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Estimating Porosity of Agglomerated Products Using Optimized Sphere Packing

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ABSTRACT

The article presents the results of studying the dynamics of changes in the porosity of two-component briquettes and pellets depending on the size of particles and the proportions of components in the mixture using an optimized packing of spheres. Knowing the patterns of change in the porosity allows to optimize the strength of the briquette and pellets as well as to improve their behavior in the reduction processes in blast furnaces, steel making furnaces and in direct reduction reactors. A computation experiment based on heuristic simulation model was designed to study the change of the estimated porosity under increasing/substituting the number of larger spherical particles in the mixture of spheres. The results obtained made it possible for the first time to reveal the extreme nature of the change in the porosity of the briquette/pellet with the addition of larger particles, depending on the fractional composition of the briquette. The results obtained open up new opportunities for optimizing the placement of fine-grained materials in the charge of metallurgical furnaces.

KEYWORDS

Briquettes, Estimated Porosity, Heuristic, Nonlinear Optimization, Sphere Packing

INTRODUCTION

The current stage of development of the ferrous metallurgy is marked by special attention to decarbonization as a key factor in reducing CO_2 emissions. The report of the Intergovernmental Panel on Climate Change (IPCC [Key World Energy Statistics, n.d.]) in 2018 set a goal to limit global warming to 1.5 °C by 2050.

Achieving this goal is largely due to the speedy introduction of the best available technologies (BAT) into metallurgical practice. The level of reduction of specific emissions in the steel industry by the introduction of BAT is estimated at 15–20% (from 1.8 to 1.44 t CO_2/t of steel [Holappa, 2020]).

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The greatest potential for reducing emissions from full-cycle steel mills comes from replacing sinter in the blast furnace charge with briquettes. The effectiveness of the synergy of briquetting and sintering with partial replacement of sinter with briquettes in a blast furnace charge was studied in detail for the first time in Bizhanov (2022).

An important role in the transformation of modern ferrous metallurgy into a green one is called upon to play cold (non-firing) briquetting. The manufacture of briquettes does not involve the consumption of carbon, in contrast to traditional industrial agglomeration technologies whereas 35–45 kg of coke breeze is consumed per 1 ton of sinter, and 18–25 m^3 of natural gas is consumed for the production of pellets. Among the criteria for belonging to BAT, one of the most important is the almost complete absence of harmful emissions in the production of briquettes.

Briquetting will not lose its relevance in the realities of green metallurgy due to the intensive pyrometallurgical nature of the main metallurgical technologies, which inevitably lead to the formation of fine materials that are promising for recycling (dust, sludge, fines, etc.). Recycling of such materials without their preliminary agglomeration is impossible. The largest mining and metallurgical company VALE announced plans for the early commissioning of briquette factories with a capacity of 6 million tons of briquettes from hematite iron ore concentrate both for blast furnaces and DRI reactors in 2024.

The reducibility of the briquette is a key factor in obtaining a product with the desired metallurgical properties. In turn, the reducibility is largely determined by the porosity of the briquette material.

In most studies known from the literature, the porosity of briquettes is investigated depending on the magnitude of the applied pressure. It is clear that the amount of pressure applied in the production of briquettes manifests itself differently in different briquette technologies. Thus, in vibropressing, the briquetted mixture is practically not subjected to compression, and the compaction process is carried out due to fluctuations in the viscosity of the mixture synchronously with the vibration phases due to the properties of thixotropy manifested by the hydrated binder. The values of the applied pressure are insignificant (0.2 MPa) and may not be taken into account in extrusion briquetting, the pressure in the working chamber of the extrusion extruder reaches values of 3-4 MPa, which is an order of magnitude less than the pressure values typical for roll briquetting (from 10 to 100 MPa).

High values of pressure exerted on the mixture briquetted by the roller press can significantly change the structure of the briquette components, the size and shape of their particles, which can cause both a decrease in porosity and its growth due to the appearance of internal cracks.

Speaking in general about the study of the metallurgical properties of briquettes, including porosity, an important remark should be made concerning the incorrectness of projecting the results of the study of laboratory briquettes, in the vast majority of cases manufactured by means available in the laboratory that have little in common with the main types of commercial briquette technologies, to the specific conditions of industrial briquetting process. A significant number of scientific studies of the briquetting process are based on the study of the properties of laboratory briquettes made by lever or piston presses, which obviously does not allow us to identify the features of the metallurgical properties of briquettes based on the studied mixtures during their manufacture by one or another briquetting equipment (roller, press, vibropress or extruder).

The method of manufacturing has a significant effect on porosity and, consequently, on the reducibility and metallization of briquettes.

The main contributions of the paper are as follows.

1) An optimized sphere packing problem is introduced to study the porosity of individual pellets (briquettes) and the porosity of layers of pellets on roasting machines and in the charges of metallurgical furnaces and reactors, depending on the particle size distribution.
2) Novel mathematical model of the optimized packing problem in the form of NLP problem is provided.
3) Intelligent solution technique is proposed based on a mulistart strategy combined with a feasible starting point algorithm and nonlinear optimization.

4) For the first time, the extreme (non-monotonic) nature of the dependence of pellet (briquette) porosity on the size of iron ore concentrate particles and the porosity of the pellet layer on their size distribution has been revealed.

The rest of the paper is organized as follows. The next section describes motivations related to the problem of determining the effect of the granulometric composition of the components of the pellet or briquette on its porosity. An optimized packing problem for spherical particles in a given 3D volume is formulated and a solution algorithm is described in section Problem Formulation and a Solution Approach. Numerical examples for two special scenarios of the packing problem, adjunction and replacement, are presented in the next section. Discussions and conclusions are presented in the last two sections.

MOTIVATION

Previously, the problem of determining the effect of the granulometric composition of the components of the pellet or briquette on its porosity was not formulated in the literature.

The influence of the fractional composition was studied in connection with the study of the porosity of the soil and the layer of multicomponent metallurgical charges. The regularities of structure formation in the process of fine-grained materials in the context of solving extreme problems of maximizing and minimizing the porosity of the charge were studied mainly. The first task is related to the need to achieve high gas permeability of a layer of lump materials in a blast furnace or on a conveyor belt of a sintering/firing machine, the second is aimed at increasing the strength of the agglomerated raw materials.

