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Modeling of temperature fields in the working chamber of the process furnace for REE synthesis

Kerbel B M [1], Ageev A Yu[1], Payusov A Yu[1], Katsnelson L M,[2] Tereshchenko E V[1] , Verkhoturova V V[3]

1. Seversk Technological Institute, MEPhI, 636036, Russia, Seversk, Tomsk region, Kommunistichesky avenue 65.
2 JSC SPE "Technologic", Russia, 863033, Rostov-on-Don, Portovaya street, 303
3. National Research Tomsk Polytechnic University, 634050, Russia, Tomsk, Lenin avenue street 30.

Email: BMKerbel@mephi.ru

Abstract. The results of mathematical modeling of temperature fields in the working chamber of the process furnace for special purposes are shown. Studied laboratory furnace is test equipment, which is used for practicing the stages of the technological process of continuous solid-phase synthesis of nanopowders of various purpose, such as obtaining of luminophore powders with rare earth elements oxides in its composition. Mathematical model adequacy is tested empirically

Studied laboratory furnace is test equipment, which is used for practicing the stages of the technological process of continuous solid-phase synthesis (CSPhS) of nanopowders of various purpose [1], for example, obtaining luminophore powders [2], with rare earth elements oxides in its composition.
Mathematical modeling of temperature fields is carried out to create an automated control system of the technical system, which appears as shaft-type laboratory furnace in this paper. Solid-phase synthesis of REE oxide powders is carried out in a high-temperature furnace chamber, it is necessary to keep determinate distribution of thermal field in closed space of the working chamber.
This distribution is caused by special features of technological process of continuous solid-phase synthesis. Design layout view of studied furnace is shown in Figure 1.

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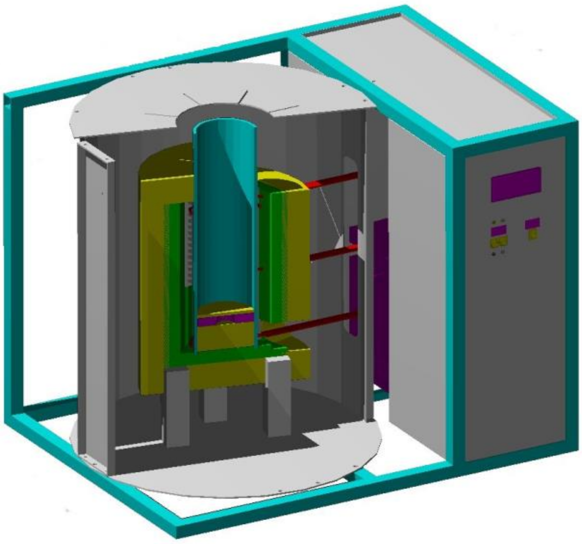


Figure 1 - High-temperature shaft-type furnace

Distinctive features of the furnace design are: relatively small dimensions, 1200°C as the upper limit of the temperatures operating range, the ability of automatic program control of the process when the furnace reaches fully operating conditions and automatically maintain this mode. In addition, distinctive features of the furnace design include dual-zone heating by the high level of the working chamber and the absence of heating on the sides (at the top (cover) and lower part (bottom)), as well as the presence of thermal capacitance "cushion" at the bottom of the chamber. Main technical characteristics of the studied furnace are shown in Table 1.

Table 1 – Main technical characteristics of the shaft-type furnace

№	Furnace parameters, items	values
1	The maximum allowable temperature, °C	1350
2	The number of thermocouples	2
3	Accuracy of temperature maintenance, not worse than, °C	±2
4	Working dimensions, not more than, mm	
	Diameter	100
	The furnace depth	300

While optimizing the furnace work, the conditions of the solid-phase reactions behavior in continuous synthesis mode should be taken into account, as well as high-speed sintering conditions. In this regard, focused research [3, 4] has been conducted to determine the factors, influencing the formation of the chemical continuity process conditions.

