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# DETERMINING EFFICIENT VALUES FOR THE THERMOPHYSICAL PROPERTIES OF BULK MATERIALS

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***Розроблено методику визначення ефективних теплофізичних властивостей сипких матеріалів різного гранулометричного та матеріального складу, що базується на поєднанні дискретного і континуального уявлень про середовище. Сформульовано задачу механотермічного стану циліндричного шару сипкого матеріалу для визначення його ефективних теплофізичних властивостей. На базі дискретно-континуальних уявлень про сипке середовище запропоновано підхід та розроблено методику розв'язання поставленої задачі. Розроблено алгоритм визначення ефективних значень теплофізичних властивостей сипких матеріалів. Числову реалізацію розробленої методики виконано з використанням вільно відкритого програмного забезпечення (LIGGGHTS, ParaView). Пропонована методика дає змогу визначити ефективні значення теплофізичних властивостей сипкого матеріалу (насипної густини, ефективного коефіцієнта теплопровідності та ефективного значення ізобарної масової теплоємності) довільного матеріального й гранулометричного складу. У цьому разі потрібне проведення мінімального обсягу складних і витратних експериментальних досліджень з наступним числовим моделюванням процесу механотермічного стану досліджуваного сипкого матеріалу. При цьому істинні фізичні властивості можна брати з довідників. На прикладі модельного матеріалу визначено ефективні теплофізичні властивості сипких матеріалів за різного гранулометричного складу та проведено верифікацію розробленої методики. Встановлено, що дані розрахунків ефективної теплопровідності за розробленою методикою відрізняються від даних, отриманих за осередненими теоретичними залежностями, в межах 0,8–9,0 %. Результати дослідження є корисними для числового аналізу в континуальному наближенні теплових режимів процесів та обладнання, де застосовуються сипкі матеріали***

***Ключові слова:** сипкий матеріал, дискретна і континуальна моделі, ефективні теплофізичні властивості, матеріальний і гранулометричний склад*

## 1. Introduction

Bulk materials, specifically grainy and granulated, have become common in many industries, particularly in the chemical, metallurgical, thermal power, construction, food, electronic.

These materials are used as fuel, raw materials, semi-finished goods, and finished products. Owing to the wide range of unique properties, such materials are applied to create composite materials for different purposes [1, 2]. In this case, bulk materials in technological and auxiliary equipment, especially during transportation and processing, are involved in various processes: mechanical, hydromechanical, thermal, mass transfer, chemical, as well as their combinations.

Development of the effective processes to process bulk materials, as well as to treat them, implies the necessity of data or methods for determining certain properties of these materials, one of the most essential among them are the thermal-physical properties. These properties are of special importance when designing equipment for obtaining and processing of bulk materials, as well as their transportation, dispensing, etc. This is critically important for determining energy-efficient parameters for equipment and its operation modes [3].

The thermal-physical properties of materials primarily include density, thermal conductivity, heat capacity and temperature conductivity. However, given that for many substances the true thermal-physical properties are known [4], for bulk materials it is typically necessary to calculate appropriate effective properties [3]. In a general case, the specified properties depend on the qualitative and quantitative composition of a material. In addition, these properties depend on the nature of interaction between components, and it is very difficult or even impossible to fully take them into consideration in the analytical determination of their values [5, 6].

Therefore, it is a relevant task to develop new methods for predicting effective thermal-physical properties for bulk materials of various material and granulometric composition in order to minimize volumes of complex and expensive experimental studies.

## 2. Literature review and problem statement

Determining effective values for the thermal-physical properties of bulk materials, in contrast to values for optical, electric, magnetic, or chemical properties [3, 5, 9], has not been much addressed by research. In this case, studies in recent years have mainly dealt with bulk nanomaterials whose properties differ significantly from traditional bulk materials with macroscopic particles [10, 11].

To determine the effective values of the thermal-physical properties of bulk materials, both experimental [12] and theoretical methods [3, 5, 6] are applied, which are based on analytical dependences and solving inverse problems [13].

Specifically, paper [12] describes experimental installations for examining an effective coefficient of thermal conductivity and specific electric resistance of granulated carbon-containing materials the size of up to 15 mm in the temperature range to 1,300 K. The paper reports results of experimental study into temperature dependences of the coefficient of thermal conductivity and specific electric resistance of granulated carbon materials of varying fractional and structural composition. The authors estimated error of the experimental research, which, for the coefficient of thermal conductivity, does not exceed 12 %, and for the specific electrical resistance, 15 %. The paper also provides an example of applying the results from measurements of the properties of physical quantities for a numerical analysis of the thermal-electric condition of graphite furnaces in order to improve their energy efficiency. The disadvantage of the approach is the need to perform additional experimental research if there is a change in the fractional and structural composition of bulk material.

Article [13] considered a procedure to solve numerically the inverse coefficient problem on thermal conductivity, which makes it possible to restore the effective thermal-physical properties at the same time. The authors developed a programming code to solve the inverse coefficient problem on thermal conductivity for determining the coefficient of thermal conductivity and mass isobaric heat capacity of bulk carbon materials. In this case, they employed experimental data from a quasi-stationary method of cylindrical sphere or coaxial cylinders. Even though this approach makes it possible to define the heat capacity additionally, it requires a significant volume of experimental research into bulk material.