The regulation of the granulometric composition of the iron ore concentrates entering the pelletizing, aims to influence the porous structure of the pellet. It should be taken into account that the initial density of the pellet has an ambiguous impact on the strengthening process. On the one hand, an increase in density leads to an increase in the number of contacts between particles and is thus favorable for strengthening. On the other hand, a decrease in porosity hinders the process of magnetite oxidation, which is a negative factor for strength. It is for these circumstances that when mixing concentrates of various sizes, it is necessary to choose their optimal mix ratio, proper pelletizing mode and rational pellet firing. Speaking about firing, it should also be borne in mind that the choice of optimal methods for organizing it for iron ore spherical pellets ranging in size from 6 to 16 mm at temperatures up to 1300 °C in a moving layer also involves solving the problem of proper placement (packing) of the fired layer.

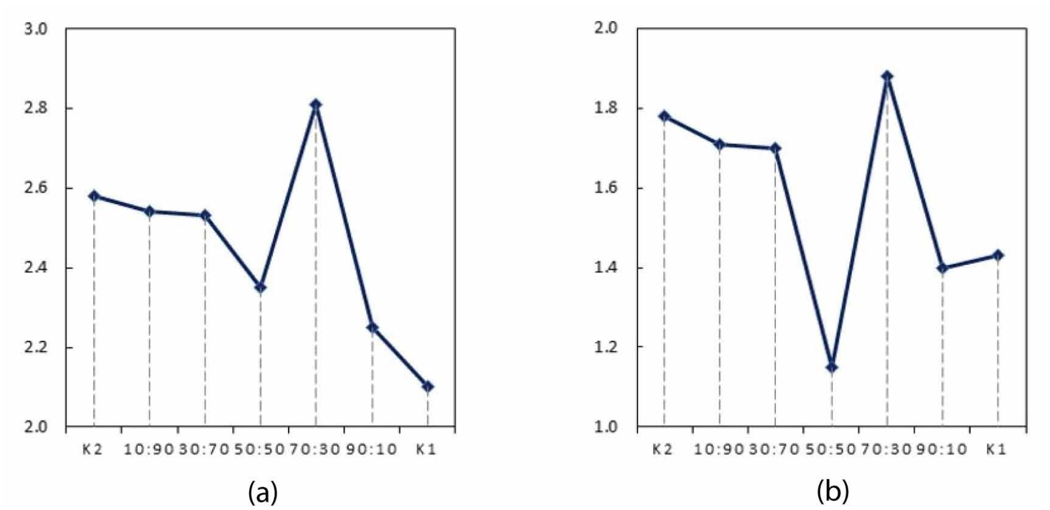
There are solutions for strengthening pellets by optimizing the structure of the granules by mixing concentrates of different dispersity. The granulometric composition of the considered concentrates is shown in Table 1.

The results of strengthening experiments on pellets with a different ratio of concentrates K_1 and K_2, respectively (10:90; 30:70; 50:50; 70:30; 90:10) are shown in Figure 1.

Table 1. Granulometric composition of concentrates for pelletizing

Fraction	The contents of the fraction, %	
	Fine concentrate K1	Coarse concentrate K2
< 0.044 mm	90.3	80.8
0,044 – 0,074 mm	8.6	15.7
> 0.074 mm	1.1	3.5

Figure 1. Cold strength of pellets made from a mixture of concentrates (roasting temperature 1280°C): a) bentonite content of 0.5%; b) the content of bentonite 0.25%. The abscissa axis denotes the ratio of the concentrates in the mixture, %; ordinate axis denotes strength of fired pellets, kN / pellet.



The best indicators of cold strength are given by the ratio of “fine” and “coarse” concentrates as 70:30 with the minimum strength of pellets in the case of a 50:50 ratio of concentrates. For the 70:30 case, the total porosity of pellet was equal to 37.09%; in case of 50:50 – 48.76%.

In application to briquetting, ensuring high strength of the briquette in itself is not a sufficient condition for obtaining agglomerated products with high metallurgical properties. Minimizing briquette porosity negatively affects its reducibility due to a decrease in the proportion of volume not occupied by the solid phase and a decrease in the surface area available for the action of reducing gases.

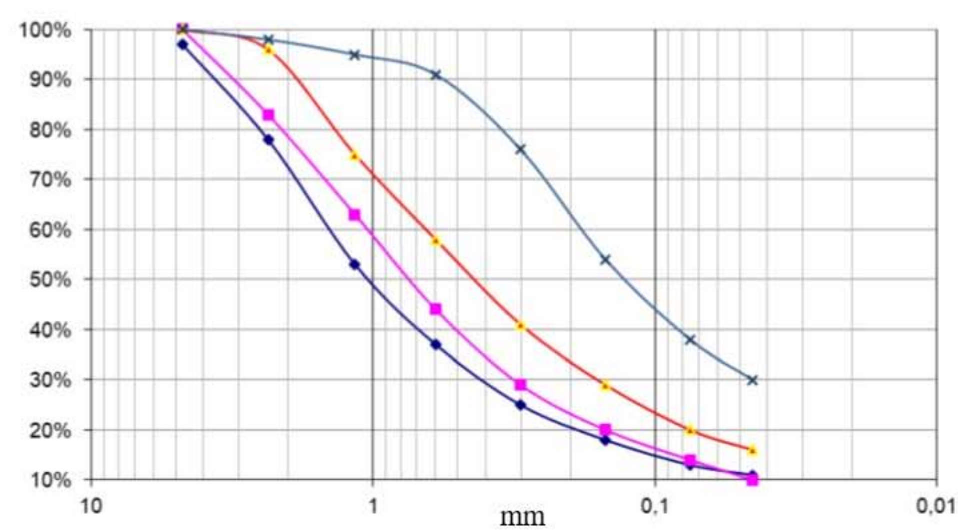
The choice of stiff extrusion technology is precisely due to the possibility of achieving mechanical strength sufficient for immediate transportation of raw extruded briquettes in combination with porosity comparable to the porosity of fired pellets.

The practice of extrusion briquetting shows that the greatest difficulties are caused by briquetting of a separate fine-grained material consisting of particles with sizes in a narrow range from tens to a hundred microns. The packing density of such particles reduces the total surface available for the action of plasticizing additives. The possibility of achieving plasticity is critical for the production of briquettes. The addition of larger particles simplifies the extrusion process. Large particles create a kind of corset that facilitates the pushing of the plasticized mixture and supports the porous structure of the briquette.

An example showing the same effect of fractions redistribution on physical properties of briquettes is given by the results of the study of briquettes made from coke breeze from a single source, pulverized in three different ways: a roller crusher, a hammer mill, and double extrusion through an extruder shearing plate. In each of the three cases considered, the granular composition of the briquetted mixture was noticeably different from the composition of the starting material (Figure 2).

