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MATHEMATICAL MODELS OF PURIFICATION OF A MELT CENTRIFUGED AT HIGH TEMPERATURES

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The authors describe mathematically the processes of metal melting and crystallization in a crucible rotating around a heater as well as a migration model of nonmetallic impurities in the melt. Numerical methods for solving problems and results of a computation experiment are described.

In a crucible of an experimental setup rotating around a heater a metal becomes heated and melts (see Fig. 1). Here, in the liquidus (melt) phase the migration of nonmetallic impurities due to a centrifugal force that develops as a result of centrifuging is observed. After some time the heater is removed from the setup and the phase of melt cooling and crystallization proceeds. Along the axis of the ingot obtained, a set of crystallization conditions, such as a cooling rate, pressure, and concentration of nonmetallic impurities are implemented. A comparison of the structure and properties of an ingot metal with crystallization conditions is of scientific and practical value [1, 2]. Up to now the greatest emphasis has been given to metallographic analysis of the problem. Theoretical studies of the purification of a centrifuged melt, based on mathematical modeling, are covered inadequately in the current literature. Related problems have been discussed, for instance, in [1, 3, 4]. Below we suggest a rational mathematical model of thermohydrodynamic processes under high-temperature centrifuging conditions that permits optimization of a full-scale experiment.

We consider the steady-state rotation of a crucible when the melt has no flows.

Thermal Processes. The dynamics of the temperature field $\vartheta(x, r, \tau)$ in an ingot may be described by the boundary-value problem

$$\rho \frac{\partial h}{\partial \tau} = \frac{1}{r} \frac{\partial}{\partial r} r\lambda \frac{\partial \vartheta}{\partial r} + \frac{\partial}{\partial x} \lambda \frac{\partial \vartheta}{\partial x}, \tag{1}$$

$$0 < \tau < \tau_e, \quad 0 < r < r_0(x), \quad 0 < x < l; \quad \vartheta|_{\tau=0} = \vartheta_0; \quad \lambda \frac{\partial \vartheta}{\partial n}\bigg|_B = q.$$

Here l is the crucible length, the function $r_0(x)$ describes its shape; ρ is the metal density; $\lambda(\vartheta)$ is the thermal conductivity; τ is the time; τ_e is the time of the technological process; ϑ_0 is the initial temperature; $h(\vartheta)$ is the enthalpy. In a first approximation we may consider that

$$h(\vartheta) = \begin{cases} c\vartheta + L/2, & \vartheta > \vartheta_f, \\ c\vartheta - L/2, & \vartheta < \vartheta_f, \end{cases} \tag{2}$$

where c is the heat capacity; L is the latent heat of melting. Problem (1), (2) is written in the form of a generalized statement of the two-phase Stefan problem [5] and allows modeling of melting-crystallization processes. Preliminary analysis of the boundary conditions showed that for real geometric and thermophysical parameters of the process the density of the heat flux q across the open surface of the crucible ($x = 0$) is by one or two orders of magnitude higher than on the walls. In this case heat is mainly transferred by diffuse radiation while heat conduction and free convection in the gap between the heater and the crucible may be neglected. Therefore the

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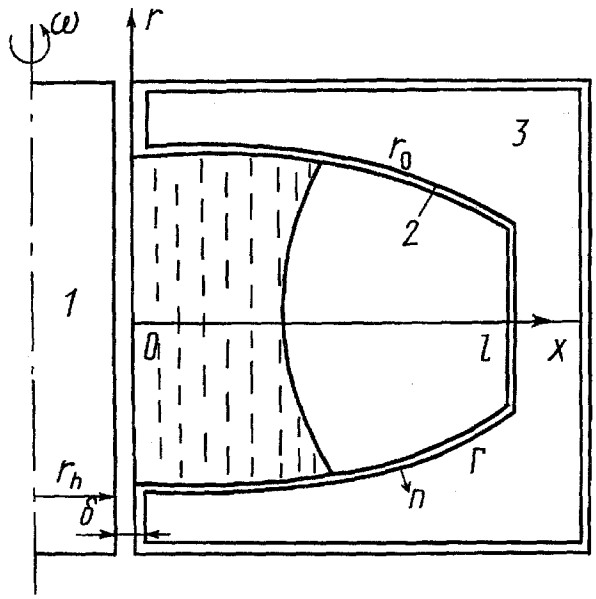