Thus, the unresolved issues related to determining the thermal-physical properties of bulk materials include the minimization of volumes of experimental research that is known to require significant resources.

At the same time, theoretical methods that are based on analytical dependences [3, 5, 6] have significant limitations. These methods are used mainly for monodisperse materials and do not take into consideration contact effects between the particles of a bulk material.

A variant that could overcome these difficulties is an alternative approach based on mathematical modeling of the mechanical-thermal behavior of bulk materials in discrete continual approximation. This should significantly accelerate and reduce the cost of obtaining relevant results.

Therefore, a promising field of research includes:

– development of an algorithm for determining effective values for thermal properties, which would not require complex and expensive experimental research;

– development of appropriate numerical models and their validation.

## 3. The aim and objectives of the study

The aim of this study is to devise a procedure for determining effective values for the thermal properties of bulk materials based on discrete-continuum representations of bulk environment using the true physical properties. This would make it possible to apply continual models for numerical simulation of thermal modes of processes and equipment where bulk materials are involved.

To accomplish the aim, the following tasks have been set:

– to state the problem on determining effective thermal-physical properties of bulk materials;

– to devise a procedure and an algorithm for determining effective values of the thermal-physical properties of bulk materials;

– to determine effective thermal-physical properties of bulk materials for different granulometric composition using an example of model material;

– to verify the procedure.

## 4. Methods to study the thermal-physical properties of bulk materials

Underlying the procedure for determining effective thermal-physical properties of bulk materials is the numeric solution to such a problem. Let there be a cylindrical volume of diameter $d$ and height $2\delta$, which is first filled with particles of a bulk material to the state of mechanical equilibrium. At the beginning of the process of equalizing the temperature in the cylinder, its lower part $(0;-\delta)$ is exposed to temperature $T_{cold}$, and the upper – $(0;+\delta)$ – $T_{hot}(T_{hot}>T_{cold})$ (Fig. 1, *a*). Next, there is an adiabatic process of equalizing the temperature for the height of the cylinder. As a result, we obtain the equilibrium temperature $T_m$ and time $\tau_{est}$, over which this temperature was established (Fig. 1, *b*).

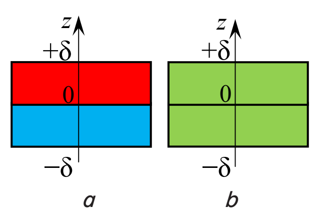



Fig. 1. Diagram of heat transfer between granules in a layer of bulk material: *a* – at the beginning of the process; *b* – balanced state

In this case, it is believed that the bulk material particles have spherical shape, and their physical properties are considered to be isotropic.

At the first stage of calculations, we simulate the mechanical process of filling a cylindrical layer (Fig. 1) with the particles of a bulk material of different granulometric composition under the action of gravitational forces to the state of mechanical equilibrium. The specified procedure is performed by solving a system of discrete equations based on a discrete element method (DEM) in the form [14–19]:

$$\begin{cases} m_i \dfrac{d\mathbf{v}_i}{d\tau} = m_i \mathbf{b} + \sum_{j=1}^{k} \mathbf{F}_{ij}; \\ I_i \dfrac{d\omega_i}{d\tau} = \sum_{j=1}^{k} \left( \mathbf{T}_{ij} + \mathbf{M}_{ij} \right), \end{cases} \quad (1)$$

where $m_i$ is the mass of the $i$-th particle, kg; $\tau$ is the time, s; $i$ is the index of a particle relative to which the system of equations (1) is considered; $\mathbf{v}_i$ is the vector of linear velocity of the center of mass of the particle, m/s; $I_i$ is the moment of inertia, kg·m$^2$; $\omega_i$ is the vector of angular velocity, rad/s; $\mathbf{b}$ is the vector of mass strength, N/kg; $\mathbf{F}_{ij}$ is the vector of the external force acting on particle $i$ through a contact with particle $j$, N; $j$ is the index of the particle that interacts with particle $i$; $k$ is the number of particles that are in contact with particle $i$; $\mathbf{T}_{ij}$ is the external torque associated with the contact interaction between particles $i$ and $j$, N·m; $\mathbf{M}_{ij}$ is the momentum of rolling resistance, N·m.

Calculations that are based on the system of equations (1) are carried out using the known values for mechanical properties of granules in a bulk material: $E$, $\nu$, $e$, $\mu_s$, $\mu_r$, $\rho$.