As evidenced above, the grinding of coke breeze is maximized after double extrusion through a shearing plate in an extruder. In this case, the effect of deep grinding is achieved through the application of high shear stresses. The use of a hammer mill for such a material was found to be ineffective, and the granulometric composition of the ground material differed weakly from that of the initial coke breeze. Briquettes were produced with a binder in the form of cement (5%) and bentonite (1%). The only difference between the briquettes was the manner in which the coke breeze was ground. The

Figure 2. Granulometric composition of coke breeze in the following states: (1) initial and (2–4) after additional grinding in a hammer mill, in a roll crusher, and double extrusion in an extruder, respectively. γ is the yield of the oversize mass, and a is the mesh size.



briquettes were classified assigned the following numbers in accordance with the method of grinding: #1 was coke breeze ground by roller crusher; #2 was coke breeze sheared twice through the shearing plate with a plurality of holes; #3 was coke breeze ground by hammer mill. Physical properties of briquettes are provided in Table 2.

With practically no change in the density of the briquette, their compressive strength varied significantly depending on the particle size distribution, despite the fact that the briquettes had identical component and chemical compositions. The transition from a coarse composition in a hammer mill to grinding with a roller crusher led to an increase in the strength of the briquette, while further grinding of coke breeze in an extruder reduced this strength.

When replacing cement (5% by weight) with particle sizes less than 32 μm in briquette intended for direct reduction reactors with lime (5% by weight) with larger particle sizes (52.6 μm) the porosity increased and amounted to 21.25% versus 20.88% before such a replacement. For other briquette from almost the same materials, replacing lime (52.6 microns, 5% by weight) with a magnesium binder (0.1-1.0 mm, 55 by weight) led to a decrease in porosity from 29.7% to 25 .4%.

Another example of the influence of the granulometric composition of the briquetted mixture on its density, porosity and strength is the experience of creating briquettes for high-temperature reduction in the ITmk^3 process. For the production of the experimental briquettes, we have used the Hematite iron ore concentrate, the Coal 1 with 73% of particles smaller than 0.6 mm and the Coal 2 with 99% of the particles smaller than 0.3 mm in size. The Portland cement (general use) has been used as the binder (5% mass). Table 3 shows the briquettes compositions and their physical properties.

Table 2. Physical properties of coke breeze briquette

Grinding method	Density,g/cm^3	Compressive strength, kgF/cm^2
#1 (roller crusher)	1.63	37.76
#2 (double shearing)	1.67	34.32
#3 (hammer mill)	1.63	20.25

Table 3. Briquettes components and physical properties

Briquette sample	Component, %			Density, g/cm^3	Porosity	CCS,
	Iron ore	Coal	Portland cement		%	kgF/cm^2
#1	63	32*	5	2.207	36.4	49.0
#2	63	32	5	2.034	36.9	24.0

*Coal 1

When a coarser fraction of coal was used in the briquette, the density increased by almost 9%, the compressive strength almost doubled, and the porosity decreased by only 1.5%.

When replacing 10% of the mass of briquette made from a mixture of equal amounts of the blast furnace sludge (43% particles with sizes less than 0.045 mm, bulk density 1.1 g/cm^3) and converter sludge (62% particles with sizes less than 0.045 mm, bulk density 1.5 g/cm^3) by coke breeze (96% of particles with sizes less than 2.36 mm, bulk density 0.6 g/cm^3) with equal amounts of binder and plasticizers, the density of the briquette of the modified composition remained unchanged (2.36 g/cm^3), and the compressive strength increased from 2.46 MPa to 3.0 MPa.

When replacing 7% of the mass of a briquette made from iron ore concentrate (39% of particles less than 0.075 mm in size, bulk density 3.0 g/cm^3) with coke breeze (96% of particles less than 2.36 mm in size, bulk density 0.6 g/cm^3) with equal amounts of binder and plasticizers, the density of the briquette of the modified composition was 3.44 g/cm3 against 3.31 g/cm^3 for original composition, and the drop strength (height 2 meters, 3 drops) did not change (8% fines with particle sizes less than 4.75 mm).

The given examples of changes in the physical properties and porosity of pellets and briquettes with a change in the granulometric composition of the mixture indicate the absence of a direct linear relationship between these parameters. The lack of a clear algorithm for optimizing the particle size distribution of a briquette (pellet) components makes this problem empirical. In this work, an attempt was made to develop a new approach to choosing the relative sizes of particles of a briquetted mixture using the theory of close packing of spheres.

Sphere Packing Problem. In this paper, the influence of the quantity and size of the added large particles on the porosity of the briquette or pellet, as a key parameter of reducibility, is studied.

In sphere packing problems a set of spheres must be allocated completely inside a container without mutual overlapping while optimizing dimension(s) or volume of the container.

Problems of packing spheres are well studied. Various solution techniques for the sphere packing are based on geometric placement presentation, probabilistic approaches, heuristics and metaheuristics, mathematical programming and hybrid approaches.

Geometric placement methods are based on geometric principles and modeling to determine the optimal sphere placement achieving uniform distribution (Conway & Sloane, 1998).

Important results were also obtained using an approach based on the use of artificial neural networks to study the strength of pellets (Chagas et al., 2015) and the porosity of the layer they are laid on a roasting machine (Dwarapudi et al., 2007).

Probabilistic methods such as Monte Carlo simulations (Abreu et al., 1999; Cheng et al., 2000) and stochastic optimization (Wu et al., 2010) algorithms are based on probabilistic models and statistical analysis.

Heuristics are practical problem-solving strategies that exploit domain-specific knowledge and intuition to guide the search for solutions making smart guesses and applying rules of thumb to explore the solution space quickly. Heuristics for sphere packing involve strategies like greedy algorithms, sequential addition, block coordinate descent method and other techniques (see, e.g., Blondel et al. 2013; Kubach et al., 2011; Mueller, 2005).

Metaheuristics are higher-level strategies that guide the search process by iteratively exploring the solution space, considering multiple candidate solutions, and gradually refining them. Unlike specific heuristics, metaheuristics are applicable to a wide range of problems. Popular metaheuristic algorithms used in sphere packing include simulated annealing (Mughal et al., 2012), genetic algorithms (Sulaiman et al., 2019), particle swarm optimization (Hifi et al., 2017), ant colony optimization (Li et al., 2013), and tabu search (Fu et al., 2013). These algorithms often incorporate randomness and mechanisms to balance searching for new solutions and exploitation of promising ones.

Mathematical programming based algorithms are used to solve sphere packing problems by formulating them as mathematical optimization problems (e.g., Litvinchev & Ozuna, 2014).

