



## Article Peculiarities of Calculating the Thermal Conductivity of Moist Autoclaved Aerated Concrete

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**Abstract**: The pore space of autoclaved aerated concretes (ACCs), regardless of their apparent density, is represented by large pores formed as a result of gas formation and fine capillary pores. With the free absorption of liquid moisture, only the capillary pores are filled. Large pores contain vaporair mixture. Considering such a bimodal pore size distribution, it is proposed to determine the thermal conductivity of moist ACC in two stages. First, an inhomogeneous ternary system that consists of a solid skeleton with a fine porous structure containing gas and liquid moisture should be considered. Then a binary system is taken into account, the first component of which is the mentioned ternary system, and the other component of which consists of isolated gas inclusions in large pores. To determine the thermal conductivity were used. The thermal conductivity of the binary system was calculated using well-known formulas. It was found that the results of thermal conductivity calculations based on the proposed two-step method deviate from the experimental data in the range from -7.29 to +5.75%, with an average deviation of -0.71%. With the one-step calculation method (assuming a unimodal pore distribution), the spread of analogous data ranges from -30.72 to -21.98%, with an average deviation of -26%.

**Keywords:** effective thermal conductivity; autoclave aerated concrete; bimodal pore size distribution; modeling of the structure of moist material; theory of generalized conductivity

### 1. Introduction

Aerated concretes are commonly used for exterior walls of buildings. In the dry state, they are characterized by a relatively low value of the effective thermal conductivity, however, during the operation of buildings, the moisture content of ACCs can increase significantly. Thus, in the work [1] on the basis of physical and computational experiments, it was shown that the average moisture content of the ACC slab used for exterior wall of a heated building exceeded the standard (normalised) value 4–5 times. This led to an increase in the thermal conductivity of the material and a deterioration in the thermal insulation of the partition.

One of the reasons for the increased dampness of shielding structures is the simultaneous impact of precipitation and wind on the outer surface of the partition, called wind-driven rain [1–4]. In the course of wind-driven rain the moisture content of the partition outer layer material depends on the intensity and duration of precipitation, as



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**Copyright:** © 2022 by the authors. Licensee MDPI, Basel, Switzerland. This article is an open access article distributed under the terms and conditions of the Creative Commons Attribution (CC BY) license (https:// creativecommons.org/licenses/by/ 4.0/). well as on the characteristics of the pore structure of the material and can increase up to the full capillary saturation [4].

The results of measurements of the pore structure of ACC samples [5–7] showed that, regardless of the apparent density of the samples, there were always two maxima in the differential pore sizes distribution. The analysis of these data shows that the pore space of the samples under consideration consists mainly of fine capillary pores ( $\approx 10^{-7}$  m) and large gas pores ( $\approx 10^{-3}$  m). Large gas pores are formed as a result of using foaming agents or foam for ACC production. Fine pores are incorporated into the solid skeleton surrounding large gas pores. In general, the porosity of ACCs is open. The results of research presented in [8] show that the content of closed pores is only 1.4%, with the total porosity at the level of 62.3%.

In order to illustrate the bimodal pore structure of ACCs, the photos taken with a scanning electron microscope are shown in Figure 1. Samples of two different apparent densities (450 and 600 kg/m<sup>3</sup>) were photographed. Regardless of the differences in the apparent density, both samples show large pores with a diameter close to  $10^{-3}$  m, which are usually enclosed by a microporous skeleton formed by mineral structures. The fine pores of the skeleton, formed together with the solid material, constitute a binary system with a continuous, interpenetrating structure.



**Figure 1.** Large gas pores of ACC samples of different apparent density ( $450 \text{ kg/m}^3$  on the left and  $600 \text{ kg/m}^3$  on the right) enclosed by the microporous skeleton of the material.

