Impact of heating conditions on the synthesis dynamics of composites in a cylindrical mold

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Abstract. The paper suggests a model of powder compact heating in a cylindrical mold. The model accounts for various conditions of the reactor wall heating by different devices available for a laboratory experiment. Different heating conditions are set as different boundary conditions. The effective thermophysical properties of the mixture in the reactor are considered to be constant. The treatise demonstrates the examples of numerical modeling for three heating conditions, which lead to different respective conditions of reaction initiation due to nonuniform temperature propagation in the compact.

1. Introduction
Heat transfer is one of the main processes in the formation of the materials’ structure and surface during their synthesis and processing. Any high-temperature process is aimed at attaining a new type of material or composition that possesses the highest properties and low cost. Different conditions of the synthesis cause different composition of the material. Therefore, the mechanical, physicochemical and operational characteristics of materials and parts are mainly determined by such thermal parameters as temperature field, thermal cycle, heating and cooling rates.

Indeed, in [1] a compacted specimen was subjected to electric-field treatment. As a result, the reaction initiated inside the compact. In [2], the authors initiated the reaction through heating a steel part—touching one of the ends of the compacted specimens—using an induction coil. The authors of [3] ignited cylindrical compacts using a tungsten coil. In all the cases, the deliverable is a high-density product. The selection of the initiation source should also take into account the reaction type and particle size of the powder mixture. In some cases, low exothermicity of the reaction between powder compact components requires preliminary heating of the system, similarly to [3]. Sometimes, selecting a more suitable heating method is required [2].

Thus, the classification of heating sources becomes of high importance. As a rule, literature sources contain classification of sources into distributed and pointed; surface and volumetric; immovable and moving; continuous and pulsed ones.

The traditional approach to synthesis modeling introduces a concept of effective heat source for different processing types, which allows distinguishing in them a general regularity and specificity. Effective heat source parameters include thermophysical and optical characteristics of a material. In this case, the temperature field is the only independent characteristic through which those remaining are determined: motion of phase boundaries, chemical reaction rates, mass transfer of alloying additives, etc.
Current work is aimed at investigating the effect of heating conditions on the dynamics of a compact heating in a cylindrical reactor.

2. Mathematical statement of the problem

The mathematical statement of the problem of powder composite heating in a cylindrical reactor (Fig. 1) includes a two-dimensional heat conductivity equation for a powder mixture:

\[
(c_a \rho_a) \frac{\partial T_A}{\partial t} = \frac{1}{r} \frac{\partial}{\partial r} \left( \lambda_r \frac{\partial T_A}{\partial r} \right) + \frac{\partial}{\partial z} \left( \lambda_z \frac{\partial T_A}{\partial z} \right) + W_H \tag{1}
\]

The equation includes the term accounting for the heating through electric fields. For the reactor’s walls, bottom and punch, equations similar to (1) are composed, but without source terms. It is assumed that the heat contact between the materials is ideal. In the center, a condition of symmetry is established.

Function \(W_H\) in eq. (1) characterizes heating due to current \(I(t)\). This value is considered to be volumetric. In this case, function \(W_H\) changes in time following a certain law:

\[
W_H = R_e I^2(t). \tag{2}
\]

In the case of heating by high-frequency currents, from the inductor at interface \(R_e\) the heat flux will be

\[
r = R_e : -\lambda_r \frac{\partial T_B}{\partial r} = \sigma \epsilon B \left( T_B^4 - T_A^4 \right) \tag{3}
\]

where \(T_B\) is the change in the temperature touching the external reactor wall obtained from the solution of a separate electromagnetic problem [4].

If the powder compact is heated through heat conductivity due to heat of bottom \(z = H_A + H_z\) and punch \(z = -H_1\), the heat source is set on the following boundaries: \(T\) \(|_{z=-H_1} = T_c\) or \(-\lambda_c \cdot \partial T / \partial z \) \(|_{z=-H_1} = q_c\); similarly, on the other surface \(T\) \(|_{z=H_A + H_z} = -T_c\) or \(\lambda_c \cdot \partial T / \partial z \) \(|_{z=H_A + H_z} = q_c\).

At the initial moment of time, the temperature in all regions is set: \(r = 0: T_A = T_{A0}, T_B = T_{B0}, T_c = T_{c0}\).

