

Experimental Determination of Inverse Heat Conduction Problem for Cement Clinker Granules

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Abstract: This paper presents the estimation method of relation between heat conduction coefficient of granulated material and temperature. It includes thermal changes for two points of granule when heated or cooled and simulation of a temperature field of granule according to these data. The method is allowed to define coefficient of heat conduction before 1000°C. There are represented the experiment and calculation of heat conduction coefficient and also research results of heat conduction of cement clinker granules.

Key words: Heat conduction • Inverse problem • Cement clinker

INTRODUCTION

Currently there are the mostly used stationary methods for heat conduction studies. These are specified by a simple experiment but have some disadvantages such as cold operating temperature and complicacy of experimental setup [1, 2]. The non-stationary and unbalanced dynamics methods based on time-dependent temperature fields, give opportunity to investigate a heat conduction of material at high temperature [3, 4]. The main problem of non-stationary methods consists in approximating mathematical model to experimental processes [5].

The method includes experimental determination of the temperature at two points of granule t_0^e and t_k^e (pic 1) when heated or cooled and simulation of temperature field of granule using the finding. The temperature approximation t_0^e and t_k^e , obtained after experiment and the temperature approximation t_0^m и t_k^m , calculated by heat conduction model (pic 2), are yielded according to change of model boundary conditions and other parameters (granule radius R, initial temperature), measurement of which has some errors. According to

change of temperature field there is calculated the heat flow which is equal the change of heat content of granule for a certain period. The calculation of heat conduction is produced by next parameters: heat flow Q, passed through the sphere with radius r_k , which restricts interior granule; sphere surface area; temperature difference with low volume on surface (Fig. 2).

It essential to note a difference of suggested method from classic inverse problem [6–8]. For considered problem adjusting the results of numerical simulation and experimental data by changing of heat conduction coefficient is impossible, because found coefficients will content a significant error, relating to inaccuracy of definition of model's parameters through irregular shape of granule and conditions for heat dissipation on surface. Here simulation is in use for calculation of quantity of heat, obtained and lost by granule. This yields the value of heat conduction coefficient.

Discrete Analog Construction: The temperature field of a spherical granule is defined by a solution of the non-stationary one-dimensional heat conduction equation in spatial spherical coordinates:

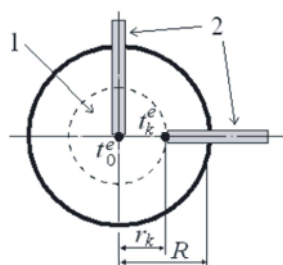


Fig. 1: Laying of thermocouples under experimental temperature measurement of granule: 1 – interior granule; 2 – thermocouples

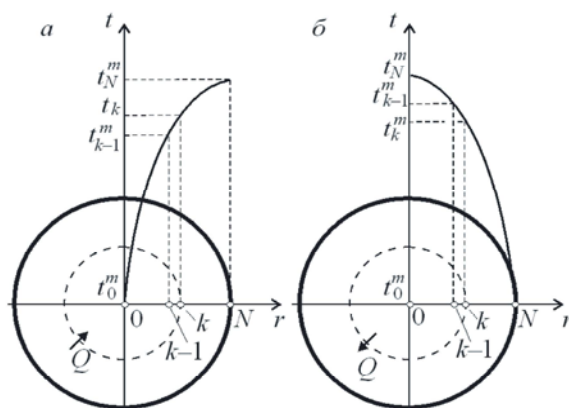


Fig. 2: Estimated temperature field of granule: A – heating; b – cooling

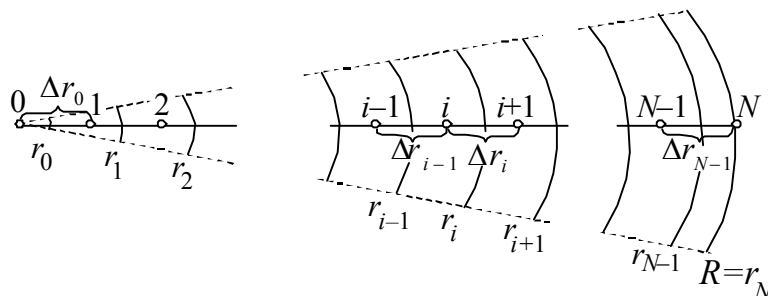


Fig. 3: Control volumes for internal and boundary points in spherical coordinates

$$\rho c \frac{\partial T}{\partial \tau} = \frac{1}{r^2} \frac{\partial}{\partial r} \left(\lambda r^2 \frac{\partial T}{\partial r} \right); \quad \frac{\partial T}{\partial r} = 0; \text{ with } r = 0; \quad \lambda \frac{\partial T}{\partial r} = \alpha (T_{env} - T), \text{ with } r = R. \quad (1)$$