With free capillary absorption, liquid moisture fills only fine pores, while large pores are filled with a mixture of vapour and air. According to the authors' own experimental data, the capillary absorption values of the ACC samples of an apparent density of 447–614 kg/m<sup>3</sup> did not exceed half of their porosity. A similar ratio was observed for the ACC samples with the apparent density of 363 and 407 kg/m<sup>3</sup> [9]. It seems, therefore, that the determination of the effective thermal conductivity of moist cellular concretes by computation should be carried out in two stages. First the heterogeneous ternary system consisting of a solid skeleton (1) and fine capillary pores containing gas (2) and liquid moisture (3) should be considered. Next, the binary system, whose first component is the above-mentioned ternary system, and whose other component is isolated gas inclusions at large pores, should be taken into account. Until now, such an approach to calculating the effective thermal conductivity of cellular concrete has not been adopted.

This paper presents a two-step method for calculating the effective thermal conductivity of materials with a bimodal pore size distribution developed by the authors. To determine the thermal conductivity of a heterogeneous ternary system, formulas constructed on the basis of the theory of generalised conductivity in combination with geometric modeling of the structure by transitioning to the unit cell [10] were used. The thermal conductivity of a binary system with insulated gas inclusions was calculated using the known formulas presented in [11]. It was found that the results of the calculations of the thermal conductivity of moist cellular concretes achieved with the proposed method practically agree with experimental values obtained by the authors. Additionally, it was shown that calculation of thermal conductivity of moist cellular concretes using the one-step method presented in [10], which does not take into account the bimodal character of pore distribution of ACCs, gives results much lower than the experimental ones.

# 2. Geometric Model of a Heterogeneous Ternary System and the Dependence to Determine Its Thermal Conductivity

When constructing a geometric model of a ternary system, it is necessary to know the volumetric concentrations of its components  $m_i$ . The cellular concrete sample volume V consists of the solid skeleton volume vs. the pores, and the volume of fine  $V_{sp}$  and large  $V_{bp}$  pores. The volume of the ternary system V' considered in this case is equal to the sum  $V_s + V_{sp}$ . The volume of the solid skeleton vs. the pores can be determined by the pycnometric method, and the volume of fine pores  $V_{sp}$  is assumed to be equal to the volume of the liquid absorbed by a sample of material immersed in water  $V_{sat}$ . The volume of fine pores  $V_{sp} = V_{sat}$  is filled with water with the volume  $V_w \leq V_{sp}$ . As a result, the following values of the volumetric concentrations of the considered components are obtained: solid  $m_1 = V_s/V'$ , liquid  $m_3 = V_w/V' = \psi_w$  ( $\psi_w$ —moisture content of the ternary system) and gas  $m_2 = (V_{sp} - V_w)/V' = P_{sp} - \psi_w$ , where  $P_{sp} = V_{sat}/V'$  is the porosity of the ternary system.

If the volume of the liquid  $V_w$  does not exceed a certain limit value  $V_w'$ , then the liquid is distributed in the porous space in the form of isolated inclusions. This case is described in detail in [11]. In what follows a ternary system for which  $V_w > V_w'$  will be considered. In a general case, the structure of such an arrangement, according to [11,12], can be represented in the form of the eighth part of the unit cell illustrated in Figure 2. Figure 2 shows that the volume of the liquid  $V_w$  covering bars of the solid skeleton with dimension  $\Delta$  can be conditionally divided into two parts of dimensions  $\Delta_x$  and  $\Delta_n$ . It is assumed that, when the pore moisture content changes, the value of  $\Delta_x$  remains constant. The justification for this assumption is given in [11].



**Figure 2.** The eighth part of the unit cell with continuous inclusions of liquid; 1, 2, 3—solid, gas and liquid components, respectively.