Hybrid methods combine multiple approaches to improve the strengths of different techniques. Hybrid methods may involve a combination of optimization algorithms, machine learning, simulation, or other approaches to get reasonable sphere placement solutions. A hybrid heuristic combining a variable neighborhood search with a local search for the NP-hard optimization problem of packing identical spheres of unit radii into the smallest sphere is considered in Fischer et al. (2023). In M'Hallah et al. (2013) the authors propose using a set of geometrical features, including the concept of packed spheres, to represent and analyze the atomic clusters. These packed spheres serve as a reduced feature representation of the cluster structures, allowing for more efficient optimization in a reduced variable space. A novel algorithm for solving the sphere packing problem is studied in Bagattini et al. (2018). By combining basic greedy procedure, intensification stage and diversification stage, the threshold search-based population algorithm seeks to achieve an optimal or near-optimal sphere packing arrangement.

PROBLEM FORMULATION AND A SOLUTION APPROACH

A packing problem is considered in the following formulation.

Let spheres S_i, $i = 1,2,...,n$, be given. Denote a sphere centered at $v_i = (x_i, y_i, z_i)$ with radius r_i by:

$$S_i(v_i) = \left\{(x,y,z) \in R^3 : (x - x_i)^2 + (y - y_i)^2 + (z - z_i)^2 - r_i^2 \le 0\right\}$$

The problem is aimed to pack the spheres in a minimum volume cube:

$$C(a) = \left\{(x,y,z) \in R^3 : 0 \le x \le a, 0 \le y \le a, 0 \le z \le a\right\}$$

Denote by I a collection of spheres S_i.

The packing problem is stated in the form of the following nonlinear programming model:

$$\min_{v,a} a \tag{1}$$

subject to:

$$\left\|v_i - v_j\right\|^2 - (r_i + r_j)^2 \ge 0, i > j \in I \tag{2}$$

$$\min\{x_i - r_i, y_i - r_i, z_i - r_i, a - x_i - r_i, a - y_i - r_i, a - z_i - r_i\} \geq 0,\ i \in I \tag{3}$$

$$v = (v_1, v_2, ..., v_n),\ v_i = (x_i, y_i, z_i),\ i \in I \tag{4}$$

In (1)-(4), the inequality (2) is responsible for a pairwise non-overlapping of spheres, i.e. $\operatorname{int} S_i(v_i) \bigcap \operatorname{int} S_j(v_j) = \varnothing$ (touching is allowed) for $i > j \in I,$ while the inequality (3) describes an arrangement of each sphere $S_i(v_i)$, $i \in I$, fully inside the cube $C(a)$, i.e. $S_i(v_i) \subset C(a) \Leftrightarrow \operatorname{int} S_i(v_i) \bigcap C^*(a) = \varnothing$, $C^*(a) = R^3 \setminus \operatorname{int} C(a)$. The latest is referred to the containment condition. Here $\operatorname{int}(\cdot)$ means the topological interior of the set $(\cdot)$.

Note that inequality (3) is equivalent to the system of inequalities $x_i - r_i \geq 0,$ $y_i - r_i \geq 0,$ $z_i - r_i \geq 0,$ $a - x_i - r_i \geq 0,$ $a - y_i - r_i \geq 0,$ $a - z_i - r_i \geq 0$ for $i \in I$.

According to the classification of packing problems (Hifi et al., 2023), model (1)-(4) belongs to ODP (Open Dimension Problem) with a variable metric characteristic a.

The problem (1)-(4) is NP-hard (Wäscher et al., 2007) and therefore a heuristic approach is used based on a mulistart strategy combined with a feasible starting point algorithm (Chazelle et al., 1989) and a decomposition technique (Duriagina et al., 2021).

Let us consider the approach in details. Assume that the radii r_i, $i \in I$, of the spheres become variable. A sphere with a variable radius $0 \leq \rho_i \leq r_i$ and variable center v_i is denoted by $S_i(v_i, \rho_i)$, $i \in I$. Then set a sufficiently large value of $a = a_0$, so that all spheres $S_i(v_i)$, $i \in I$ are fitting the cube $C(a_0)$ undoubtedly.

Then we formulate the following optimization problem:

$$\max_{v,\rho} \sum_{i \in I_n} \rho_i \tag{5}$$

$$\left\| v_i - v_j \right\|^2 - (\rho_i + \rho_j)^2 \geq 0,\ j > i \in I \tag{6}$$

$$\begin{gathered} x_i - \rho_i \geq 0, y_i - \rho_i \geq 0, z_i - \rho_i \geq 0, i \in I, \\ a_0 - x_i - \rho_i \geq 0, a_0 - y_i - \rho_i \geq 0, a_0 - z_i - \rho_i \geq 0, i \in I \end{gathered} \tag{7}$$

$$0 \leq \rho_i \leq r_i, i \in I \tag{8}$$

$$v = (v_1, v_2, ..., v_n), \rho = (\rho_1, \rho_2, ..., \rho_n) \tag{9}$$

If, as a result of solving problem (5)-(9), we obtain $\max\limits_{v,\rho} \sum\limits_{i \in I_n} \rho_i = \sum\limits_{i \in I} r_i$, then the local maximum point $(v_1^*, \rho_1^* = r_1, v_2^*, \rho_2^* = r_2, \ldots, v_n^*, \rho_n^* = r_n)$ corresponds to a feasible point $(v_1^*, v_2^*, \ldots, v_n^*, a_0)$ of problem (1)-(4). This point is considered as a starting point for problem (1)-(4).

Generating feasible starting points for the problem (5)-(9) is also an important stage.

A heuristic algorithm is proposed that takes into account the metric characteristics of the placed spheres and the cubic container.

Algorithm for generating feasible starting points (GFSP) of problem (5)-(9).

Assume spheres $S_i(v_i, \rho_i)$, $i \in I$, are ordered with respect to descending their original radii r_i, $i \in I$.
Step 1. Set $k := 1$, $\rho_k = r_k$. Choose randomly v_k such that $S_k(v_k, \rho_k) \subset C(a_0)$.
Step 2. Set $k := k + 1$.
Step 3. If $k > n$ then stop algorithm.
Step 4. Set $\rho_k := r_k$.
Step 5. Set $t := 0$.
Step 6. Set $t := t + 1$.
Step 7. Choose randomly v_k such that $S_k(v_k, \rho_k) \subset ! \,(a_0)$.
Step 8. If $\operatorname{int} S_k(v_k, \rho_k) \cap \operatorname{int} S_j(v_j, \rho_j) = \varnothing$ for $j = 1, \ldots, k$, then go to Step 2. Otherwise go to
Step 9. If $t = m + 1$, then set $\rho_k := \rho_k \cdot \mu \ (0 < \mu < 1)$ and go to Step5. Otherwise go to Step 6.