Fig. 1. Schematic of the experimental setup: 1) heater; 2) crucible; 3) refractory lining.

value of q in boundary condition (1) may be assumed equal to zero everywhere with the exception of the open surface, $x = 0$, where in the heating stage we have [6]:

$$-\lambda \frac{\partial \vartheta}{\partial x} = \sigma \hat{\vartheta}_h^4 (1 - \hat{\vartheta}^4/\hat{\vartheta}_h^4), \quad x = 0, \quad \tau < \tau_h. \tag{3}$$

In (3), $\sigma = 5.67 \cdot 10^{-8}$ W/(m$^2 \cdot$ K^4) is the Stefan-Boltzmann constant; τ_h is the time of source action; and the sign $\hat{}$ indicates the absolute temperature $\hat{\vartheta} = \vartheta + 273$. At the cooling stage ($\tau_\eta < \tau < \tau_\varepsilon$) q may be determined by solving the problem of radiative heat transfer. Under the assumption that the temperature of the open crucible surface and that of the refractory lining are equal, we employ the well-known solution of the problem of the radiation of the inner surface of a cylindrical groove [6] and obtain the following rough estimate:

$$q = -0.14 \sigma \hat{\vartheta}_h^4, \quad x = 0, \quad \tau > \tau_h. \tag{4}$$

Note that along with condition (4) other models of cooling, e.g., by water, may be considered. In model (1)-(4) we pass to the dimensionless quantities

$$X = \frac{x}{l}, \quad R = \frac{r}{l}, \quad t = \frac{\tau a^0}{l^2}, \quad k = \frac{\lambda}{\lambda^0}, \quad T = \frac{\vartheta - \vartheta_f}{\vartheta_f - \vartheta_0}, \quad H = \frac{h - c\vartheta_f}{c(\vartheta_f - \vartheta_0)},$$

$$\mathrm{Ko} = \frac{L}{c(\vartheta_f - \vartheta_0)}, \quad Q = \frac{ql}{\lambda^0 (\vartheta_f - \vartheta_0)}, \quad Q_h = \frac{\sigma \hat{\vartheta}^4 l}{\lambda^0 (\vartheta_f - \vartheta_0)}, \quad Q_c = 0.14 Q_h. \tag{5}$$

In formulas (5) the superscript "0" indicates quantities calculated at some "characteristic" temperature ϑ^0; $a^0 = \lambda^0/c\rho$ is the thermal diffusivity; Ko is the Kosovich number. Relations (1)-(4) acquire the form

$$\frac{\partial H}{\partial t} = \frac{1}{R} \frac{\partial}{\partial R} Rk \frac{\partial T}{\partial R} + \frac{\partial}{\partial X} k \frac{\partial T}{\partial X}, \tag{6}$$

$$0 < t < t_e, \quad 0 < X < 1, \quad 0 < R < R_0(X);$$

$$H(T) = T + \mathrm{sgn}(T)\, \mathrm{Ko}/2; \quad t = 0; \quad T = -1;$$

$$k\frac{\partial T}{\partial n}=\begin{cases} Q_h(1-\tilde{T}^4), & t<t_h, \quad X=0, \\ -Q_c\tilde{T}^4, & t_h<t<t_e, \quad X=0, \\ 0, & X\neq 0. \end{cases} \tag{7}$$

In formula (7) the expression

$$\tilde{T}=\hat{\vartheta}/\hat{\vartheta}_h=[\vartheta_f+273+T(\vartheta_f-\vartheta_0)]/[\vartheta_f+273+T_h(\vartheta_f-\vartheta_0)]$$

may be simplified if we take into account that $\vartheta_0 < \vartheta_f$, $273 < \vartheta_f$. Then

$$\tilde{T}\approx\frac{1+T}{1+T_h}, \quad T_h=\frac{\vartheta_h-\vartheta_f}{\vartheta_f-\vartheta_0}. \tag{8}$$