The dimension  $\Delta_x$  is related to the volume of the liquid  $V_k$  in the node of the skeleton mesh  $V_k = (\Delta_x - \Delta)^3 + 3\Delta(\Delta_x - \Delta)^2$ . After determining the difference  $(\Delta_x - \Delta) = x$  the dependence  $V_k = x^3 + 3\Delta x^2$  is obtained. After the division of the left and right sides of this equality by the volume of the unit cell  $V = L^3$ , the cubic equation combining the volumetric concentration of the liquid in the mesh node  $\psi_k = V_k/L^3$  with the geometric parameters  $c = \Delta/L$  and  $d = x/L = \Delta_x/L - \Delta/L = c_x - c$  is obtained:

$$\psi_k = d^3 + 3cd^2. \tag{1}$$

The value of *c* depends on the volumetric concentration of the solid skeleton and is determined by the formula [13]

$$c = 0.5 + \sin\left[\frac{\arcsin(2m_1 - 1)}{3}\right].$$
(2)

The volumetric concentration of the liquid in the network node  $\psi_k$  is determined by the formula

$$\psi_k = \psi'_p p_{sp} , \qquad (3)$$

where  $\psi'_p = V_w / V_{sp}$  is the boundary value of pore moisture at which the transition from isolated liquid inclusions to continuous liquid inclusions (and vice versa) takes place. According to [14,15], the value of  $\psi'_p$  depends on *c* and the wetting angle  $\theta$ . For example, at  $\theta = 45^\circ$  we have

$$\psi'_p = \frac{1+8c}{6(1+2c)}.\tag{4}$$

With the known values of  $\psi_k$  and *c* a positive, physically justified, root *d* is determined using formula (1). Then the geometric parameter  $c_x = c + d$ .

The second part of the liquid volume  $V_n = V_w - V_k$  (see Figure 2) is equal to  $V_n = 3(\Delta_n^2 - \Delta^2)(L - \Delta_x)$ . After dividing both sides of this equation by the volume of the unit cell  $V = L^3$ , the quadratic equation is obtained

$$\psi_n = \psi_w - \psi_k = 3(c_n^2 - c^2)(1 - c_x), \tag{5}$$

solving which the geometric parameter  $c_n$  can be found.

In this way, with the known volumetric concentrations of the ternary system components and the assumed wetting angle  $\theta$ , it is possible to determine the parameters of the structure of the geometric model under consideration (Figure 2). For this model, using the procedure described in [10,15], dependencies were constructed that allow to estimation of the effective thermal conductivity of the ternary system at known values of the thermal conductivity of its components  $\lambda_i$  (i = 1, 2, 3).

By dividing the unit cell (Figure 2) with adiabatic planes parallel to the heat flux, a formula was obtained that gives the lower estimate of the thermal conductivity of the ternary system  $\lambda'_a$ :

$$\frac{\lambda'_{a}}{\lambda_{1}} = c^{2} + \nu^{2}(c_{n} - c)^{2} + \frac{2\nu_{2}c(c_{n} - c)}{1 - c + \nu_{2}c} + \frac{2\nu_{1}\nu_{2}c(c_{x} - c_{n})}{\nu_{2}(1 - c_{x}) + \nu_{1}(c_{x} - c) + \nu_{1}\nu_{2}c} + \frac{2\nu_{1}\nu_{2}(c_{x} - c_{n})^{2}}{\nu_{2}(1 - c_{x}) + \nu_{1}c_{x}} + \frac{2\nu_{1}\nu_{2}c(1 - c_{x})}{\nu_{2}(1 - c_{n}) + \nu_{1}(c_{n} - c) + \nu_{1}\nu_{2}c} + \frac{2\nu_{1}\nu_{2}(c_{n} - c)(1 - c_{x})}{\nu_{2}(1 - c_{n}) + \nu_{1}c_{n}} + \nu_{1}\left[\left(1 - c_{n}^{2}\right) - (c_{x} - c_{n})^{2}\right].$$
(6)

where  $\nu_1 = \lambda_2 / \lambda_1$ ,  $\nu_2 = \lambda_3 / \lambda$ ,  $c = \Delta / L$ ,  $c_n = \Delta_n / L$  and  $c_x = \Delta_x / L$ .

By dividing the same unit cell with isothermal planes perpendicular to the heat flux, a formula was obtained determining the upper estimate of the thermal conductivity of the ternary system  $\lambda'_{iz}$ :

As in (6),  $\nu_1 = \lambda_2 / \lambda_1$ ,  $\nu_2 = \lambda_3 / \lambda$ ,  $c = \Delta / L$ ,  $c_n = \Delta_n / \text{Li } c_x = \Delta_x / L$ .