Sampling of the equation (1) was produced according to the method discussed in this paper [9]. In the center of the granule where was located origin of coordinate, rated operating conditions are divided by a grid, containing $N+1$ junctions. The junction № 0 was located in the center of granule, the junction № N was on its surface (Fig. 3). The control volume representing a spherical layer which borders are spheres with radius r_i is allocated near every junction. Every junction is equidistance from the boundary of the volume corresponding to it.

For ensuring equality of the masses being contained in each control volume, the non-uniform mesh is applied. According to experimental conditions one of model's points has to coincide with a place of a laying of the thermocouple, this section is set by number k and radius r_k , determining the distance from a point to the center by which radius r'_k is determined for boundary of control volume. The mesh is formed when control volumes located relative to this boundary of granule outside or inside are all equal. Borders of partitions are defined as:

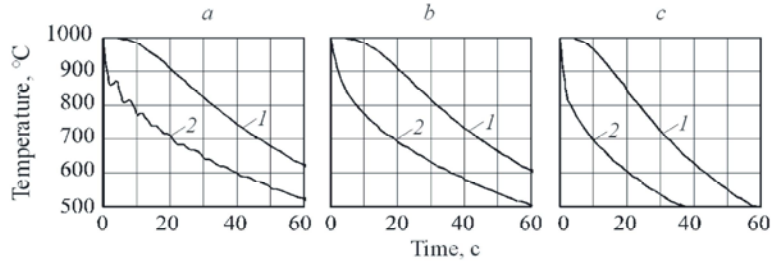


Fig. 4: Results of modeling of cooling of granule with diameter of 1 cm with various schemes of sampling: 1 – temperature of the center of granule; 2 – surface temperature; a – Kranka-Nicholson's scheme; b – Kranka-Nicholson's scheme with implicit discrete analog for the last junction; c – implicit scheme

$$r'_i = \frac{r'_k}{\sqrt[3]{\frac{k+1}{i+1}}}, i \leq k; \quad r_i = \sqrt[3]{(r'_k)^3 + \left(R^3 - (r'_k)^3\right) \frac{i-k}{N-k}}, i \leq k; \quad r'_i = \frac{2r_k}{1 + \sqrt[3]{\frac{k}{k+1}}}.$$

Due to the symmetry of area for the left border (the center of granule) there was defined the boundary condition of the second genus when the heat flow was equal to zero. For the right border (a granule surface) the boundary condition of the third genus was obtained:

$$\alpha = \varphi(\alpha_{con} + \alpha_{rad}). \quad (2)$$

In accordance with results of experimental measurement of temperature in studied heated or cooled clinker granules, time change of temperatures is close to the linear for studied points. Therefore the Kranka- Nicholson's scheme has to provide the greatest accuracy when sampling the differential equation. This disadvantage is variation of decision with insufficiently small values of steps on time. In the this case the variation was from the point lying on a surface of a granule (Fig. 4). The implicit scheme hasn't this, but includes low accuracy which results to fast cooling (Fig. 4).

For the required accuracy and acceptable time of calculation to be provided it is necessary to sample the equations at all junctions of the mesh according to Kranka-Nicholson's scheme and use the implicit scheme for the last junction located on surface of granule. As a result accuracy of solving remains when increasing step on time and variation of temperature values in a boundary point (Fig. 4) is deleted.