Analyzing obtained data, the following requirements appear that dictate the optimum temperature conditions, which are necessary to provide within the considered experimental furnace:

- The higher the specific surface area of the synthesized material, the lower temperature and the shorter time period are needed to complete the continuous synthesis of a particular material;
- Synthesis temperature has the most significant impact on minimizing its duration;

- Boundary conditions of the continuous synthesis are determined by prehistory of mechanical mixture, including its specific surface area;
- ceteris paribus, the intensity of the solid-phase reactions behavior in continuous synthesis is determined by the temperature-time characteristics of the synthesis;
- maximum quality of the synthesized oxide material is achieved at maximum intensity coefficient value of continuous solid-phase synthesis.

It has been found that the synthesis required quality could be achieved under certain interdependency of synthesis temperature and time. The tendency is that that the reduction of the synthesis time leads to synthesis temperature increase and, accordingly, has a direct impact on the installation capacity, in general. It is clear that the time-temperature interdependence has the restrictions, determined by criticality of particular oxide material to the conditions of synthesis.

During the oxide materials synthesis using the technology of continuous solid-phase synthesis, nanomodule formation occurs with following self-assembly of nanostructured macro-objects having constant particle size distribution in one technological process:

- control of the oxide material dispersion directly during the process of its synthesis allows avoiding grinding of the synthesized material from the classical ceramic technology specifications, which naturally brings to the end all the problems associated with the technological specifications, that are particularly significant for the functional materials with sensitivity to contamination;
- regulation of the powders particle size composition during CSPhS process eliminates the problem of molding ultra- and nano-level powders, which is rather complicated technological problem for real ceramic manufacturing;
-
- ceteris paribus, ceramic materials get the most preferred parameters values in comparison with traditional ceramic technology of their producing.

Initial oxides grinding, occurring in the first few seconds, as if precedes a new phase synthesis, although, it is not possible to separate these two processes, because they occur simultaneously at the initial moment (seconds), and, then, the quality and dispersion of synthesis are formed.

The necessity to carry out the experiments on baking the powders batches of various volumes using CSPhS technology determined the necessity to assess the parameters of the temperature of non-gradient zone (NGZ) in the furnace working chamber.

Traditionally, quantitative description of the heat transfer process is based on the theory of mathematical physics, using a system of differential equations in partial derivatives, with imposing the necessary boundary (Neumann coefficients) and initial (Dirichlet coefficients) conditions [5] on this system. However, due to the bulkiness of the mathematical apparatus, such approach is not always convenient.

Alternative method, which is successfully applied in everyday engineering practice, appears as the calculation of the temperature in a given three-dimensional object space using analytical expressions, obtained with processing of experimental data.

Let us consider the experimental data as a result of some process realization disturbed with the interference, which is certainly determined by the unknown function of the $y = f(x)$ form. In most cases, the experimental data of this kind are represented as tables or charts, which display the tables

Obviously, the charts are the simplest means, widely used for a long time in various fields of human activity, for cognitive representation of the experimental data that allows visualizing the qualitative features of the process and evaluate them, despite the interference and measurement inaccuracy.

The charts that show the same process and the characteristics of a certain object may differ significantly from one another by scale, by the number of measurements used, by the level of interference, and so on. At the same time, the distinctive features of the chart type describe the parameters of the imaged object or the process. Automatic or automated processing of such charts includes the comparison of their types to determine whether different charts describe the same or different processes or objects.

Wherein, the situation, when the experimental data set with sufficient accuracy for engineering practice could be approximated by a function, is typical enough.

The most common method of the experimental data approximation is the method of the least squares [6, 7]. This method allows using approximating functions of any kind, and belongs to the global methods group. Polynomial approximation of various degree is one of the least squares method variation.

The requirement for the minimum sum of squared deviations from the approximating function to the data points is the criteria of the least squares method accuracy:

$$\mathrm{F} = \sum_{i=1}^{n}(y_i - f(x_i))^2 \to min,$$

where y – some known values, x - a set of unknown (desired) variables.

Thus, this method does not require from approximating function to go through all given points. This is significant at approximation of experimental data with some inaccuracy.

Applying to the studied shaft-type furnace, series of measurements were carried out on the temperature profile of the furnace - temperature change at the vertical geometric axis of the working chamber depending on the depth of immersion therein. These measurements were conducted for different sections of the working temperature range of the furnace - for the initial zone, the central zone and high zone. The numerical values of the set the temperatures in this case were: 200, 500, 800, 1000 and 1200 ° C.