Thus, the thermal processes in an ingot are described by model (6)-(8), which contains six dimensionless parameters, namely, the heating and cooling intensities Q_h, T_h, Q_c, the duration of the phases of the technological process t_h, t_e, the criterion Ko, and also the function $k(T)$. The last two quantities are unambiguously determined by the thermophysical properties of a metal, and therefore a variety of technological situations are determined, in fact, by the first five parameters. Naturally, the crucible shape $R_0(X)$ also influences the solution of the problem. However, it is close to a cylinder and there are no heat fluxes at the boundary $R = R_0$. In this case the temperature field will depend weakly on the radius R. Therefore in practical calculations instead of (6) we may use the quasi-one-dimensional equation that is valid along the ingot axis $R = 0$:

$$\frac{\partial H}{\partial t}=\frac{1}{R_0^2}\frac{\partial}{\partial X}R_0^2\,k\frac{\partial T}{\partial X}, \quad 0<t<t_e, \quad 0<X<1. \tag{9}$$

In this formulation, the function $R_0(X)$ has the meaning of the radius of a heat flux tube and is determined up to a multiplier.

Migration of Particles. Impurities contained in the metal may rise to the melt surface due to centrifuging with the velocity

$$v=\frac{2}{g}(1-K_\rho)\frac{gA^2}{\nu}, \quad g=\omega^2(r_h+\delta+x). \tag{10}$$

In the Stokes formula (10) r_h is the heater radius; δ is the gap (see Fig. 1); ω is the angular velocity; $\nu(\vartheta)$ is the kinematic viscosity of the melt; A is the effective radius of a particle; $K_\rho = \rho_*/\rho$, ρ_* is the density of nonmetallic inclusions. As a result, there is a change in the particle concentration. For low impurity concentrations $c(x, r, \tau)$ typical of metals this process is adequately described by the equation

$$\frac{\partial c}{\partial \tau}=\nabla(d\nabla c+vc). \tag{11}$$

Equations (10), (11), valid only in the liquid phase, may be extended to the entire region by defining the viscosity and diffusion coefficients in the solid phase in the following way: $\nu = \infty$, $d = 0$ at $\vartheta \geq \vartheta_f$. Then in order to formulate the problem of the concentration it is sufficient to prescribe the boundary conditions

$$c=c_0 \quad \text{at} \quad \tau=0, \quad d\frac{\partial c}{\partial n}+vc=0 \quad \text{on} \quad \Gamma. \tag{12}$$

Passing to variables (5) in (11), (12) and introducing additionally the quantities

$$D=d/d^0, \quad C=c/c_0, \quad K_\nu=\nu/\nu^0, \quad K_a=A/A_0, \quad \mathrm{Pr}=\frac{d^0}{a^0}, \quad V=\frac{X+X_1}{1+X_1}K_\nu^{-1}, \tag{13}$$

$$X_1 = \frac{r_h + \delta}{l}, \quad \mathrm{Pe} = \frac{\nu^0 l K_a^2}{a^0}, \quad \nu^0 = \frac{2(1 - K_\rho)\omega^2 (r_h + \delta + l) A_0^2}{9\nu^0},$$

we obtain the formulation of the convective diffusion problem in dimensionless form. By analogy with the heat problem we may write at once the model of particle migration along the ingot axis

$$\frac{\partial C}{\partial t} = \frac{1}{R_0^2} \frac{\partial}{\partial X} R_0^2 Q, \quad 0 < X < 1, \quad 0 < t < t_e,$$
$$Q \equiv \mathrm{Pr} D \frac{\partial C}{\partial X} + \mathrm{Pe} V C; \quad Q|_{X=0} = Q|_{X=1} = 0; \quad C|_{t=0} = 1. \tag{14}$$

In the conversion formulas (13) the superscript 0, as before, points to the characteristic temperature ϑ^0, while A_0 is some fixed size of a particle. The criterion K_a is introduced to describe the dynamics of the concentration field of particles of different size using model (14). For this, as follows from (13), a series of solutions of problem (14) must be obtained for different Peclet numbers. Since the design dimension X_1 is practically constant, the functions K_ν and D are determined by the temperature T, and the Prandtl number Pr depends only on the material, Pe is the main similarity parameter and provides information on the size of the particles, their density, the rotational speed, and the geometric size of the setup in the problem under consideration.