As a result of sampling of the equation (1) on the mesh given on Fig. 3, there are obtained the system with $N+1$ equations: (Fig. 4).

$$\begin{cases} K_0(T_0^1 - T_0^0) = k_0(T_1^1 + T_1^0 - T_0^1 - T_0^0); \\ K_i(T_i^1 - T_i^0) = k_i(T_{i+1}^1 + T_{i+1}^0 - T_i^1 - T_i^0) - k_{i-1}(T_i^1 + T_i^0 - T_{i-1}^1 - T_{i-1}^0); \quad i = 1 \dots N-1; \\ K_N(T_N^1 - T_N^0) = k_{lm}(T_{env} - T_N^1) - 2k_{N-1}(T_N^1 - T_{N-1}^1); \end{cases} \quad (3)$$

where the following coefficients are used:

$$K_0 = \frac{\rho c_0}{\Delta \tau} \frac{r_0^3}{3}; \quad K_0 = \frac{\rho C_0 r_0^3}{\Delta \tau \cdot 3}; \quad K_i = \frac{\rho c_i}{\Delta \tau} \frac{r_i^3 - r_{i-1}^3}{3}, \quad i = 1 \dots N-1; \quad K_N = \frac{\rho c_N}{\Delta \tau} \frac{R^3 - r_{N-1}^3}{3};$$

$$k_i = (r_i - r_{i-1})/2 \cdot (i / (\Delta r_i)), \quad i = 0 \dots N;$$

$$k_{lm} = \alpha R^2;$$

$$\lambda_i = f\left(\frac{T_{i+1}^1 + T_{i+1}^0 + T_i^1 + T_i^0}{4}\right)$$

$$C_i = f\left(\frac{T_i^1 - T_i^0}{2}\right); \quad \Delta r_0 = 0,5(r_1 + r_0);$$

$$A_{ri} = 0,5(r_{i+1} - r_{i-1}), \quad i = 1 \dots N-2;$$

$$\Delta r_{N-1} = R - 0,5(r_{N-1} + r_{N-2}). \quad \Delta r_{N-1} = R - 0,5(r_{N-1} + r_{N-2})$$

For realization of the sweep method the system (3) is presented in standard form

$$\begin{cases} a_0 T_1^1 + b_0 T_0^1 + d_0 = 0; \\ \dots \\ a_i T_{i+1}^1 + b_i T_i^1 + e_i T_{i-1}^1 + d_i = 0; \quad i = 1 \dots N-1; \\ \dots \\ b_N T_N^1 + e_N T_{N-1}^1 + d_N = 0, \end{cases}$$

where

$$a_0 = -k_0; \quad b_0 = K_0 + k_0; \quad d_0 = (k_0 - K_0) T_0^0 - k_0 T_1^0;$$

$$a_i = -k_i; \quad b_i = K_i + k_{i-1} + k_i; \quad e_i = -k_{i-1}; \quad d_i = (k_i + k_{i-1} - K_i) T_i^0 - k_i T_{i+1}^0 - k_{i-1} T_{i-1}^0;$$

$$b_N = K_N + k_{lm} + 2k_{N-l}; \quad e_N = -2k_{N-l}; \quad d_N = -K_N T_{N-1}^0 - k_{lm} T_{env}^0.$$

Calculation of Heat Conduction Coefficient: The result of experimental measurement of temperatures of the granule when heated or cooled is L_e values of temperatures in the center of granule (point 0) and at distance of $\frac{1}{2}$ radiuses from it (point k), measured in time intervals Δt_e :

$$t_{0,p}^e \text{ и } t_{k,p}^e, \quad p = 1 \dots L_e.$$

According to losses of time for granule extraction from the muffle furnace (or set it in the furnace) and connection of thermocouples, the first sample time Δt doesn't correspond to initial time of cooling (heating), that is $\Delta t \gtrless$.

For the experimental errors and the gradation of the graphics caused by gradation of a scale electronic millivoltmeter in 0,1 V (that is observed when using software thermocouples with small termo-EDS) to be excepted experimental data are smoothed out with their approximation by a polynom of 2, 3 or 4 degrees. As result there are yielded L_e values of temperatures

$$t_{0,p}^a \text{ и } t_{k,p}^a, \quad p = 1 \dots L_e.$$

Result of the decision of system of the equations of discrete analog of the equation of heat conductivity is distribution of temperatures in a granule through the set periods

$$t_{i,j}^m, \quad i = 0 \dots N, j = 0 \dots L_m.$$

For a choice of number of steps on L_m time in mathematical model there are used conditions:

– when cooled

$$\left(t_{0,L_m}^m \leq t_{0,L_e}^a\right) \vee \left(t_{k,L_m}^m \leq t_{k,L_e}^a\right) \vee (L_m \rightarrow \min);$$