The results of measurements were taken into account for building appropriate interdependences - furnace temperature profiles for taking the temperature set points. For example, Figure 2 shows a series of temperature profiles obtained (the points on the charts show the temperature values for each of its profiles).

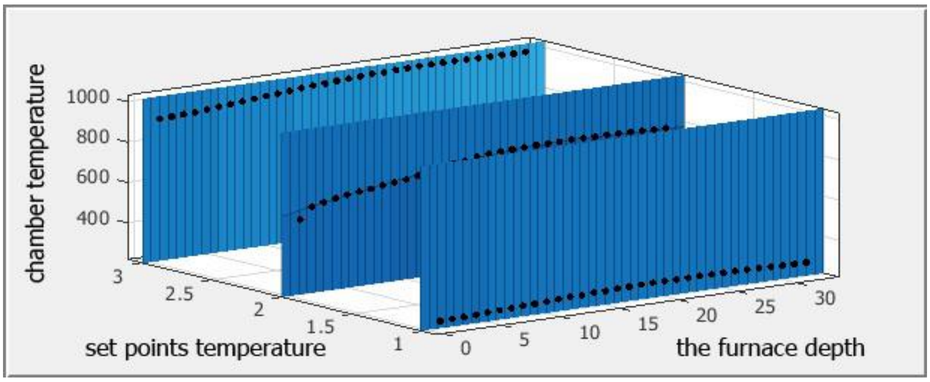
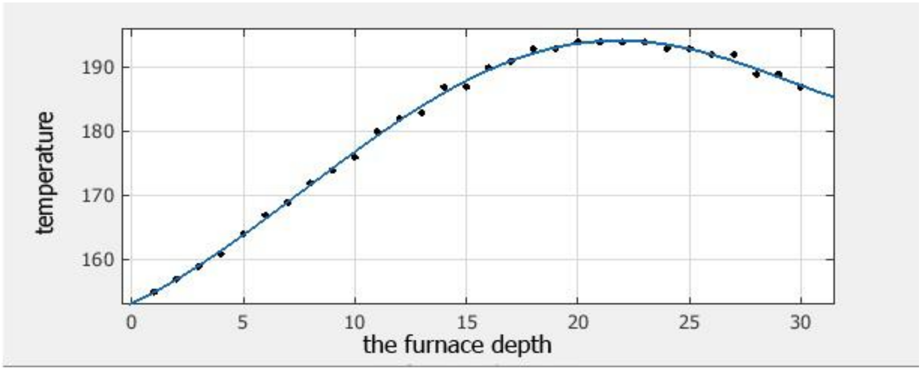
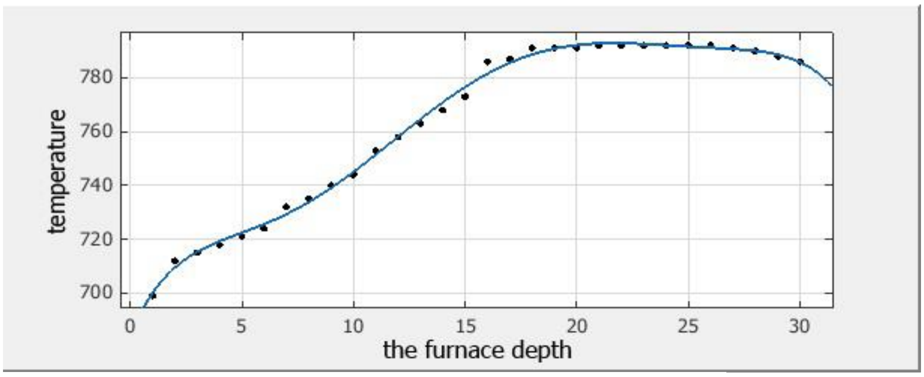


Figure 2 – Experimental temperature profiles of the studied furnace

For the mathematical processing of the experimental data polynomial approximation with polynom of the 5th order was used. Thus, each of the temperature profile was approximated by this function. The results of the temperature profiles approximation for set points of 200 and 800 ° C are shown in Figure 3. As it is seen from the Figure, the deviation of the calculated and experimental values of the temperature does not exceed XºC or Y%, which is sufficient accuracy for engineering calculations.



a) the experimental and calculated furnace profiles at 200 °C set point



b) the experimental and calculated profiles at 800 °C set point

Figure 3 – Comparison of the calculated and experimental furnace profiles

Surface approximation was performed to obtain more universal tool, which allows analytically evaluating the temperature profile parameters of the studied furnace at arbitrary set point (Figure 4).