Algorithm of Numerical Implementation. To solve Stefan problem (7)-(9), we adopt the approach [7] based on the representation

$$\frac{\partial H}{\partial t} = [1 + \mathrm{Ko}\, \delta(T)] \frac{\partial T}{\partial t} \tag{15}$$

and "smearing" of the Dirac δ-function. We use the approximation

$$\delta(T) = \begin{cases} 0, & |T| > \varepsilon, \\ \dfrac{4\pi}{4\varepsilon} \cos\left(\dfrac{\pi}{2\varepsilon} T\right), & |T| < \varepsilon, \end{cases} \tag{16}$$

where ε is the regularization parameter. For the problem obtained after substitution of (15) into Eq. (9), we have written an implicit two-layer difference scheme. It represents a system of nonlinear equations where the nonlinearity "sources" are the representation (15), (16), the dependence $k(T)$ in Eq. (9), and boundary condition (7). In connection with this, the iteration technique has been employed to solve the problem on each time layer. Two iteration levels are considered: in the external cycle the functions $k(T)$ and $\delta(T)$ are refined using the newly calculated values of T, while in the internal Newton process a boundary value is determined from condition (7). The linearized system of equations is solved by the elimination method [7]. To check the accuracy of the algorithm we made a series of calculations using denser networks and compared numerical solutions with exact self-similar solutions of the Stefan problem and calculation results obtained by other numerical methods [8, 9]. In the course of testing, optimum values of the scheme parameters (ε, network steps with respect to X and t) have been determined.

The problem of impurity migration is linear; however a numerical solution of it presents difficulties because the coefficients D and V decrease sharply to zero in a small neighborhood of a phase boundary. Moreover, and the Prandtl number is small, the Peclet criterion may change in a very wide range due, mainly, to the need to model the migration of particles of different sizes. In particular, at $\mathrm{Pe} \gg 1$ near the open surface, $X = 0$, a boundary layer is inevitably formed. Taking into account these circumstances, we used a nonuniform network in the calculations that becomes denser as $X \to 0$, and we approximated, in building the difference scheme, the convective part of the operator with account for the sign of V so as to intensify the diagonal predominance of the matrix of the system of finite-difference equations. The numerical algorithm was tested using a sequence of denser networks. It was confirmed that the difference network was conservative and provided constancy of the total concentration of particles

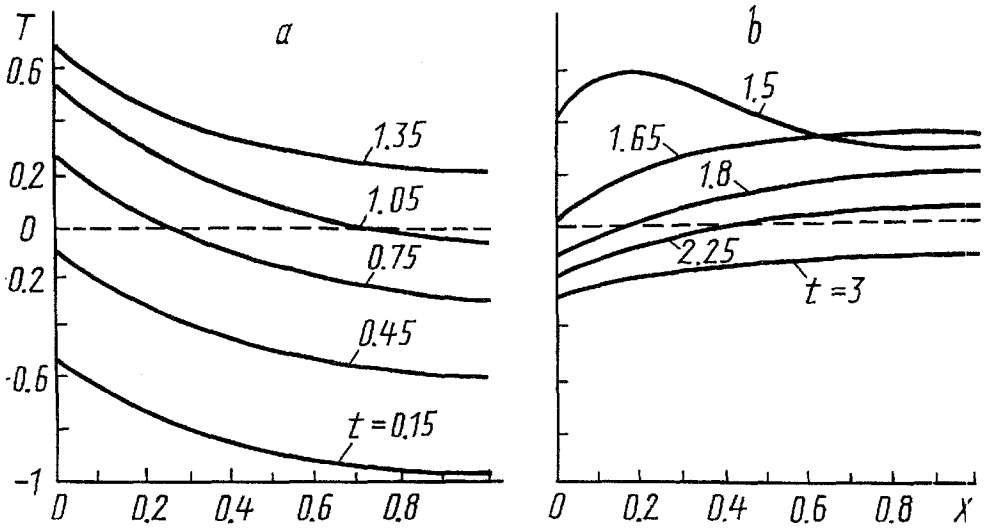

Fig. 2. Dynamics of the temperature field: a) heating and melting; b) cooling and crystallization. The dashed line indicates the dimensionless temperature of phase transitions $T_f = 0$.