– when heated

$$(t_{0,L_m}^m \geq t_{0,L_e}^a) \vee (t_{k,L_m}^m \geq t_{k,L_e}^a) \vee (L_m \rightarrow \min);$$

temperature of model in points with numbers 0 and k, corresponding to time of experimental measurements are chosen among the received temperature distribution, as a result from L_m only L_e points remains:

$$t_{0,p}^m \text{ и } t_{k,p}^m, p = 1 \dots L_e.$$

It is necessary to make approach of experimental temperature $t_{0,p}^a$, $t_{k,p}^a$ and model $t_{0,p}^m$ and $t_{k,p}^m$ for determination of heat conduction coefficient. Criterion of a deviation of settlement and experimental temperatures is the sum of squares of differences of temperature deviations at every point and deviations of differences of temperature of the center and the point with number k:

$$S = \sum_{p=1}^{L_e} \left[(t_{0,p}^m - t_{0,p}^a)^2 + (t_{k,p}^m - t_{k,p}^a)^2 + \left[(t_{0,p}^m - t_{k,p}^m) + (t_{0,p}^a - t_{k,p}^a) \right]^2 \right].$$

$$S = \sum_{p=1}^{L_e} \left[(t_{0,p}^m - t_{0,p}^a)^2 + (t_{k,p}^m - t_{k,p}^a)^2 + \left[(t_{0,p}^m - t_{k,p}^m) + (t_{0,p}^a - t_{k,p}^a) \right]^2 \right]. \quad (4)$$

For minimization of value S there should be changed the coefficient φ from the equation (2). Other parameters of the model which measurement is connected with a certain error should be specified: initial temperature of a granule when cooled or environment temperatures in the muffle case when heated; time interval before initial measurement \square_0 ; radius R. of granule.

After minimization it is impossible to achieve absolute coincidence of experimental temperature and model, especially in the first iterations. for calculation of heat conduction coefficient there are used the settlement temperature field coinciding with experimental temperature at points 0 and k and corresponding to pattern of temperature change on radius of granule in model for other points is used:

$$t_{i,p} = t_{0,p}^a - (t_{0,p}^m - t_{i,p}^m) \frac{t_{0,p}^a - t_{k,p}^a}{t_{0,p}^m - t_{k,p}^m}, \quad i = 0 \dots k; m = 1 \dots L_e$$

Calculation of heat conduction coefficients \square_p is obtained by quantity of the heat, lost or received by internal part of granule for every moment of time of experimental measurements:

$$\lambda_p = \frac{(Q_{p-1} - Q_p)(r_k - r_{k-1})}{2F_k \Delta t_p (\tau_p - \tau_{p-1})}, \quad t_p = \frac{t_{k-1} + t_k}{2}, \quad p = 1 \dots L_e,$$

where Q_{p-1} , Q_p are quantities of heat for internal part of a granule (Fig. 1) in the moments of time of two measurements τ_{p-1} and τ_p ; F_k is the surface area restricting internal part of a granule; r_k and r_{k-1} are radiuses of points between which the difference of temperatures $\square t$ is taken t_p is temperature corresponding to the received coefficient of \square_p .

For calculation of heat conduction coefficient the difference of temperatures $\square t$ is taken in two next points of settlement mesh of the model one of which is the point with number k, corresponding to the place of laying of the thermocouple, the second – the point next to it. As the difference of temperatures at k and k-1 points during $\square \square_e$ changes, $\square t$ is calculated as a logarithmic average between periods \square_{p-1} and \square_p .

The heat content of internal part of a granule is determined by its temperature field:

$$Q_p = \sum_{i=1}^n \rho \frac{4}{3} \pi (r_i^3 - r_{i-1}^3) c t_{i,p},$$

where the thermal capacity is calculated according to work subject to temperature [10].

After determination of heat conduction coefficient in every moment of time according to the received tabular dependence $\lambda_p(t_p)$, $p = 1 \dots L_p$, coefficients x_0 , x_1 , x_2 of linear or square dependence are estimated:

$$\lambda = \lambda_p: \lambda = x_0 + x_1 t \vee \lambda = x_0 + x_1 t + x_2 t^2. \quad (5)$$

As when modeling of cooling the coefficient of heat conduction of a material is used in the equation (1), the calculation is produced with use of the dependence received in the previous iteration (5).

According to the considered technique the software is developed for modeling of a temperature field of a granule, analysis of experiment and determination of dependence coefficients of heat conductivity coefficient from temperature [10, 11]. There is presented algorithm for the program work.

