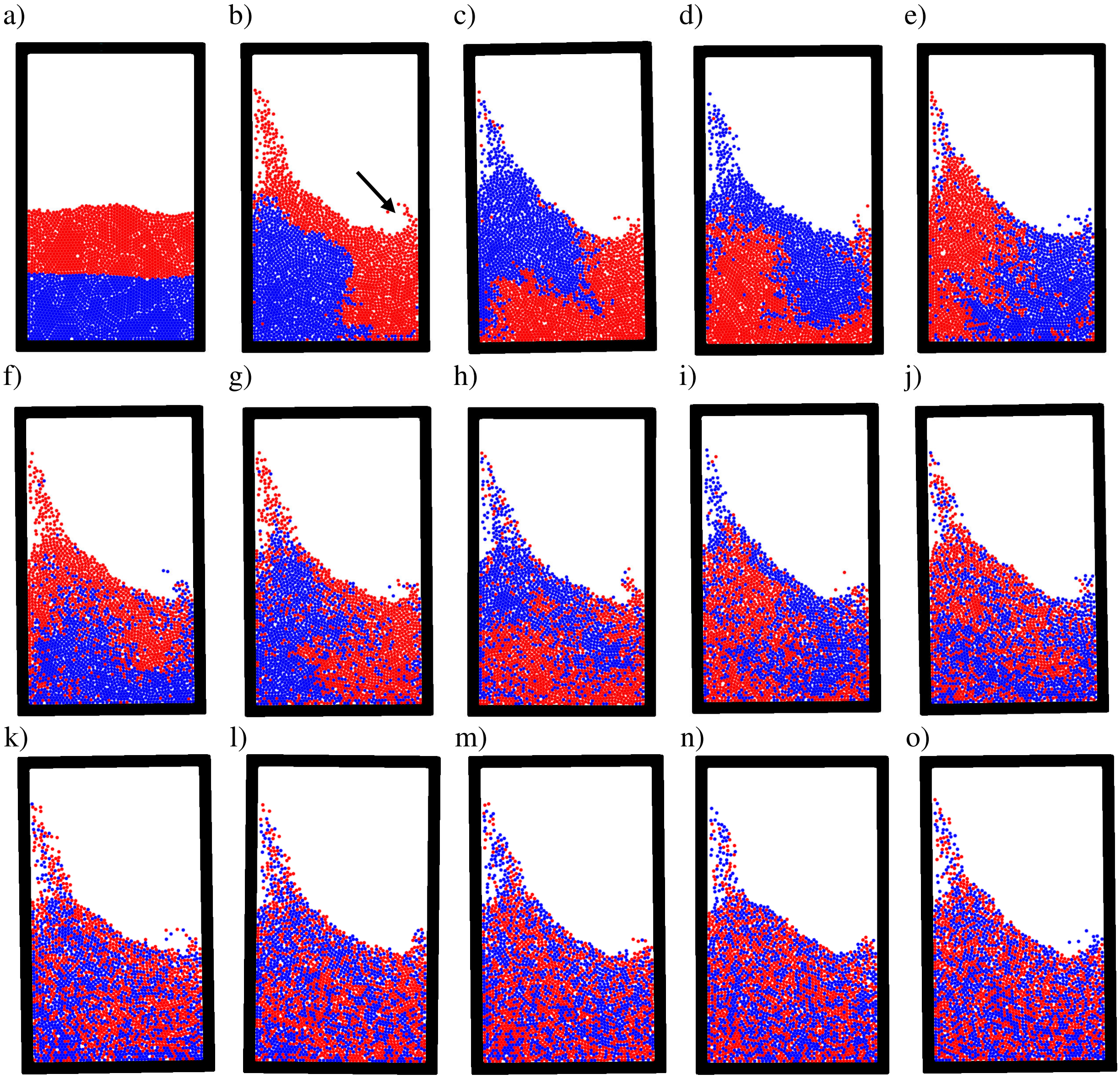

Fig. 4. The consecutive stages of the mixing process calculated for the drum blender, the pictures present particles after: 0 a), 1 b), 2 c), 3 d), 4 e), 5 f), 6 g), 7 h), 8 i), 9 j), 10 k), 11 l), 12 m), 13 n) and 14 o) rotations

The diffusion process can be observed in Figs. 2f, 3f, 4f. An analysis of the results tends to conclusion that the diffusion process is the most intensive in drum blender, while the diffusion process in IBC blender is slightly less intensive. At the same time the diffusion process in double cone blender is less intensive than in IBC blender. After nine rotations blend in drum blender, is the most homogeneous comparing with IBC and double cone blenders; it is difficult to find the spiral shape (Fig. 4j). That is a result of the intensive diffusion process and chaotic dynamics. Finally after fourteen rotations blends in drum blender and IBC blender are homoheneus and a progress of the mixing process is not as significant, as has been observed on the early stage (Figs. 3o, 4o). While in in double cone blender, sets of blue and red particles are observed (Fig. 2o).

Results of simulation obtained with DEM has been compared against experinental results published previously [34]. A good agerrement between results tends to conclusion, that discrete element method can provide a valid information about mixing process.

3. Conclusions

The presented computational results show mixing process of two granular ingredients within three blenders. Apart from the three basic mixing mechanisms: diffusion, convection and shear, one more mechanism has been observed. The mechanism is the baker's transformation and diffusion. The baker's transformation leads to a spiral shape of ingredients. Then the diffusion process finally destroys the spiral shape, which makes a blend more homogeneous. That is the point of mixing. The diffusion process can be coupled with the butterfly effect, which is typical for chaotic systems. The mixing process is the most intensive on the early stage; while after some period of time the progress of the mixing process is not significant. The phenomenon has been observed experimentally and described in literature.

Summarising this, the mixing process can take less time if the diffusion process is more intensive - granular flow is more chaotic, and the baker's transformation - "vortex" is faster; that is practical conclusion. Moreover designers can use the discrete element method to improve blenders.

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