Figure 4 shows the approximated surface of the temperature profiles of the studied furnace, which is described by expression:

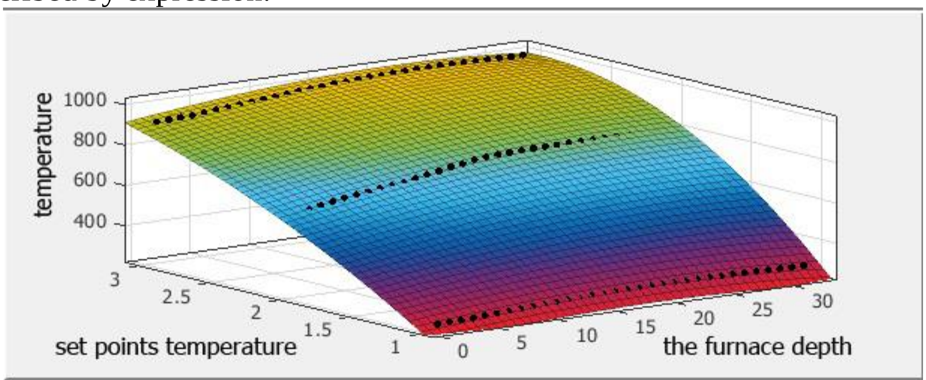


Figure 4 – Temperature profiles approximation with surface

$$f(x,y) = p00 + p10x + p01y + p20x^2 + p11xy + p02y^2 + p30x^3\ p21x^2y + p12xy^2,$$

Where the values of the respective coefficients are:

$$p00 = -276{,}9\ (-307{,}8;\ -246);$$
$$p10 = -6{,}441\ (-9{,}65;\ -3{,}233);$$
$$p01 = 577{,}4\ (545{,}1;\ 609{,}6);$$
$$p20 = -0{,}05262\ (-0{,}2112;\ 0{,}1059);$$
$$p11 = 14{,}9\ (12{,}97;\ 16{,}84);$$
$$p02 = -62{,}3\ (-70{,}16;\ -54{,}44);$$
$$p30 = -0{,}001724\ (-0{,}004664;\ 0{,}001217);$$
$$p21 = -0{,}01679\ (-0{,}04589;\ 0{,}0123);$$
$$p12 = -3{,}396\ (-3{,}811;\ -2{,}98).$$

The resulting approximated surface allows calculating the furnace temperature profile for any arbitrary set point at the temperature.

To assess the adequacy and accuracy of the values, obtained using the approximated surface, a comparison of the calculated and experimental parameters was carried out for a number of set points, which were not used in the original mathematical processing. For example, Figures 5 and 6 show the calculated and experimental temperature profiles of the furnace for 300 и 1000 °C set points, respectively.

As it is seen from the Figures, the discrepancy in the parameters, determined with the approximated surface and measured temperature profiles, does not exceed ±3 °C, which is in accordance with the requirements for practical engineering calculations.