- Readout from the file of experimental data: radius R , density of a granule ρ , time from the beginning of heating (cooling) before measurements of λ_0 , temperatures $t_{0,p}^e$ and $t_{k,p}^e$, $p = 1 \dots L'_e$.
- Removal of the experimental points, not entering into the set range of temperatures, smoothing of experimental data by polynom of the set degree, result – temperatures $t_{0,p}^a$ and $t_{k,p}^a$, $p = 1 \dots L_e$.
- Calculation of a temperature field of a granule, $t_{i,j}^m$, $i = 0 \dots N$, $j = 0 \dots L_m$.
- Minimization of a deviation S of experimental and settlement temperatures S calculated on the equation (4), by change of the set parameters according to alternating-variable descent method with step crushing (iterative calculation of item 3, 4 before stabilization of coefficients regression equations)
- Calculation of heat conduction coefficient of $\lambda_p(t_p)$, $p = 1 \dots L_e$ and coefficients of the regression equation $\lambda = \lambda(t)$ (iterative calculation of item 3-5 before stabilization of coefficients regression equations) visually

The graphic interface of the program allows to estimate the accuracy of approximation of experimental data by polynom, degree of approximation of temperatures of model and experiment, a type of received dependence for heat conduction coefficient, gives the opportunity to select the most successful way of calculation. Use of the graphic dialogue interface and evident representation and results of calculation rendered also big help when developing and debugging algorithm of the program.

For program testing as basic data the distribution of temperatures was set by the analytical solution of the equation of non-stationary heat conduction [12]. Results of calculation of heat conduction coefficient with various options of parameters of process (density, a thermal capacity, heat dissipation coefficient) didn't differ from set with the analytical decision more than 0,5%.

Experimental Research Results: For determination of heat conduction there were used factory clinker granules of ZAO (close corporation) “Belgorodsky cement” (BTsZ) and ZAO (close corporation) “Oskolcement” (SOTsZ) with a diameter of 35 ... 50 mm and the granules received in vitro by roasting in the high-temperature furnace (L) with a diameter of 25 ... of 40 mm. Laboratory granules were prepared from a factory raw mix of BTsZ, in part from them the raw mix was corrected by limy, clay and ferriferous components for increase or reduction of saturation coefficient with constant aluminous and silica modules. Porosity of factory granules composed 10,5 ... 11,1%, laboratory granules – 17%.

Two holes with a diameter of 3 or 4 mm were bored in granules, one to the center of granule, another on depth which is equal to a half of radius (this distance is chosen for prevention of influence of the thermocouple channel on the process of heat conduction in it). The thermocouples of type Pt-10%Rh / Pt placed in ceramic tubes were inserted into the received holes. The location of thermal junctions was defined by graphic construction of plane projection of the granule and thermocouples. Thermo-emf was measured by electronic millivoltmeters.

Before experiments there were defined the volume and the apparent density of the granule which helps to obtain equivalent radius. Heating was carried out in the muffle furnace with a temperature of 1000 ... 1200°C, cooling – out of the furnace under natural conditions. The experiment is duplicated from two to four times

Table 1: Heat conduction of clinker granule on temperature interval 300...900°C, W/m•K

Name of granule	Change range, W/m•K	Average values $\bar{\lambda}$, W/m•K	Change $\Delta\lambda$, when increasing temperature on 100°C (100 x_1), W/m•K	Errpr! 100%	Correlation between coefficient x_0 and x_1
BtsZ	0,6...0,95	0,80	0,053	6,6	-0,56
SOTsZ	0,7...1,0	0,84	0,054	6,4	-0,72
Laboratory	0,5...0,75	0,60	0,042	7,0	-0,33

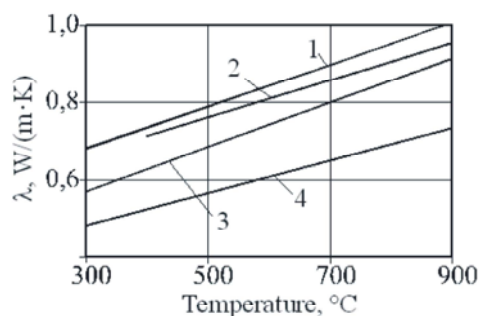


Fig. 5: Average heat conduction of clinker granules:
1 – SOTsZ; 2 – BtsZ, heating; 3 – BtsZ, cooling;
4 – laboratory