Next, we calculate heat transfer in the cylinder filled with a bulk material with known true values for the thermal-physical properties of granules: $c_p$, $\lambda$, $\rho$. A discrete equation of heat transfer for a bulk environment, consisting of individual particles, takes the form [20]

$$m_{pi}c_{pi}\frac{dT_{pi}}{d\tau}=\sum_{\text{contacts } i-j}\dot{Q}_{pi-pj}, \tag{2}$$

where $m_{pi}$ is the mass of the $i$-th particle, kg; $c_{pi}$ is the heat capacity of the $i$-th particle, J/(kg·K); $T_{pi}$ is the absolute temperature of the $i$-th particle, K; $\dot{Q}_{pi-pj}=h_{ci-j}\Delta T_{pi-pj}$ is the amount of heat that is transmitted through contacts between particles $i$ and $j$, J/s(W);

$$h_{ci-j}=\frac{4\lambda_{pi}\lambda_{pj}}{\lambda_{pi}+\lambda_{pj}}\sqrt{A_{contact\ i-j}}$$

is the coefficient of heat transfer between particles through their contacts, W/K; $\lambda_{pi}$ is the coefficient of heat conductivity of the $i$-th particle, W/(m·K); $A_{contact\ i-j}$ is the area of contact between particles $i$ and $j$, m$^2$.

Magnitude $\dfrac{\sum_{\text{contacts } i-j}\dot{Q}_{pi-pj}}{V_{pi}}$ (W/m$^3$) is the divergence of density of heat flow of the $i$-th particle, where $V_{pi}$ is the volume of the $i$-th particle, m$^3$. Therefore, to determine the power of the heat flow of the bulk material particles, for example, at the top of the cylinder (Fig. 1), one can use a simple summation

$$N=\sum_{k=1}^{K}\left(\sum_{\text{contacts } i-j}\dot{Q}_{pi-pj}\right)_k, \tag{3}$$

where $K$ is the number of particles in a bulk material.

The calculation of effective values $a$, $\lambda$, $c_p$ employs the analytical solution to the non-stationary equation of thermal conductivity for a half of the unlimited plate under the boundary conditions of first order and the adiabatic condition in the middle of the plate in continual approximation.

A one-dimensional equation of the linear nonstationary thermal conductivity of solid medium takes the form

$$\frac{\partial T}{\partial\tau}=a\frac{\partial^2 T}{\partial z^2}, \tag{4}$$

where $T$ is the absolute temperature, K; $\tau$ is the time, s; $a=\dfrac{\lambda}{c_p\rho}$ is the temperature conductivity, m$^2$/s; $\lambda$ is the coefficient of thermal conductivity, W/(m·K); $c_p$ is the mass isobaric heat capacity, J/(kg·K); $\rho$ is the density, kg/m$^3$; $z$ is the longitudinal coordinate, m.

Initial conditions for (4):

$$T(z)\big|_{\tau=0}=T_0, \tag{5}$$

where $T_0$=$T_{hot}$ is the initial temperature, K.

Boundary conditions (4) for $\tau$>0:

$$\left.\frac{dT}{dz}\right|_{z=\pm\delta}=0, \tag{6}$$

$$T\big|_{z=0}=T_c, \tag{7}$$

where $T_c$ is the temperature of the wall (or balanced temperature $T_m$), K.

An analytical solution by Fourier (4) to (7) by Lykov [21] for determining a temperature distribution takes the form

$$T(z,\tau)= \\ =T_c+(T_0-T_c)\sum_{n=1}^{\infty}(-1)^{n+1}\frac{2}{\mu_n}\cos\left(\mu_n\frac{z}{\delta}\right)\exp\left(\mu_n^2\text{Fo}\right), \tag{8}$$

where

$$\mu_n=(2n-1)\frac{\pi}{2};$$

$\delta$ is half the height of the cylinder, m;

$$\text{Fo}=\frac{a\tau}{\delta^2}$$

is the Fourier number.

By differentiating (8), one can obtain a distribution of the temperature gradient in the half-plate

$$\frac{dT(z,\tau)}{dz}=(T_0-T_c)\sum_{n=1}^{\infty}(-1)^{n}\frac{2}{\delta}\sin\left(\mu_n\frac{z}{\delta}\right)\exp\left(\mu_n^2\text{Fo}\right). \tag{9}$$

Hence the distribution of density of heat flow is found from formula

$$q(z,\tau)=-\lambda\frac{dT(z,\tau)}{dz}. \tag{10}$$

The considered procedure for determining effective thermal-physical properties of bulk materials (1) to (10) does not imply consideration of heat exchange through convection and radiation.

## 5. The algorithm for determining effective values of the thermal-physical properties of bulk materials

An algorithm for solving the stated problem can include the following:

1) Solve a system of equations (1) and model the mechanical process of filling a cylindrical layer (Fig. 1) with the particles of a bulk material of different granulometric composition to the state of mechanical equilibrium under condition of the same temperature. Determine the bulk density of a bulk material layer from formula

$$\rho_{bulk} = \frac{\sum_{m=1}^{M} \rho_m N_m V_m}{2\delta A}, \qquad (11)$$

where $\rho_m$ is the true density of granules, kg/m$^3$; $A$ is the area of base of the cylinder, m$^2$; $2\delta$ is the height of the cylinder, m; $M$ is the number of dimensions of particles in the granulometric composition of a bulk material; $N_m$ is the number of particles of the $m$-th size, m$^3$; $V_m = \frac{4}{3}\pi r_m^3$ is the volume of particles of the $m$-th size, m$^3$; $r_m$ is the radius of particles of the $m$-th size, m.