It is easy to establish that Formulas (6) and (7) are transformed from the formula obtained in [15] for isolated inclusions of the liquid. For  $c_n = c_x$  Formulas (6) and (7) are transformed into the form of relationships constructed for the steady distribution of the liquid on the surface of the solid skeleton bars [15]. However, with such a distribution of the liquid, a smooth transition to isolated liquid inclusions is not ensured, and comparative calculations yield significant differences. For example, at the wetting angle  $\theta = 45^{\circ}$  and the pore boundary moisture content  $\psi_p' = 0.417$ , with concentrations of the components of the system  $m_1 = 0.5$ ;  $m_2 = 0.2915$ ;  $m_3 = 0.2085$  and their thermal conductivities  $\lambda_1 = 1.0$  W/(m·K),  $\lambda_2 = 0.03$  W/(m·K),  $\lambda_3 = 0.6$  W/(m·K), the effective thermal conductivity of such a system, determined by formulas (6) and (7), is equal to  $\lambda = 0.4065$  W/(m·K) while, according to formulas from [15], for the steady distribution of the liquid  $\lambda = 0.5455$  W/(m·K). From a physical point of view, the first result, which is 25.5% lower than the other, gives a more accurate estimate.

If the material is dry ( $c_n = c$  and  $c_x = c$ ) Formulas (6) and (7) are transformed into known formulas for a system with two interpenetrating components [11] at adiabatic

$$\frac{\lambda_a}{\lambda_1} = c^2 + \nu (1-c)^2 + 2\nu c (1-c) (\nu c + 1 - c)^{-1},$$
(8)

and isometric division of the unit cell

$$\frac{\lambda_{iz}}{\lambda_1} = \left[\frac{1-c}{c^2 + \nu(1-c^2)} + \frac{c}{c(2-c) + \nu(1-c)^2}\right]^{-1},\tag{9}$$

where  $\nu = \nu_1 = \lambda_2 / \lambda_1$ .

In order to perform calculations according to Formulas (6) and (7) it is necessary to determine the volumetric concentration of the components  $m_i$  and their thermal conductivities  $\lambda_i$ .

The thermal conductivity of the solid component  $\lambda_1$  at the first approximation can be determined by Formulas (8) and (9) in which  $\lambda_1^a$  and  $\lambda_1^{iz}$  are assumed to be equal to the experimental value of the thermal conductivity of dry material  $\lambda_{dry}$ , and then the thermal conductivity of the solid component is calculated by an iterative method with adiabatic  $\lambda_1^a$  and isothermal  $\lambda_1^{iz}$  unit division. For further calculations, the average value  $\lambda_1 = 0.5(\lambda_1^a + \lambda_1^{iz})$  is adopted.

The thermal conductivity of the vapour-air mixture  $\lambda_2$  (gas component) is the sum of the thermal conductivity of dry air  $\lambda_{air}$  and the thermal conductivity of vapour  $\lambda_{ws}$  caused by the diffusion transfer of vapour in the pore space. The first element of the sum is described by the formula [16]:

$$\lambda_{air} = 0.0257[1 + 0.003(t - 20)], \tag{10}$$

where *t* is the temperature,  $^{\circ}$ C.

The other element is determined by the formula presented in the work [11], based on the Krisher relationship [17],

$$\lambda_{ws} = \frac{D}{\mu} \cdot \frac{M}{RT} \cdot \frac{P_{va}}{P_{va} - P_v} \cdot \frac{dP_v}{dt} q_t, \tag{11}$$

where:

*D*—water vapour diffusion coefficient in stationary air,  $m^2/s$ ; *M*—coefficient of resistance of vapour diffusion in the pore space; *M*—molecular weight of water vapour, kg/mol;

*R*—universal gas constant, J/(mol·K);

*T*—water vapour temperature, K;

 $p_{va}$ —total water vapour and air pressure, Pa;

*p*<sub>v</sub>—partial water vapour pressure, Pa;

 $q_t$ —specific heat of evaporation at temperature t, J/kg.