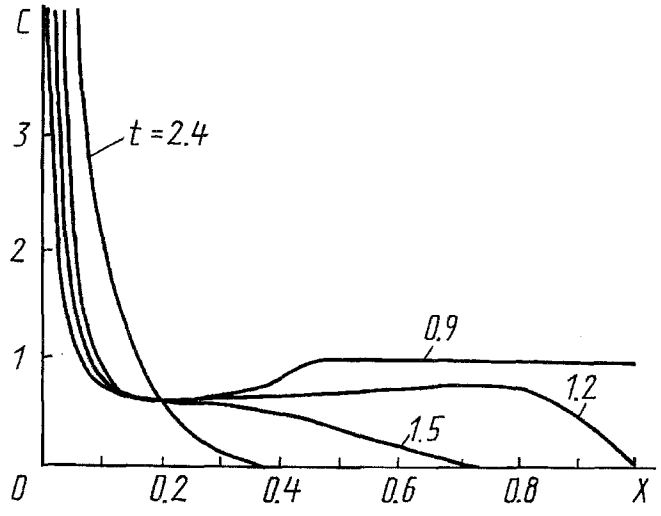

Fig. 3. Concentration along the ingot axis versus time; Pr = 0.016; Pe = 1.47.

in an ingot. Network parameters were found that ensured acceptable accuracy in a wide range of the coefficients of problem (14). As already mentioned, the coefficients V and D are prescribed as functions of the temperature T. Therefore in solving the problem for the concentration the function $T(X, t)$ was reproduced bilinearly on the rectangle $X_i < X < X_{i+1}$, $t_j < t < t_{j+1}$ using the solution of the heat problem as nodal values.

Calculation Results. We shall consider a model centrifuging process for a cast iron ingot. The thermophysical properties of the metal are prescribed as follows: $\vartheta_f = 1153^\circ C$, $\lambda^0 = 17$ W/(m·K), $c = 962$ J/(kg·K), $L = 285$ kg/kg, $\rho = 7000$ kg/m^3, $\nu^0 = 3 \cdot 10^{-7}$ m^2/sec, $d^0 = 4 \cdot 10^{-8}$ m^2/sec [10]. The temperature $\vartheta^0 = 1250\ ^\circ C$ is chosen as the characteristic one, and at the initial moment $\vartheta = \vartheta_0 = 25^\circ C$. We assume that nonmetallic impurities have the characteristic size $A^0 = 2 \cdot 10^{-6}$ m and density $\rho^* = 2.25$ kg/m^3 and the geometric dimensions are as follows: $l = 52$ mm, $r_0(0) = 22$ mm, $r_0(l) = 16$ mm, $\delta = 3$ mm. The heat source is heated to the temperature $\vartheta_h = 2000^\circ C$ and its time of action is $\tau_h = 30$ min; the total time of the process is $\tau_e = 60$ min. The rotational speed is $\omega = 60$ sec^{-1}. Using formulas (5), (13), we determine characteristic scales of the process such as the velocity of floating up of the particles $v^0 \approx 7 \cdot 10^{-5}$ m/sec, the specific heat flux $q^0 = \lambda^0(\vartheta_f - \vartheta_0)/l \approx 10^5$ W/m^2, the ingot heating time $\tau^0 = l^2/a^0 \approx 17$ min, the time of melt purification from particles with size A^0 $l/v^0 \approx 12$ min. The pressure along the ingot axis increases from 0.01 MPa at $x = 0$ to 0.03 MPa at $x = l$. Simultaneously, we calculate the