In general case, the problem is a set of equations that allows deriving the temperature distribution at any time for different composition of powder mixtures and different materials that may comprise the cylindrical reactor walls. The result will be also affected by the reactor wall thickness and porosity of the powder mixture, because by accumulating the heat, the reactor walls become an additional heat source for the mixture.

The problem was solved numerically using implicit difference scheme of second-order approximation in space and first-order approximation in time using splitting in coordinates and the linear sweep method. The calculations yielded temperature fields along the whole studied region for different heating variants.

In the case of electric heating (2), the electrical resistance, in general case, depends on such parameters as structure, medium composition, temperature and porosity, i.e. it changes in time. Volumetric heat sources feature relatively large heating time up to the working temperature. The energy concentration in such sources is usually small.

In the case of heating by high-frequency currents by inductor (3), the inner reactor surface heats up and then the heat propagates through heat conductivity inside the system. An important role is played by the current density in this case. An electromagnetic problem [4] was solved separately. Its solution gave the dependence of the heater temperature on the magnetic field strength. The body that is characterized by this changing temperature are reactor walls heated by radiation. Then, the powder mixture is heated by the walls through heat conductivity. The processed results showed that the
temperature rise can be described by a straight line \( T_n(t, H) = at + b \), where the coefficients depend on \( H \).

In case (4), the calculations used constant temperature on the upper and lower boundaries of the reactor.

As an example, let us consider a compact comprised of Ni and Al powder mixture. The effective properties of the mixture obey the following rule:

\[
\left( c_A \rho_A \right)^0 = c_N \rho_N \xi + c_A \rho_A (1 - \xi); \\
\lambda_A^0 = \lambda_N \xi + \lambda_A (1 - \xi);
\]

\( \xi \) is the mass fraction of nickel in the initial mixture, \( \rho_A \), \( \rho_N \), \( c_A \), \( c_N \) are density and heat capacity of pure elements in the mixture. Hence, \( \left( c_A \rho_A \right)^0 = 4.04; \lambda_A^0 = 1.024 \).

In general case, the material of the reactor walls, bottom and punch may be different. The material of the reactor walls was steel E235 with the following properties: \( c_b = c_c = 0.462 \, [J/(g \cdot K)]; \rho_b = \rho_c = 7.87 \, [g/cm^3]; \lambda_b = \lambda_c = 0.46 \, [W/(cm \cdot K)]. \)

The calculations were made with the following parameters [6]: \( R_i = 3, \ R_s = 4.5 \, [cm], \ 
\sigma = 5.67 \times 10^{-12} \, [W/cm^2 \cdot K^4], \ \varepsilon = 0.4, \ c_N = 0.482; \ c_A = 0.951 \, [J/(g \cdot K)]; \ 
\rho_N = 8.9; \ \rho_A = 2.7 \, [g/cm^3]; \lambda_N = 0.8; \lambda_A = 2.4 \, [W/(cm \cdot K)]. \)

3. Results and Discussion

Below are the calculation examples for different heating conditions (Fig. 2–4).

In the case of powder compact heating, the heat propagates from upper and lower reactor parts (bottom and punch) through the heat conductivity of the materials. The reaction mixture gradually heats up. Since the side walls of the reactor, in this case, are the heat sinks (they should also heat up), the temperature distribution at the initial stage is nonuniform.

In the figures, the reactor bottom is at the top, while the punch is at the bottom.

![Figure 2](image-url)

**Figure 2.** Temperature fields corresponding to heating of bottom and punch at different moments of time: a) 40 s; b) 70 s; c) 100 s; d) 200 s.

In the case of electric heating inside the powder compact, all reactor walls are heat sinks. Uniform heating of the powder compact is evident. However, since the reactor bottom thickness is smaller than that of the punch, it will require less heat for the heat-up. Therefore, more uniform temperature is expected to be closer to the reactor's bottom.
Figure 3. Temperature fields at different moments of time during heating by volumetric source (through Joule heating): a) 40 s; b) 70 s; c) 100 s; d) 200 s.

Heating by high-frequency currents by an inductor provides uniform heating from side surfaces. However, evidently from Fig. 4, the heat-up is nonuniform along the specimen.

Figure 4. Temperature fields at different moments of time during heating by high-frequency currents from inductor a) 40 s; b) 70 s; c) 100 s; d) 200 s.

4. Conclusion
Thus, different heating conditions create different conditions for reaction initiation, which should be accounted when selecting the synthesis conditions and interpreting experimental data.

Acknowledgments
This work has been performed under the program of fundamental research project III. 23.2.2.

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