When determining the water vapour diffusion coefficient, the following formula [17] was used

$$D = \frac{2.305 \cdot 10^{-5} p_0}{p_{va}} \left(\frac{T}{273}\right)^{1.81}, p_0 = 101,323 \text{ Pa},$$
(12)

proposed by R. Schirmer in 1938.

The derivative  $\frac{dp_v}{dt}$  can be determined from reference data or from formula [17]

$$\frac{dp_v}{dt} = \frac{2.44314 \cdot 10^6}{\left(234.175 + t\right)^2} \cdot exp\left(\frac{17.08085t}{234.175 + t}\right), \ (0^\circ \le t \le 109.9^\circ \text{C}).$$
(13)

The dependence of the specific heat of evaporation on the temperature after approximation of the reference data is in the form of:

$$q_t = (2.5 - 0.0024t) \cdot 10^6. \tag{14}$$

The water vapour diffusion resistance coefficient  $\mu$  for the continuous gas component, according to [14,18], can be determined by the formula

$$\mu = \frac{m_2}{c_*^4},$$
 (15)

where  $c_*$  should be calculated by formula (2) in which the concentration of the solid component  $m_1$  is replaced by the concentration of the gas component  $m_2$ . For insulated gas inclusions  $\mu = 1.0$  [11].

The thermal conductivity of the liquid component (water)  $\lambda_3$  is determined by the formula obtained after approximation of data from the work [5],

$$\lambda_3 = 0.551 + 0.256 \cdot 10^{-2}t - 0.124 \cdot 10^{-4}t^2.$$
<sup>(16)</sup>

Now, using formulas (6) and (7), it is possible to determine the thermal conductivities  $\lambda_a'$  and  $\lambda_{iz}'$  and their mean value  $\lambda' = 0.5(\lambda_a' + \lambda_{iz}')$ , which is assumed to be the effective thermal conductivity of the ternary system with the volume V' considered at the first stage of calculation. Then the calculation of the binary system can be performed.

#### 3. Calculation of the Binary System

In the binary system with the volume  $V = V' + V_{bp}$  ( $V_{bp}$ —volume of large pores) the first component is the considered ternary system with the volume V', thermal conductivity  $\lambda_1 = \lambda'$  and volumetric concentration  $m_1 = V'/V$ , and the other includes closed large pores with the volumetric concentration  $m_2 = 1 - m_1$ . The thermal conductivity  $\lambda_2$  of the mixture of vapour and air filling large pores is determined by Formulas (10)–(14) with a vapour diffusion resistance coefficient  $\mu = 1$ .

When determining the thermal conductivity of a binary system the following formulas from [11] can be used:

when dividing the unit cell by adiabatic planes

$$\frac{\lambda_a}{\lambda_1} = \frac{\nu - (\nu - 1)\left(1 - m_2^{2/3}\right) \cdot m_2^{1/3}}{\nu - m_2^{1/3}(\nu - 1)},\tag{17}$$

when dividing the unit cell by isothermal planes

$$\frac{\lambda_{iz}}{\lambda_1} = \frac{1 + (\nu - 1)m_2^{2/3}}{1 + (\nu - 1)m_2^{2/3} \cdot \left(1 - m_2^{1/3}\right)},\tag{18}$$

where  $\nu = \lambda_2 / \lambda_1$ .

The average value  $\lambda = 0.5(\lambda_a + \lambda_{iz})$  gives an estimate of the effective thermal conductivity of the moist material with a bimodal distribution of the pore volume by size.

#### 4. Results of the Physical and Computational Experiment

#### 4.1. Results of the Physical Experiment

In order to confirm the accuracy of the proposed method of calculating the thermal conductivity of moist materials with a bimodal pore size distribution, an experiment was carried out using ACC specimens of different apparent density  $\rho$  and equal volume V (24 × 24 × 5 cm), which were cut from masonry units (blocks). Four series were considered, each of which consisted of three specimens of a similar apparent density. Using pycnometry, the density of the solid skeleton  $\rho_s$  was determined, at which its volume concentration  $m_s = \rho/\rho_s$  and porosity of the material  $P = 1 - m_s$  were calculated. Water absorption  $\psi_{sat} = V_{sat}/V$  was determined by immersing the specimens in water. The thermal conductivity of dry  $\lambda_{dry}$  and moist samples  $\lambda_h$  was measured by the stationary method. All measurements were carried out at room temperature  $t \approx 20$  °C. The values of experimental data necessary to calculate the effective thermal conductivity  $\lambda$  of moist materials are given in Table 1.