Formula (11) implies its application for both the mono- and polydisperse layer (for the same or different diameters of particles). Regarding the fractional composition of the examined model mixtures, its structure is given below in the text (Fig. 3, 5, 6).

2) Assign to the top half of the cylinder (Fig. 1*a*) temperature $T_{hot}$, to the bottom – $T_{cold}$. Solve a nonstationary problem on thermal conductivity (2) and model the adiabatic process of equalizing the temperature in the cylindrical layer of a bulk material and plot diagrams of change in the temperature of particles (a discrete environment) depending on the $z$ coordinate and time $T^D(z,\tau)$, $\tau<\tau_{est}$. Determine the power of heat flow of the bulk material particles in the upper and lower parts of the cylindrical layer of a bulk material from formula (3) for time $\tau<\tau_{est}$.

3) Derive the effective value for a temperature conductivity coefficient $a_{eff}$ of continual environment by building the plot $T(z,\tau)$ (approximating function, equivalent to $T^D(z,\tau)$, according to formula (8), using the condition $\max\limits_{[0;+\delta]} R^2$. Here

$$R^2 = 1 - \frac{\sum_{i=1}^{N} \left(T_i^D - T_i\right)^2}{\sum_{i=1}^{N} \left(T_i^D - \bar{T}^D\right)^2}$$

is the coefficient of determination; $N$ is the number of particles over interval $[0; +\delta]$; $T_i^D$ is the temperature of particles in a bulk material over interval $[0; +\delta]$, determined based on the solution to discrete equation (2), K.; $T_i$ is the continual field temperature over interval $[0;+\delta]$, obtained from (8), K;

$$\bar{T}^D = \frac{1}{N}\sum_{i=1}^{N} T_i^D$$

is the arithmetic mean, K.

Determine the temperature gradient $\mathrm{grad}T\big|_{\substack{z=0+\\ \tau<\tau_{est}}}$ from formula (9).

4) Determine for time $\tau<\tau_{est}$:

density of the heat flow from formula

$$q(0,\tau) = \frac{N(\tau)}{A}, \qquad (12)$$

where $N(\tau)$ is the power of heat flow of the bulk material particles in the upper

half of a cylindrical layer (Fig. 1), determined from formula (3), W; $A=\pi R^2$ is the area of base of the cylinder, m$^2$;

– effective coefficient of thermal conductivity (10)

$$\lambda_{\mathrm{eff}} = -\frac{q(0,\tau)}{\mathrm{grad}T\big|_{\substack{z=0+\\ \tau<\tau_{est}}}}; \qquad (13)$$

– effective value for the isobaric mass heat capacity

$$c_{p\ \mathrm{eff}} = \frac{\lambda_{\mathrm{eff}}}{a_{\mathrm{eff}}\rho_{\mathrm{bulk}}}. \qquad (14)$$

The described algorithm (11) to (14) for determining effective values for the thermal-physical properties of bulk materials is appropriate to implement using DEM.

## 6. Results of numerical study into determining the effective thermal-physical properties of bulk materials. Verification of the procedure

Determining effective values for the thermal-physical properties of bulk materials employs the open source programming code LIGGGHTS [22], built on DEM [14–20]. In this case, to simplify the mathematical notation of the statics and dynamics of a bulk medium, granules are accepted to be spherical particles with their corresponding equivalent diameters according to the granulometric composition.

Determining effective values for the thermal-physical properties of a bulk material was performed using an example of model material of different granulometric composition.

The estimation values for true physical properties of the model material are as follows:

– modulus of elasticity $E$=5.0 MPa;
– Poisson's ratio $\nu$=0.45;
– coefficient of restitution $e$=0.7;
– coefficient of slipping friction $\mu_s$=0.05;
– coefficient of rolling friction $\mu_r$=0.0;
– density $\rho$=2,000 kg/m$^3$;
– coefficient of thermal conductivity $\lambda$=5 W/(m·K);
– mass isobaric heat capacity $c_p$=500 J/(kg·K).

Results from numerical studies into mechanical-thermal state of the cylindrical layer of a bulk environment based on the discrete and continual models are shown in Fig. 2–6. To visualize the dynamics of physical fields in the course of the adiabatic equalizing of temperature in the layer of a bulk material (Fig. 2, 3), we used files in the standard *.vtk and the free open source graphic package for interactive visualization ParaView [23].