This algorithm allows effectively use the free space in the cube.

To solve problem (1)-(4), the multistart strategy is used, i.e. several feasible starting points are selected, obtained by solving problem (5)-(9).

General solution strategy is illustrated in Figure 3.

COMPUTATIONAL RESULTS

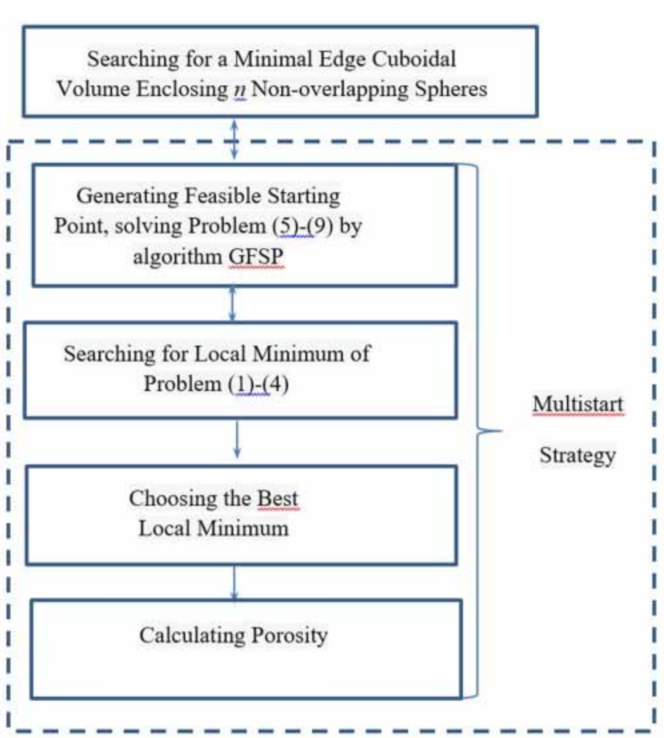
In the computational experiment two special cases to construct the set I of spheres are considered. In both cases the set I consists of two subsets, I_{i0} and I_{ik} such that $I = I_{i0} \cup I_{ik}$. The set I_{i0} consists of n_{io} equal spheres having radius r_{io}, while the set I_{ik} is composed of n_{ik} equal spheres with radius r_{ik} which are added to the spheres r_{io}.

In the first case the number n_{io} of spheres is fixed and n_{ik} is gradually increased. That is, we simply add the spheres r_{ik} to the spheres r_{io} and the total volume of the spheres is increased.

In the second case the spheres r_{ik} are added, but some spheres r_{io} are withdrawn from I_{i0} such that the total volume of added spheres is approximately equal to the volume of the withdrawn spheres. The aim is to maintain the total volume of all spheres approximately constant. More specifically, let V_{ik} be the volume of all added spheres and V_{i0} be the volume of the sphere r_{io}:

$$V_{ik} = n_{ik}(4/3)\pi(r_{ik})^3, \; V_{i0} = (4/3)\pi(r_{i0})^3$$

Figure 3. Flow chart of general solution strategy



We would like to define the maximal integer number $\bar{n}_{io}$ such that $V_{ik} \geq \bar{n}_{io} V_{io}$. The corresponding value be:

$$\bar{n}_{io} = \left\lfloor \frac{V_{ik}}{V_{io}} \right\rfloor = \left\lfloor \frac{n_{ik} r_{ik}^3}{r_{i0}^3} \right\rfloor$$

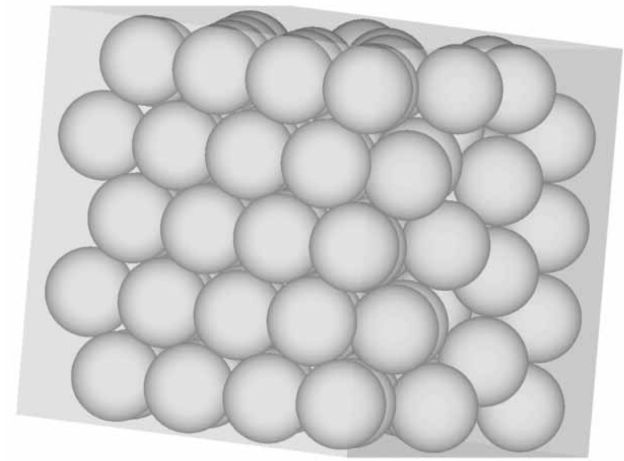
where $\lfloor \bullet \rfloor$ denotes the integer part of the number. Correspondingly, the number of spheres in I_{i0} is defined as $n_{io} := n_{io} - \bar{n}_{io}$.

Computational Results for the First Case (Adjunction Scenario)

In computational experiments, 100 starting points are generated, $\mu = 0.95$, $m = 5000$.

Computational experiments are carried out for one- and two-component mixtures of spheres. The first group (fraction) of spheres consists of 100 spheres with radius $r = 1$. The second group (fraction) includes 5, 10, ..., 25 equal spheres with a larger radius $r =$ 3, 4, …, 15. For different proportions of spheres mixed with these radii, the length of the cube edge is minimized and the resulting porosity coefficient is calculated. Strictly speaking, the porosity coefficient in the formulation under consideration differs from porosity in its classical definition (the fraction of the volume of a material not occupied by solid mass), since in such an idealization it is assumed that only whole spheres are located inside the cube. Fragments of spheres from areas of the briquette adjacent to the cube are not taken into account.

Figure 4. Packing of 100 spheres with a radius of 1



First, the case of identical spheres $r = 1$, $n = 100$ is considered. The resulting porosity value is 0.4383 with a minimum cube edge length of $a = 9.0701$ (Figure 4). The remaining experimental results are shown in Table 4. The first column of the table shows the radii of the spheres that make up the second group. In subsequent columns – the values of the obtained minimum cube length / porosity coefficient for the mixture, which is 100 spheres with a radius of 1 and 5, 10, ..., 25 spheres with the corresponding radii indicated in the first column. For example, for a mixture containing 100 spheres of radius 1 and 20 spheres of radius 7, the minimum cube edge length is $a = 39.2361$ and the porosity coefficient is 0.5173. All values of cube length and porosity coefficient are given rounded to the fourth decimal place.

Figure 5 shows packings of a two-component mixture of 100 spheres. The first mixture is of 100 spheres of radius 1 and 10 spheres of radius 3. The second is 100 spheres of radius 1 and 15 spheres of radius 3.