**Table 1.** Experimental mean values of the apparent density  $\rho$ , absolute skeleton density  $\rho_s$ , water absorption  $\psi_{sat}$ , porosity *P* and thermal conductivity in the dry state  $\lambda_{dry}$  of specimens in four series.

Series nr	ho, kg/m <sup>3</sup>	$ ho_{ m s}$ , kg/m $^3$	$\psi_{sat}$	Р	$\lambda_{dry}$ , W/(m·K)
1	447	1980	0.2924	0.7742	0.1189
2	530	2110	0.3004	0.7488	0.1399
3	577	2204	0.3215	0.7382	0.1496
4	614	2285	0.3451	0.7312	0.1601

#### 4.2. Example of Calculation According to the Two-Step Procedure

The procedure of calculating the thermal conductivity of moist ACCs will be considered based on the data obtained for specimens from the first series with the average apparent density  $\rho = 447 \text{ kg/m}^3$  and the thermal conductivity in the moist state  $\lambda_h = 0.278 \text{ W/(m \cdot K)}$  at the moisture content  $\psi = V_w/V = 0.232$ , which corresponds to the state of saturation with free capillary water absorption.

At the first stage of the calculation, the ternary system with the volume V' is considered, which consists of the volume of the solid skeleton (solid phase) vs. and the volume of fine pores  $V_{sp} = V_{sat}$ . The volumetric concentration of this system is  $m' = (V_s + V_{sat})/V = m_s + \psi_{sat} = 0.5182$ . The volumetric concentrations of the components of the ternary system are: solid phase  $m_1 = m_s/m' = 0.4357$ ; liquid  $m_3 = \psi/m' = 0.4477$  and gas  $m_2 = 1 - m_1 - m_3 = 0.1166$ . The geometric parameter of the solid skeleton c = 0.4572 is calculated by Formula (2). Before determining the geometrical parameters of the liquid component, the value of the wetting angle should be assumed. Taking into account the data from [14,19], a wetting angle equal to  $\theta = 45^{\circ}$  was assumed. In this case, the pore boundary moisture content  $\psi'_p = 0.4055$  calculated on the basis of Formula (4) did not exceed the actual moisture content of the pores  $\psi_p = m_3(1 - m_1) = 0.7934$ . This means that the liquid in the pore space is distributed as a continuous component, and that the geometrical parameters  $c_x$  and  $c_n$  are determined by Formulas (1), (3) and (5), and the thermal conductivity of the system should be calculated by Formulas (6) and (7).

The calculation gave the following values  $c_x = 0.8204$  and  $c_n = 0.7844$ . After performing the iterative procedure described earlier, the thermal conductivity of the solid skeleton  $\lambda_1 = 0.84 \text{ W/(m·K)}$  was determined. The thermal conductivity of the gas component was determined by Formulas (10)–(15) and is  $\lambda_2 = 0.0269 \text{ W/(m·K)}$ . The thermal conductivity of water calculated by Formula (16) is  $\lambda_3 = 0.597 \text{ W/(m·K)}$ . Formula (6) was employed to determine the thermal conductivity of the system for the adiabatic division of the unit cell  $\lambda_a' = 0.4845 \text{ W/(m·K)}$ , whereas Formula (7) was used for the isothermal division of the unit cell  $\lambda_{iz}' = 0.6109 \text{ W/(m·K)}$ . Their average is taken as the estimate of the effective thermal conductivity of the ternary system  $\lambda' = 0.5(0.4845 + 0.6109) = 0.5477 \text{ W/(m·K)}$ .