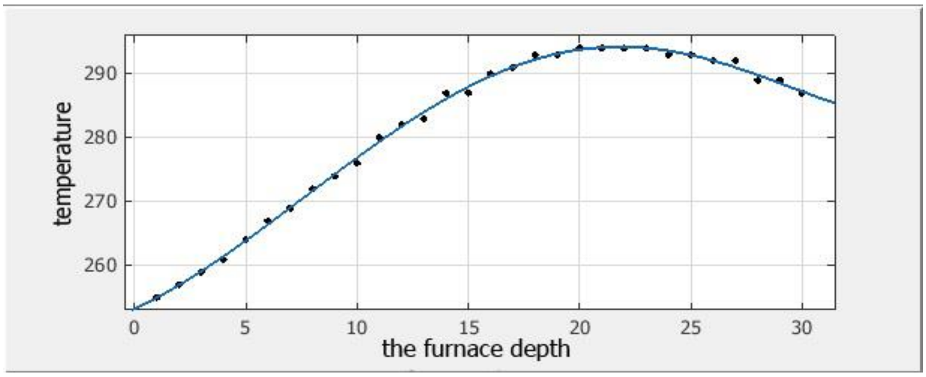


Figure 5 – Calculated and measured profiles for 300 °C set point

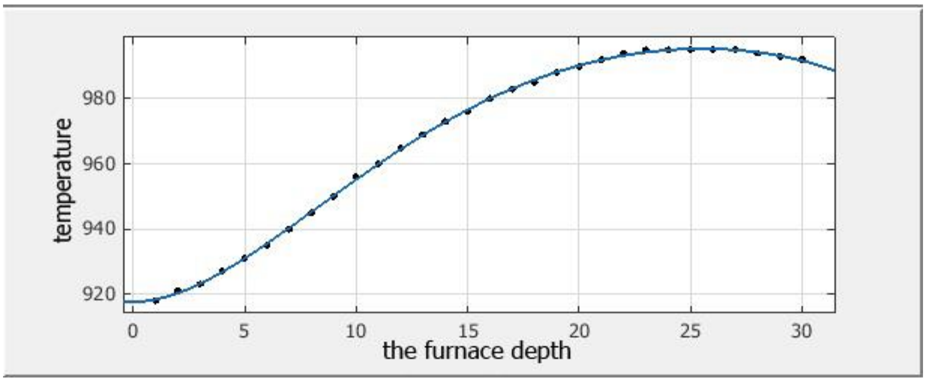


Figure 6 – Calculated and measured profiles for 1000 °C set point

The resulting analytical expression, which describes approximated surface of the temperature profiles of the studied furnace, allows evaluating only the vertical size of the non-gradient zone (NGZ) of the working chamber . The studies are the first step in working towards the application of approximating expressions for assessing the full set of NGZ parameters of the shaft-type furnace. At subsequent stages the evaluation of the radial temperature change in the furnace working chamber will be conducted.

Thus, this work shows the permissibility of using relatively simple approximating analytical expressions to assess the parameters of non-gradient zone (NGZ) of the shaft-type furnace working chamber. The furnace temperature profile may be analytically determined and graphically constructed for any arbitrary set point from the operating temperature range. The accuracy of the temperature profile design and an assessment of the NGZ axial dimension with its use is acceptable for practical engineering calculations.

Additional positive feature of this approach is the convenience and ease of programming the considered approximated surface and its use in the software of the furnace controller. This gives the opportunity of almost instantaneous construction of the furnace calculated temperature profile on the computer screen of the operator when setting a new set point by the temperature.

Developed furnace design and the levels of temperature fields in its working chamber allows carrying out the experiments on a continuous solid-phase synthesis of almost any oxide materials: ferrites, luminophores, semiconductors, posistors, piezoelectric materials, high-temperature superconductors, structural, condensed and other materials.

References

1. Katsnelson L M, Kerbel B.M. Continuous solid-phase synthesis of ultra- and nano powders of oxide materials for producting high-functional ceramics *Non-ferrous metal* 2012, **1,** 34-37
2. Kerbel B.M., Katsnelson L.M., Buynovskiy A.S., Tereschenko E.V., Daneikina N.V. Synthesis of photoluminophors using a continuous solid-phase technology *Procedia Chemistry*, 2014, **1**, 152–157
3. Katznelson L.M., Kerbel B.M. Production of technologically equilibrium oxide functional materials with increased electrophysical parameters. South Siberian Scientific Bulletin; 2013, **1(3),** 34-46; Online access: http://s-sibsb.ru/issues-of-the-journal.html?catid=21.
4. Katznelson L.M., Kerbel B.M. Installation of a continuous solid-phase synthesis of nanostructured powders and ultra-oxide materials in a real ceramic production. *Non-ferrous metals*., 2012, **1**, 75 – 78.
5. Laptev G.I., Laptev G.G. Mathematical physics equations. M.: *Nauka*, 2003.
6. Numerical methods: using MATLAB: translated from English. / D.G. Matthews, K.D. Fink; Ed. Y.V. Kozachenko. – **3-rd Ed**. - Moscow: Williams, 2001. - 720 p.
7. Heat and mass transfer. /A.S. Telegin, V.S. Shvydkoi, Yu.G.Yaroshenko, Moscow, Metallurgy, 1995