It should be understood that in this approach a fraction of larger particles is added to the initial fraction. In reality, there is usually a replacement of part of the fine fraction by larger particles. It is clear that the above results can simply be brought into line with reality by simple recalculation. So, when adding 20 spheres to the original 100, the share of large spheres is about 17% of the total number, and when replacing 20 spheres with larger ones, their total number remains unchanged, and large spheres make up 20% of the total number of spheres.

Figure 6 shows graphs of the dependence of the porosity on the number of spheres from the second group with radii from 3 to 15 according to Table 4.

Figure 7 shows the dependence of the porosity coefficient on the radius of the added particles for various volumes of adding a large fraction (5, 10, 15, 25%). Such a presentation of the results obtained corresponds to the situation with a fixed amount of coarse fraction, determined by the volume of its formation in metallurgical processes. It is clear that the added spheres 5, 10, 15, 20 and 25.

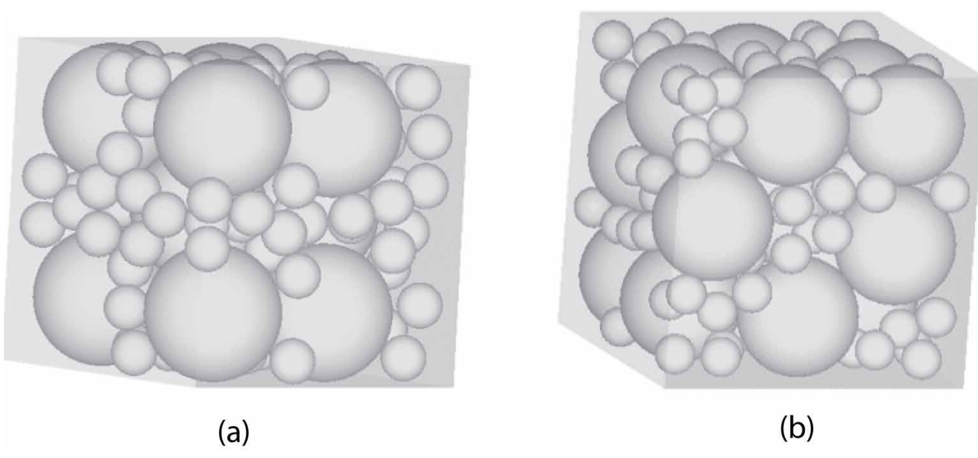
Computational Results for the Second Case (Replacement Scenario)

In some cases, it becomes necessary to consider a different scenario in modeling the porosity of briquettes – when replacing a fixed proportion of its mass with a material consisting of larger sizes, with a constant total volume of the briquette. The fact is that due to the specifics of briquette technologies, based on roller pressing and vibrocompression, the volume of the briquette and its shape are constant. In the case of extrusion agglomeration, the dimensions of the briquette can change, which makes the first scenario described above (adjunction) applicable in this case.

Table 4. Results of computational experiments for the first case: values of porosity

	n=5	*n*=10	*n*=15	*n*=20	*n*=25
r=3	11.8101/0.4023	14/0.4352	15.6/0.4428	16.8155/0.4362	17.878/0.4319
r=4	15.1554/0.4946	18.6667/0.5234	20.8/0.5066	22.4206/0.4871	23.8373/0.4743
r=5	18.9443/0.5533	23.3333/0.5549	26/0.5293	28.0258/0.5052	29.7967/0.4893
r=6	22.7331/0.5793	28/0.5687	31.2/0.5393	33.6309/0.5132	35.756/0.4960
r=7	26.522/0.5925	32.6667/0.5758	36.4/0.5444	39.2361/0.5173	41.7153/0.4994
r=8	30.3108/0.5999	37.3333/0.5798	41.6/0.5473	44.8412/0.5196	47.6746/0.5013
r=9	34.0997/0.6044	42/0.5822	46.8/0.5490	50.4464/0.5210	53.634/0.5025
r=10	37.8885/0.6072	46.6667/0.5837	52/0.5501	56.0515/0.5219	59.5933/0.5032
r=11	41.6774/0.6091	51.3333/0.5847	57.2/0.5509	61.6567/0.5225	65.5526/0.5037
r=12	45.4663/0.6105	56/0.5854	62.4/0.5514	67.2619/0.5229	71.5120/0.5040
r=13	49.2551/0.6114	60.6667/0.5859	67.6/0.5518	72.867/0.5232	77.4713/0.5043
r=14	53.044/0.6121	65.3333/0.5863	72.8/0.5520	78.4722/0.5234	83.4306/0.5045
r=15	56.8328/0.6126	70/0.5866	78/0.5522	84.0773/0.5236	89.39/0.5046

Figure 5. Optimized packings of a two-component mixture of spheres: a) 100 spheres with radius 1 and 10 spheres with radius 3; b) 100 spheres of radius 1 and 15 spheres of radius 3



We consider n_0 =500 spheres of radii $r_{io} = 1$, i=1,...,n, in the minimum size volume with the porosity value of 41.835028% (Figure 8).

Then we replace η^s (in %) of the total volume of the spheres $V_0 = \sum_{i=1}^{n} V_{i0}$ consequently with the same volume of spheres of radii r_{ik}, $k = 1,...,6$, such that $\eta^{(s)} V_0 \approx \sum_{i=1}^{n_k} V_{ik}$, where $\eta^{(s)}$ for $s = 1,2,3$ takes values of 5%, 10%, 20%, i.e., $\eta^{(1)} = 5\%, \eta^{(2)} = 10\%, \eta^{(3)} = 20\%$, while $r_{i1} = 1.1$, $r_{i1} = 1.2$, $r_{i1} = 1.3$, $r_{i1} = 1.4$, $r_{i1} = 1.5$, $r_{i1} = 2.0$.