It should be noted that, if the actual pore moisture content  $\psi_p$  does not exceed the boundary value  $\psi_p'$ , then the liquid is distributed in the porous material in the form of isolated inclusions. Then the thermal conductivity of the system can be determined by the formulas from [14] or by Formulas (6) and (7), taking  $c_n = c$  and determining  $c_x$  from Formula (1), in which the actual moisture should be used  $m_3 = \psi/m'$  instead of the volumetric concentration of the liquid in the node of the network  $\psi_k$ .

In the second stage, calculations are made for a binary system in which the volumetric concentration of the first component is  $m_1 = m' = 0.5182$ , and the thermal conductivity  $\lambda_1 = \lambda' = 0.5477 \text{ W/ (m·K)}$ . The volumetric concentration of the other component (gas) is  $m_2 = 1 - m_1 = 0.4812$ . The thermal conductivity of the vapour-air mixture in closed large pores  $\lambda_2 = 0.0962 \text{ W/(m·K)}$  is calculated by Formulas (10)–(14), assuming that the coefficient of vapour diffusion resistance in closed pores  $\mu = 1$ . The thermal conductivity of the binary system was determined by Formulas (17) and (18), respectively, when the unit cell is divided by adiabatic planes  $\lambda_a = 0.2833 \text{ W/(m·K)}$  and isothermal planes  $\lambda_{iz} = 0.3037 \text{ W/(m·K)}$ . The calculated estimate value of the effective thermal conductivity of the material  $\lambda = 0.5(\lambda_a + \lambda_{iz}) = 0.2935 \text{ W/(m·K)}$  exceeds the average experimental value  $\lambda_h = 0.278 \text{ W/(m·K)}$  by 5.57%.

#### 4.3. Example of Calculation According to The One-Step Procedure

For the purpose of comparison, calculation of the thermal conductivity  $\lambda$  for the same ACC specimens was performed using the one-step procedure proposed in [10], which does not take into account the bimodal pore distribution. In this case, the following values of the volumetric concentrations of the components are obtained: solid phase  $m_1 = m_s = 0.2258$ , liquid  $m_3 = \psi = 0.232$  and gas  $m_2 = 1 - m_1 - m_3 = 0.5422$ . Thermal conductivity of the solid skeleton  $\lambda_1 = 0.84$  W/(m·K) and water  $\lambda_3 = 0.597$  W/(m·K) remains the same, and the thermal conductivity and the vapour-air mixture calculated by Formulas (10)–(15) is  $\lambda_2 = 0.0358$  W/(m·K). The geometric parameter of the solid skeleton c = 0.3075 is determined by Formula (2) at  $m_1 = 0.2257$ . The pore boundary moisture content calculated by formula (4) was  $\psi'_p = 0.3571$  and exceeded the actual moisture content  $\psi_p = \psi/P = \psi/(1 - m_1) = 0.2997$ . From this it follows that the liquid is distributed in the pores of the material in the form of isolated inclusions. In this case, Formulas (6) and (7) or dependencies from [15] constructed specifically for insulated liquid inclusions may be used to calculate the effective thermal conductivity of the material.

Using Formulas (6) and (7) for isolated liquid inclusions  $c_n = c = 0.3075$  was adopted, and  $c_x = c + d = 0.7238$  were obtained from the solution of cubic Equation (1) at  $\psi_k = \psi = 0.232$ and d = 0.4163. Next, the thermal conductivity values of the ternary system were determined when dividing the unit cell by adiabatic planes  $\lambda_a = 0.1476 \text{ W/(m·K)}$  and isothermal planes  $\lambda_{iz} = 0.2377 \text{ W/(m·K)}$ . Their average value was taken as the estimate of the effective thermal conductivity of the material  $\hat{\lambda} = 0.5(\lambda_a + \lambda_{iz}) = 0.1926 \text{ W/(m·K)}$ . This value turned out to be 30.7% lower than the experimental value  $\lambda_h = 0.278 \text{ W/(m·K)}$ .