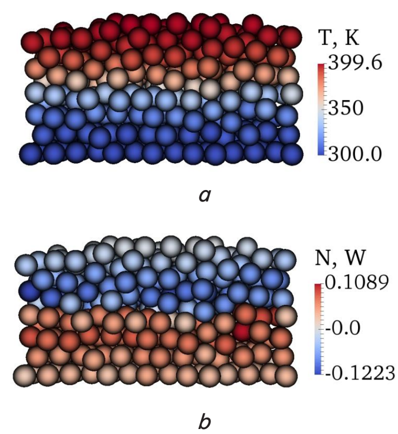
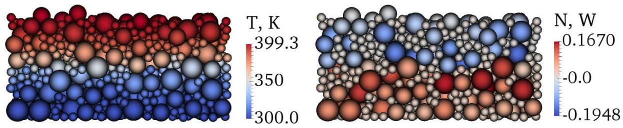
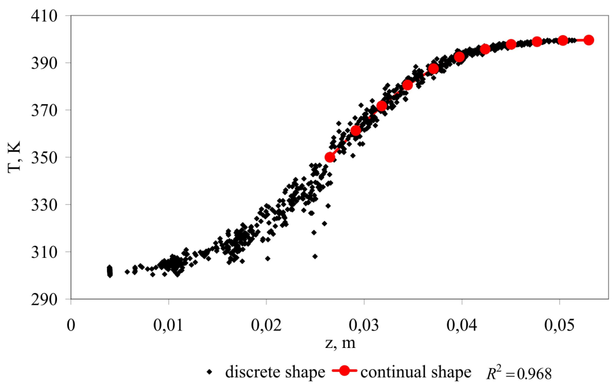



Fig. 2. Results of numerical simulation of heat transfer between particles of a bulk material in the course of the adiabatic equalizing of temperature under condition $\tau$=40 s; $d$=8 mm (100 %): *a* – temperature, K; *b* – power of heat flow

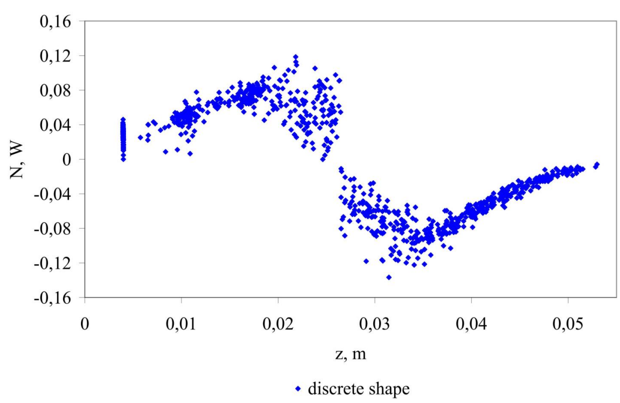



*a* *b*

Fig. 3. Results of numerical simulation of heat transfer between particles of a bulk material in the course of the adiabatic equalizing of temperature under condition $\tau$=40 s; *d*=4 mm (30 %), *d*=8 mm (40 %), *d*=10 mm (30 %): *a* — temperature, K; *b* — power of heat flow




*a*




*b*

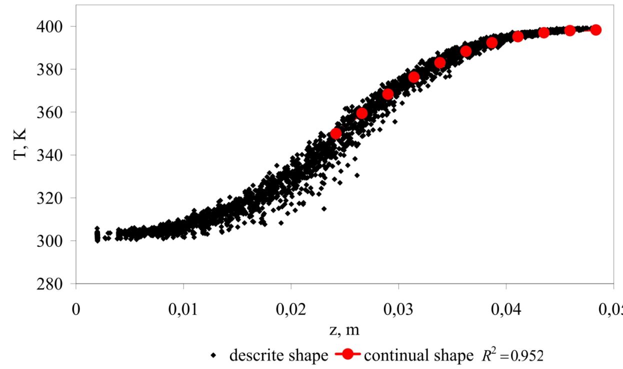
Fig. 4. Results of calculation of heat transfer between particles of a bulk material in the course of the adiabatic equalizing of temperature ($\tau$=40 s); for granulometric composition *d*=8 mm (100 %): *a* — temperature field (discrete and continual shapes); *b* — power of heat flow of particles (discrete shape)

To verify the proposed procedure, we applied formulae for determining effective values for the mixtures conductivity ratios by Zamotrinska [24] and Dulnev [25]

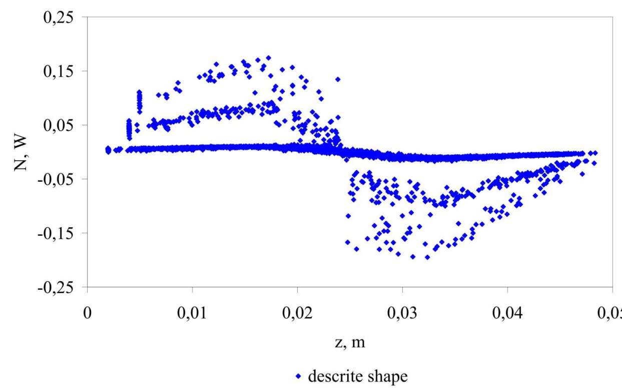
$$\lambda_{\text{eff}} = \lambda\left(1 - \frac{1-\alpha}{1/(1-v) - \alpha/3}\right), \tag{15}$$

$$\lambda_{\text{eff}} = \lambda\left(C^2 + v(1-C)^2 + \frac{2vC(1-C)}{vC+1-C}\right), \tag{16}$$

where $v = \lambda_{\text{air}}/\lambda$; $\lambda_{\text{air}}$ is the coefficient of air thermal conductivity, W/(m·K); $\lambda$ is the true coefficient of thermal conductivity of a bulk material, W/(m·K)); $\alpha$ is the volumetric share of air in a bulk material; $\beta$ is the volumetric share of particles in a bulk material; *C* is the parameter for a bulk material that is determined from equation $2C^3 - 3C^2 + 1 = \beta$.