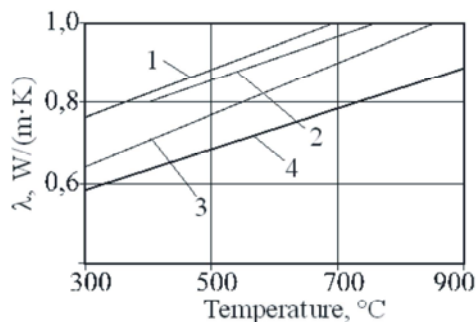


Fig. 6: Average estimated heat conduction of ideal dense clinker:
1 – SOTsZ; 2 – BtsZ, heating; 3 – BtsZ, cooling;
4 – laboratory

(with integrity of granules). After measurements the petrographic analysis of granules was made and their real density was defined by the bottle method.

For experimental studies time interval between measurements is, with numerical modeling the quantity of points of a grid was set by equal $N = 75$, a step on time.

Dependences of heat conduction coefficient on temperature, received after research, are presented in Fig. 5, 6.

For all granules growth of heat conduction coefficient with increase in temperature is observed. Heat conduction of granules of SOTsZ is higher, than BtsZ and laboratory below, than factory. It is connected with various porosity of granules. The analysis of the received dependences is provided in Tab. 1.

For studied granules there is revealed dependence of increase of heat conduction coefficient with 0,04 ... 0,05 W/m with temperature rise on 100 °C. Despite distinction in absolute values of heat conduction coefficient, the relation of coefficient x_1 to average value of heat conduction coefficient for the studied granules is equal. Therefore, at the studied granules the identical relative increase of heat conduction coefficient is observed at increase in temperature.

There is an invert correlation between two factors x_0 and x_1 . It can be explained by experimental error which causes turn of a regression straight line with the rotation center in the middle of the range of temperatures at which the heat conduction coefficient was defined. But averaging of coefficients of the regression equation allows to get rid of this error. So, despite quite wide spacing in coefficients for granules of one type, average values of coefficients are close among themselves.

In the paper [13] there have been represented the results of complex research of heat conduction of cement raw mixes and clinker including with use of the offered method, confirming adequacy. The developed model, algorithm and results of studies are successfully applied at the solution of a number of problems of modeling and experimental research [14-16].

According to considered investigation we can make a conclusion that the developed research technique, the algorithm of calculation of heat conduction coefficient and the software allow to define of heat conduction coefficient of the granulated material with temperatures before 1000 °C with a fine precision.

Nomenclature:

- a, b, e, d - Coefficients of the system of linear equations;
- C - Specific heat capacity, J/kg•K;
- \square - Dependence equation of heat conduction coefficient on the temperature coefficient;
- F - Surface area of the spherical granule section, m²;
- Q - Heat flow passing through the sphere with radius r_b , V;
- K, k - Coefficients of the discrete analogue;

L	- Number of time steps in the experiment and model;
N	- номер узловой точки на поверхности гранулы;
r	- Distance from the granule center, m;
r'	- Distance between the granule center and border of control volume, m;
R	- Granule radius, m;
S	- Sum of squared differences of temperatures obtained by measurement and calculated according to the mathematical model;
T	- Temperature, K;
t	- Temperature, °C;
x	- Coefficients of the polynomial dependence of the coefficient of heat conduction on temperature;
\square	- Heat dissipation coefficient on surface of granule, $V/m^2 \cdot K$;
φ	- The coefficient considering not sphericity of a surface of a studied granule;;
λ	- Heat conduction coefficient, $W/m \cdot K$;
$\square\square$	- Step of time iteration, sec;
$\square r$	- Step of grid, m;
$\square t$	- Temperature difference in two junction points located near the second thermopair;
ρ	- Density, kg/m^3 ;
τ	- Time, sec;

Superscripts:

1	- Current time iteration;
0	- Previous time iteration;
m	- Temperature calculated by mathematical model;
e	- Temperature derived experimentally

Subscripts:

0	- Junction point, met the center of granule (first thermopair location);
i	- Number of junction point;
j	- Number of time iteration in mathematical model;
k	- Junction point, located between center and granule surface (the second thermopair location);
m	- Number of experimental temperature measurement;
lm	- Discrete analog factors for control volume at the outer area boundary;
rad	- Radiation;
con	- Convective;
env	- Environment

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