#### 4.4. Results and Discussion

Similarly to the above examples, calculations were performed for all four series of ACC specimens using both procedures, the results of which, together with the experimental data, are presented in Table 2. The analysis of this table shows that the results of the

calculation of the thermal conductivity  $\lambda$  using the two-step procedure quite accurately predict experimental values  $\lambda_h$ . The deviations of computational and experimental values  $\Delta$ , determined by the ratio  $\Delta = (\lambda - \lambda_h) \cdot 100\% / \lambda_h$ , ranged from -7.29 to +5.75% with the average  $\overline{\Delta} = -0.71\%$ . The mean square deviation of the measured values of the thermal conductivity  $\lambda_h$  is s = 0.011 W/(m·K) at 16 degrees of freedom. The deviation of the calculated values does not exceed two mean square deviations of experimental ones. The calculated values of  $\lambda$  are within the confidence interval for the measured values with the probability of 0.94. Statistical analysis proves that the proposed two-step method, taking into account the bimodal pore size distribution, can predict the thermal conductivity of moist ACCs with high accuracy.

Series nr	ho, kg/m <sup>3</sup>	ψ	$\lambda_{h}$ , W/(m·K)	$\lambda$ , W/(m·K)	$\hat{\lambda}$ , W/(m·K)
1	447	0.1030	0.2100	0.2000	0.1587
1	447	0.2320	0.2780	0.2935	0.1926
2	530	0.1323	0.2540	0.2362	0.1923
Z	530	0.2413	0.3035	0.3235	0.2202
2	577	0.1420	0.2675	0.2480	0.2044
3	577	0.2604	0.3358	0.3450	0.2389
4	614	0.1520	0.2810	0.2606	0.2060
	614	0.3165	0.3771	0.3988	0.2942

**Table 2.** Thermal conductivity values of moist cellular concrete samples determined experimentally  $\lambda_h$  and computationally according to the two-step method  $\lambda$  and one-step method  $\hat{\lambda}$ , apparent density  $\rho$  and moisture content  $\psi$  of the samples in four series.

In contrast, the previously proposed one-step method, which does not take into account the bimodal pore size distribution, gives individual deviations in the range from -30.72 to -21.98% with an average  $\overline{\Delta} = -26\%$ . This means that the thermal conductivity values  $\hat{\lambda}$  calculated by the method proposed previously are much lower than the experimental data  $\lambda_h$ .

The above results therefore indicate that the currently proposed two-step method should be used to determine the thermal conductivity of moist cellular concretes, up to the state of water saturation with free capillary absorption.

#### 5. Conclusions

A method for calculating the effective thermal conductivity of cellular concretes with a bimodal pore size distribution has been proposed. The calculation should be carried out in two stages to take into account this property of the pore structure. First, the ternary system is considered, consisting of the solid skeleton and gas and liquid contained at fine (capillary) pores. The volumetric concentration of the fine pores is determined on the basis of the water absorption of samples previously immersed in water. Then, the binary system is taken into account, consisting of the mentioned ternary system, the effective thermal conductivity of which is determined by the formula constructed using the theory of generalised conductivity and large gas pores. The thermal conductivity of the binary system is calculated using well-known formulas.

The thermal conductivity of samples of cellular concretes was measured under laboratory conditions, the moisture content of which was increased until free capillary saturation. On the basis of experimental data, the thermal conductivity of the samples was calculated using the currently proposed and previous methods. It was found that the results of the calculation of the thermal conductivity using the currently proposed method practically agree with the experimental values, whereas the previous method of calculation yielded much lower results compared to the experimental values. Author Contributions: Conceptualisation, B.B.-B. and V.I.N.; methodology B.B.-B., V.I.N. and A.A.; software, S.K.N.; validation, A.A., and B.B.-B.; formal analysis, A.A.; investigation, B.B.-B. and W.R.; resources, A.A. and B.B.-B.; data curation, B.B.-B.; writing—original draft preparation, V.I.N.; writing—review and editing, B.B.-B.; visualisation, S.K.N.; supervision, A.A.; project administration, B.B.-B.; funding acquisition, A.A. and B.B.-B. All authors have read and agreed to the published version of the manuscript.

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