*a*




*b*

Fig. 5. Results of calculation of heat transfer between particles of a bulk material in the course of the adiabatic equalizing of temperature ($\tau$=40 s) for the polydisperse granulometric composition *d*=4 mm (30 %), *d*=8 mm (40 %), *d*=10 mm (30 %): *a* — temperature field (discrete and continual shapes); *b* — power of heat flow of particles (discrete shape)

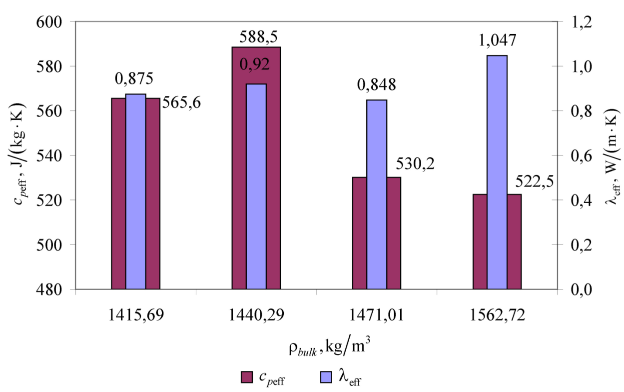



Fig. 6. Results from calculating effective values for the thermal-physical properties of a bulk material depending on granulometric composition: *d*=8 mm (100 %) — $\rho_{bulk}$=1,415.69 kg/m$^3$; *d*=10 mm (100 %) — $\rho_{bulk}$=1,440.29 kg/m$^3$; *d*=6 mm (100 %) — $\rho_{bulk}$=1,471.01 kg/m$^3$; *d*=4 mm (30 %), *d*=8 mm (40 %), *d*=10 mm (30 %) — $\rho_{bulk}$=1,562.72 kg/m$^3$

Results of comparison are given in Table 1 and shown in Fig. 7.

Table 1

Comparison of results from calculating effective values for the coefficient of thermal conductivity of a bulk material

| Calculation technique | $d$=6 mm, β=0.736 | $d$=8 mm, β=0.708 | $d$=10 mm, β=0.722 | $d$=4 mm (30 %), $d$=8 mm (40 %), $d$=10 mm (30 %), β=0.781 |
|---|---|---|---|---|
| $\lambda_{eff}$ (W/(m·K)), procedure (1) to (14) | 0.848 | 0.878 | 0.921 | 1.047 |
| $\lambda_{eff}^{(15)}/\delta\lambda$ (W/(m·K))/%), formula (15) | 0.989/16.72 | 1.101/25.45 | 1.045/13.46 | 0.811/22.54 |
| $\lambda_{eff}^{(16)}/\delta\lambda$ (W/(m·K))/%), formula (16) | 0.597/29.54 | 0.668/23.86 | 0.632/31.33 | 0.485/53.64 |
| $\lambda_{eff}^{m}/\delta\lambda$ (W/(m·K))/%), mean from formulae (15), (16) | 0.793/6.49 | 0.885/0.79 | 0.838/9.01 | 0.648/38.11 |

*Note:* $\delta\lambda = \frac{\lambda_{eff} - \lambda_{eff}^{(15)}}{\lambda_{eff}} 100, \ \lambda_{eff}^{m} = \frac{\lambda_{eff}^{(15)} + \lambda_{eff}^{(16)}}{2}$.

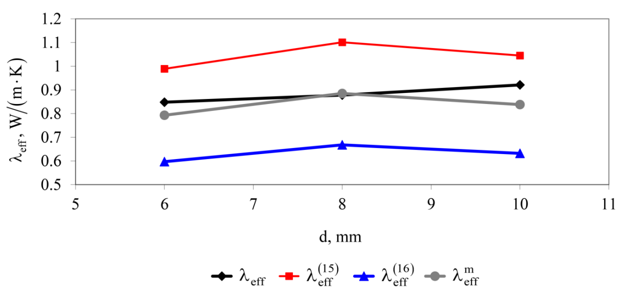



Fig. 7. Results from calculating effective values for the coefficient of thermal conductivity of a monodisperse bulk material depending on the diameter of spherical granules

In contrast to equation (2), formulae (15), (16) do not implicitly take into consideration the granulometric composition and contact pairs with a direct interaction between the particles of a bulk material with a certain thermal resistance. These are the factors that significantly influence the effective value for a coefficient of thermal conductivity in a discrete system.

It follows from the verification results that data from the calculations of effective thermal conductivity based on the developed methodology (1) to (14) differ from those data that were obtained based on the averaged theoretical dependences (15), (16), within 0.8 9.0 %. Given the fact that the bulk density of a bulk material is defined, when applying the presented procedure, precisely, then the estimation of error in determining the effective isobaric mass heat capacity must not be worse than the effective coefficient of thermal conductivity.