Figure 6. Graphs of the dependence of the porosity coefficient on the number of added spheres with radii from 3 to 15

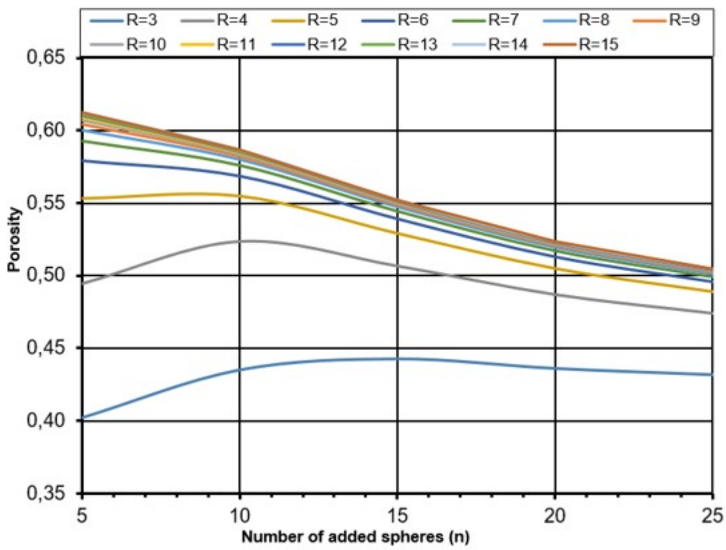


Figure 7. Graphs of porosity coefficient dependence on the sphere radius with number of the added spheres 5, 10, 15, 20 and 25

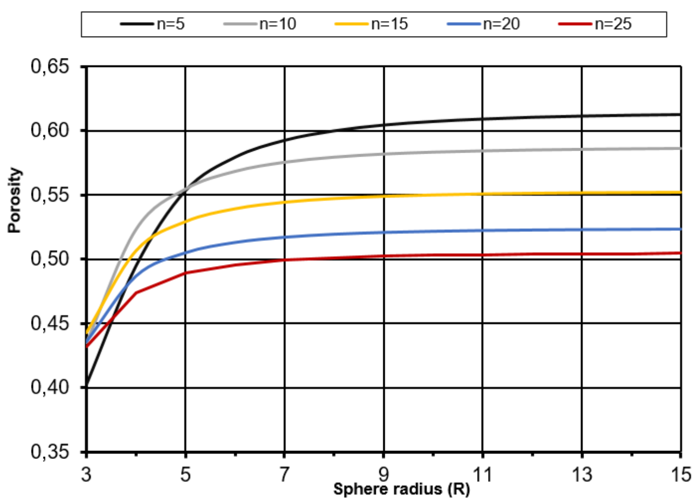


Table 5 provides the porosity for each of the combinations of $\eta^{(s)}$, $s = 1,2,3$ and r_{ik}, $k = 1,\ldots,6$.

Two optimized sphere packings are shown in Figure 9: 1) $n = 473$ spheres, where n_0 =450 spheres of radius $r_{io} = 1$ and n_3=23 spheres of radius $r_{i3} = 1.3$ for replacement volume $20\% V_0$ with the porosity 42.059; 2) $n = 477$ spheres, where n_0 =475 spheres of radius $r_{io} = 1$ and n_3=2 spheres of radius $r_{i6} = 2.0$ for replacement volume $20\% V_0$ with the porosity 41.598.

Figure 10 illustrates 3D bar chats for the combinations of $\eta^{(s)}$, $s = 1,2,3$ and r_{ik}, $k = 1,\ldots,6$. The minimum porosity found by our algorithm is 41,387 for $\eta^{(3)} = 20\%$ and $r_{i6} = 2.0$.

Figure 8. Packing 500 spheres with radii 1

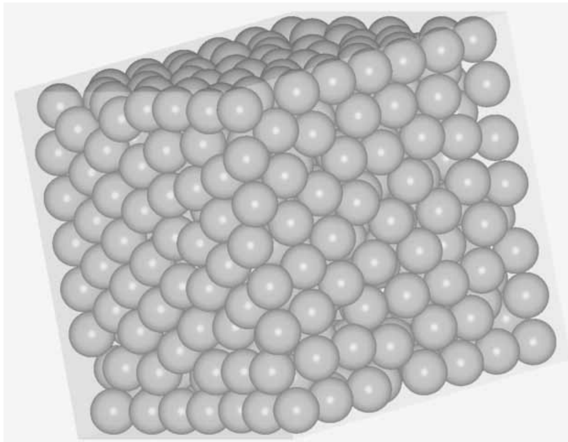
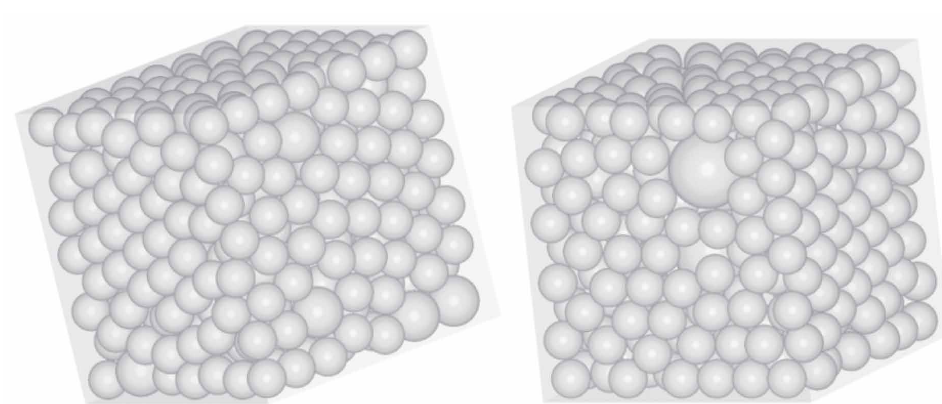


Table 5. Results of computational experiments for the second case: values of porosity

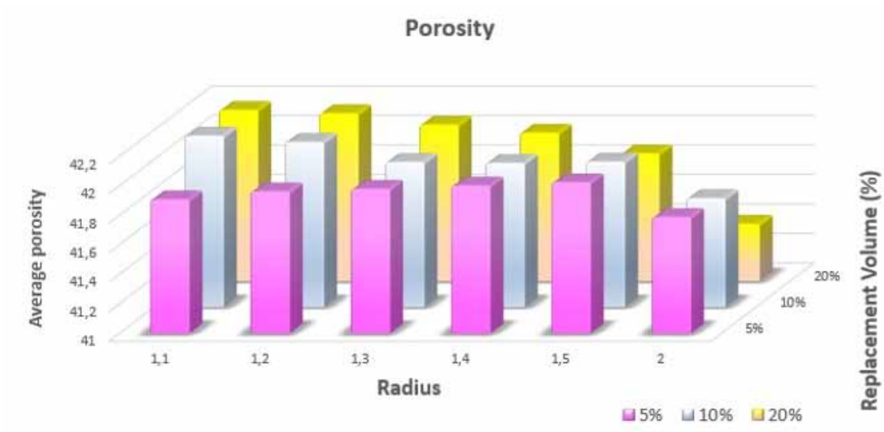
Replacement sphere radus, r_{ik}	Replacement Volume (%)		
	$\eta^{(1)}$ =5%	$\eta^{(2)}$ =10%	$\eta^{(3)}$ =20%
r_{i1}=1.1	41.907	42.161	42.159
r_{i2}=1.2	41.961	42.119	42.137
r_{i3}=1.3	41.978	41.983	42.059
r_{i4}=1.4	42.0	41.978	42.005
r_{i5}=1.5	42.023	41.986	41.865
r_{i6}=2.0	41.787	41.738	41.598

Figure 9. Optimized sphere packings: a) 450 spheres with radius 1 and 23 spheres of radius 1.3; b) 475 spheres with radius 1 and 2 spheres of radius 2.0



(a) (b)

Figure 10. The porosity distribution for different replacement volume $\eta^{(s)}$, $s = 1,2,3$ and radii r_{ik}, $k = 1,\dots,6$



In this version of the scenario, we also observe an extreme behavior of porosity depending on the relative radius of the replacing large particles.