## 7. Discussion of results of numerical modeling of efficient values for the thermophysical properties of bulk materials

When determining effective thermal-physical properties of a bulk material, the cylindrical volume, filled with it, must be taken under condition that its diameter is not less than 20 magnitudes of the equivalent size of particles of the largest faction. In this case, the ratio of its height to diameter should vary from 0.5 to 1.5.

An analysis of the results obtained has shown that the power of heat flow depends on the size of particles in the layer of a bulk material (see Fig. 3, *b,* 5, *b*). In this case, there is a clear delayering of the layer of a bulk material for the magnitude of power of the heat flow depending on the particles' size. Thus, a polydisperse bulk material is characterized by a greater heterogeneity of temperature (Fig. 5, *a*) compared with a monodisperse material (Fig. 4, *a*).

It is shown that an increase in the size of spherical particles in a monodisperse bulk model material from 6 mm to 10 mm leads to an increase in effective coefficient of thermal conductivity by 8.6 %, while the isobaric mass heat capacity, on the contrary, reduces by 11.0 % (Fig. 6).

The benefits of our study include:

– the proposed procedure enables determining effective values for the thermal-physical properties of a bulk material (bulk density, effective coefficient of thermal-conductivity and effective value for the isobaric mass heat capacity) of any material and granulometric composition. This makes it possible to perform a minimum volume of complex and expensive experimental studies, replacing them with numerical simulation of the process of the mechanical-thermal state of the examined bulk material. In this case, true physical properties can be taken from reference books [26];

– consideration of the contact thermal resistance between particles of a bulk material;

– the numerical implementation of the developed procedure was performed using the free open source software (LIGGGHTS, ParaView).

The drawbacks of our research include:

– the considered procedure for determining effective thermal-physical properties of bulk materials does not imply consideration of heat exchange through convection and radiation, therefore its use is limited to the level of temperatures close to the ambient temperature;

– the application of the simplest spherical shape of equivalent diameter for granules (particles) of a bulk material.

Results of our study are useful for numerical analysis of thermal modes of processes and equipment in the continual approximation, where bulk materials are used; they continue earlier studies [12, 13, 19, 27, 28].

The further research is planned to address the consideration of heat transfer through convection and radiation for predicting effective thermal-physical properties at high temperatures and for the shape of granules that differs from spherical.

## 8. Conclusions

1. We have stated a problem on the mechanical-thermal state of a cylindrical layer of a bulk material to determine its

effective thermal-physical properties. In contrast to many experimental approaches, such a problem statement makes it possible to simultaneously investigate two thermal-physical properties: coefficient of thermal conductivity and the isobaric mass heat capacity.

2. Based on the discrete-continuum representations of a bulk environment, we have formulated a theoretical base for the methodology of the stated problem and developed the algorithm for determining effective values for the thermal-physical properties of bulk materials. Provided reference books contain data on true values for the physical properties of the materials, the proposed procedure makes it possible to abandon complex and expensive experimental studies.

3. Based on the devised procedure, we have performed a numerical study into effective values for the thermal-physical properties of bulk materials using an example of model material. It has been shown that an increase in the size of spherical particles in a monodisperse bulk model material from 6 mm to 10 mm leads to an increase in the effective coefficient of thermal conductivity by 8.6 %, while the isobaric mass heat capacity, on the contrary, reduces by 11.0 %.

4. We have verified the devised procedure, which showed convergence between results from calculations and those data that were obtained based on the averaged theoretical dependences within 0.8–9.0 %. This provides a basis for the application of the devised procedure for numerical analysis of thermal modes in the continual approximation of processes and equipment where bulk materials are used.

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## References


1. Chung, D. D. L. (2010). Composite Materials: Science and Applications. Springer, 349. doi: https://doi.org/10.1007/978-1-84882-831-5
2. Mikulenok, I. O. (2012). Klassifikaciya termoplasticheskih kompozicionnyh materialov i ih napolniteley. Plasticheskie massy, 9, 29–38.
3. Mikulenok, I. O. (2013). Determining the Thermophysical Properties of Thermoplastic Composite Materials. International Polymer Science and Technology, 40 (9), 23–28. doi: https://doi.org/10.1177/0307174x1304000905
4. Yaws, C. L. (1999). Chemical properties handbook: physical, thermodynamic, environmental, transport, and health related properties for organic and inorganic chemicals. New York: The McGraw-Hill Companies, 779.
5. Piven', A. N., Novikov, V. V. (1989). Metody rascheta teplo- i temperaturoprovodnosti polimernyh materialov. Kyiv: UMK VO, 108.
6. Lipatov, Yu. S. (Ed.) (1986). Fizikohimiya mnogokomponentnyh polimernyh sistem. Vol. 1-2. Napolnennye polimery. Polimernye smesi i splavy. Kyiv: Nauk. dumka, 376, 384.
7. Djellal, L., Bouguelia, A., Trari, M. (2008). Physical and photoelectrochemical properties of p-CuInSe2 bulk material. Materials Chemistry and Physics, 109 (1), 99–104. doi: https://doi.org/10.1016/j.matchemphys.2007.10.038
8. Katter, M., Zellmann, V., Reppel, G. W., Uestuener, K. (2008). Magnetocaloric Properties of La(Fe, Co, Si)13 Bulk Material Prepared by Powder Metallurgy. IEEE Transactions on Magnetics, 44 (11), 3044–3047. doi: https://doi.org/10.1109/tmag.2008.2002523
9. Kleinke, H. (2010). New bulk Materials for Thermoelectric Power Generation: Clathrates and Complex Antimonides. Chemistry of Materials, 22 (3), 604–611. doi: https://doi.org/10.1021/cm901591d
10. Zehetbauer, M. J., Zhu, Y. T. (Eds.) (2009). Bulk Nanostructured Materials. Wiley, 736. doi: https://doi.org/10.1002/9783527626892
11. Valiev, R. Z., Zhilyaev, A. P., Langdon, T. G. (2014). Bulk Nanostructured Materials: Fundamentals and Applications. Wiley, 470. doi: https://doi.org/10.1002/9781118742679
12. Karvatskii, A. Y., Vasilchenko, G. M., Panov, E. M., Leleka, S. V., Lazariev, T. V., Pedchenko, A. Y., Chirka, T. V. (2019). Thermoelectric Properties of Granular Carbon Materials. Advanced Thermoelectric Materials, 437–467. doi: https://doi.org/10.1002/9781119407348.ch10
13. Karvatskii, A. Ya., Vasilchenko, G. M., Korolenko, K. M., Chirka, T. V. (2017). Renewal of thermal and physical properties of granular materials using the inverse heat conduction problem solution. Visnyk Khmelnytskoho natsionalnoho universytetu. Seriya: Tekhnichni nauky, 4, 159–166.
14. Göncü, F. (2012). Mechanics of granular materials: constitutive behavior and pattern transformation. Ipskamp Drukkers, 144.
15. Rao, K. K., Nott, P. R. (2008). An Introduction to Granular Flow. New York: Cambridge University Press, 490. doi: https://doi.org/10.1017/cbo9780511611513
16. Pöschel, T., Schwager, T. (2005). Computational granular dynamics. Models and algorithms. Springer, 322. doi: https://doi.org/10.1007/3-540-27720-x
17. Ai, J., Chen, J.-F., Rotter, J. M., Ooi, J. Y. (2011). Assessment of rolling resistance models in discrete element simulations. Powder Technology, 206 (3), 269–282. doi: https://doi.org/10.1016/j.powtec.2010.09.030
18. Makse, H. A., Gland, N., Johnson, D. L., Schwartz, L. (2004). Granular packings: Nonlinear elasticity, sound propagation, and collective relaxation dynamics. Physical Review E, 70 (6). doi: https://doi.org/10.1103/physreve.70.061302

19. Karvatskii, A. Y., Lazarev, T. V. (2014). Evaluation of the Discrete Element Method for Predicting the Behavior of Granular Media Using Petroleum Coke as an Example. Chemical and Petroleum Engineering, 50 (3-4), 186–192. doi: https://doi.org/10.1007/s10556-014-9877-y
20. Chaudhuri, B., Muzzio, F. J., Tomassone, M. S. (2006). Modeling of heat transfer in granular flow in rotating vessels. Chemical Engineering Science, 61 (19). 6348–6360. doi: https://doi.org/10.1016/j.ces.2006.05.034
21. Lykov, V. I. (1967). Teoriya teploprovodnosti. Moscow: Vysshaya shkola, 600.
22. LIGGGHTS Open Source Discrete Element Method Particle Simulation Code. Available at: https://www.cfdem.com/liggghts-open-source-discrete-element-method-particle-simulation-code
23. ParaView. An open-source, multi-platform data analysis and visualization application. Available at: http://www.paraview.org/
24. Zamotrinskaya, E. A., Nesterov, V. M., Mihaylova, T. S. (1976). Ob elektroprovodnosti smesey, soderzhashchih komponenty s bol'shoy provodimost'yu. Izvestiya vuzov. Fizika, 9, 117–119.
25. Dul'nev, G. N., Zarichnyak, Yu. P. (1974). Teploprovodnost' smesey i kompozicionnyh materialov. Leningrad: Energiya, 264.
26. Grigor'ev, I. S., Meylihov, E. Z. (Eds.) (1991). Fizicheskie velichiny. Moscow: Energoatomizdat, 1232.
27. Kutuzov, S. V., Buryak, V. V., Derkach, V. V., Panov, E. N., Karvatskii, A. Y., Vasil'chenko, G. N. et. al. (2014). Making the Heat-Insulating Charge of Acheson Graphitization Furnaces More Efficient. Refractories and Industrial Ceramics, 55 (1), 15–16. doi: https://doi.org/10.1007/s11148-014-9648-5
28. Karvatskii, A., Leleka, S., Pedchenko, A., Lazariev, T. (2016). Numerical analysis of the physical fields in the process of electrode blanks graphitization in the castner furnace. Eastern-European Journal of Enterprise Technologies, 6 (5 (84)), 19–25. doi: https://doi.org/10.15587/1729-4061.2016.83191