DISCUSSION

When applied to the above-considered cases of controlling the properties of agglomerated products (pellets and briquettes) by changing the granulometric composition, the results obtained make it possible to qualitatively correctly describe the dynamics of changes in their physical and mechanical properties, including porosity.

In particular, for iron ore concentrates pelletization it is clear that with the addition of 10% of the coarse fraction of concentrate K2 to the fine concentrate K1, the strength of the fired pellet increased, which corresponds to a decrease in its porosity. From the data in Table 3 it follows that when the radius of the added particles is close to 3, the porosity decreases when 10 such particles are added from 0.4383 to 0.4352.

For the coke fines briquetting, the average particle size of coke briquette No.1 is 1.2 mm (80% of particles), and briquette No.2 is 0.3 mm (80% of particles) as follows from Figure 2. When the particle radius of the added spheres is 4 and their number is 20, there will be a decrease in porosity from 0.4743 to 0.4383, which is consistent with an increase in the density of the coke briquette during the transition from coke breeze crushed in a roller crusher to material double pushed through the shearing plate of the extruder (briquette No.2).

The obtained results made it possible for the first time to establish the extreme nature of the dependence of porosity on the number of added spheres with relative values of the radii of the added spheres in the range from 3 to 5. With an increase in the number of added spheres, porosity initially increases and then monotonically decreases. At the same time, the maximum porosity values are lower than when adding 5% of larger spheres (with radii from 6 to 15).

As can be seen from Figure 6 maximum porosity values (larger than 0.6) can be achieved by adding 5% particles with radii from 12 to 15 radii of the original particles. With an increase in the number of added spheres with such radii, the porosity of the briquette decreases to 0.5. The approach proposed in this article will avoid unnecessary costs for optimizing the amount of added material and quantify the expected partial changes in porosity. Recall that it is the porosity in the end, all other things being equal, that determines the degree of reducibility of the agglomerated products (pellets and briquettes).

Modeling the behavior of porosity depending on the size and proportion of replacement particles also revealed the nonlinear nature of this dependence. As shown in Figure 10, the nature of the dependence of maximum porosity on the number of replacement particles at a fixed radius ratio changes, starting from a radius ratio of 1.5. As the proportion of replacement particles increases, the porosity first increases and then decreases (at $\eta^{(3)} = 20\%$). When the ratio of the radii of the replacement and original particles is equal to 2, in this case a minimum of porosity is observed.

The nonmonotonic nature of the change in porosity depending on the ratio of particle radii was also described in paper (Vasant et al., 2020), in which the material deposition process was simulated using the particle method. When studying the effect of the particle size ratio on the porosity of a material with a particle radius ratio in the range from 1:1 to 1:5, it was found that the porosity decreases with increasing size ratio in the range from 1:1 to 1:1.5, while the minimum porosity is 31.92% at a ratio of 1:1.5. Then, as the ratio increases from 1:1.5 to 1:5, the porosity also increases (Vasant et al., 2020).

Figure 7 shows that when more than 10 more spheres of the second fraction are added, the porosity values of the modified briquette approach asymptomatic values (0.5- 0.6) at relative radii in the range from 7 to 11 and remain almost constant at large radii. The establishment of such dependencies will also eliminate unnecessary costs for conducting research to optimize the optimal particle sizes of the added fraction.

Thus, an effective algorithm has been obtained for predicting qualitative changes in the physical and mechanical properties of briquettes when the granulometric composition of the briquetted mixture changes. The algorithm allows you to determine the optimal level of additions and particle size of the added coarse fraction to achieve the required level of metallurgical properties of briquettes (mechanical strength, porosity, reducibility). Optimizing the granulometric composition of the briquetted material will reduce the costs of preparing the briquette charge, expensive binders and heat treatment of raw briquettes.

The computational experiments were designed for the case where each of the sets I_{i0}, I_{ik} include only one type of radius. However, it is not hard to verify that the model (1)-(4) and the heuristic algorithm remain valid for the case where I_{i0}, I_{ik} include different radii, such that mixtures of spheres can be considered in the definition of the sets I_{i0}, I_{ik} . In this case, it is possible to model the actual granulometric composition of the agglomerated material.

CONCLUSION

In this paper packing spherical particles was considered. However, in many applications more sophisticated shapes arise. Considering, e.g., ellipsoidal (Septiawan et al., 2016), polyhedral or irregular (Pankratov et al., 2020; Romanova et al., 2020) shapes for the particles is an interesting area of future research. Throughout the paper it was implicitly assumed that the particles are rigid, i.e., do not change their shapes under pressure. Considering soft particles allows more realistic modelling of qualitative changes in physical and mechanical properties. Corresponding modelling and optimization tools one can find in Litvinchev et al. (2022) and Romanova et al. (2023). Lagrangian techniques (Litvinchev, 2007; Litvinchev et al., 2010; Manshahia et al., 2023) can be used for the large-scale nonlinear optimization problem (1)-(4) to use structural properties of the original model. Some results in these directions are on the way.

The results obtained open up new opportunities for optimizing the placement of fine-grained materials in the charge of metallurgical furnaces and units, leading to a reduction in energy costs and, accordingly, emissions during the firing of the sinter charge and pellets, during the smelting of cast iron and steel and the production of direct reduced iron.

A detailed consideration of optimizing the charge layer in blast furnaces, steel-smelting and ferroalloy furnaces and direct reduction reactors will be the subject of the following publications by the authors. Different particles shapes and their compressibility will also be considered.

The paper discusses basically the results obtained by mathematical modeling. Comparing modeling results with those obtained by real world experimentation is an interesting area for future research.

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CONFLICTS OF INTEREST

We wish to confirm that there are no known conflicts of interest associated with this publication and there has been no significant financial support for this work that could have influenced its outcome.

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