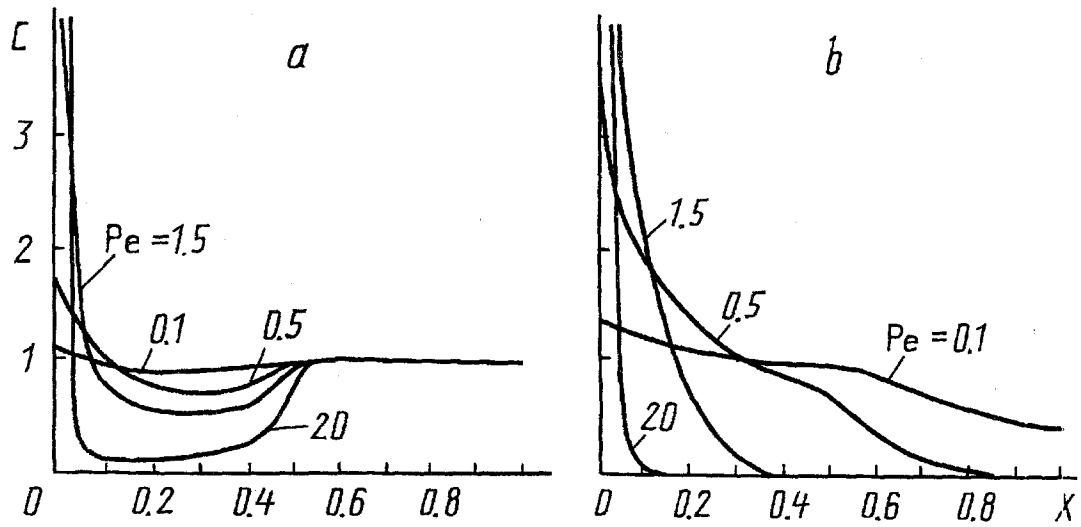

Fig. 4. Concentration distribution versus the Pe number: a) $t = 0.9$, b) 3.

dimensionless parameters that are the initial data for mathematical model (7), (9), (14). We obtain Ko = 0.26, Pr = 0.016, Pe = 1.47, $t_h = 1.5$, $t_e = 3$, $Q_h = 3.48$, $Q_c = 0.48$, $T_h = 0.66$, $K_\rho = 0.32$, $K_a = 1$, $X_1 \approx 0.5$. In the calculations given below, instead of $Q_c = 0.48$, which corresponds to natural cooling by radiation, the value $Q_c = 8$ is adopted, which gives a more dynamic picture of the process. In some sense such a high intensity of heat release may be interpreted as forced cooling.

Figure 2 shows the dynamics of the temperature field $T(X, t)$, the heating stage is depicted in Fig. 2a, and the cooling phase in Fig. 2b. We may follow the propagation of the melting-crystallization front using the intersection of the graphs of T with the level $T_f = 0$.

The distribution of the relative concentration along the X-axis at different moments of time is shown in Fig. 3. The rise of particles to the free surface, the formation of a boundary layer there, and the melt purification in the main part of the ingot are clearly seen. These results are obtained for particles of the same size $K_a = 1$. In a real metal, there are, naturally, impurity particles of different sizes. Within the framework of the suggested model, the dynamics of the concentration field of particles of each size may be studied independently by prescribing the Peclet number corresponding to this size. The dependence of the process on the Pe number is shown in Fig. 4. Note that under the chosen conditions the melt is quickly purified of comparatively coarse particles (Pe > 1), while fine (Pe < 1) foreign particles are centrifuged to a substantially lesser degree. Knowing the dependence of C on Pe, it is easy to follow the changes in the size distribution function of particles in the cross section X = const during centrifuging. Our results of computer-aided modeling show that in the main part of the ingot the maximum of the distribution function shifts toward low values of K_a with a simultaneous decrease of its value. The resultant curves (at the moment t_e) differ substantially from each other in different cross sections X = const. These data may serve as a criterion of the adequacy of the model when it is identified using experimental data.

The theoretical analysis of high-temperature centrifuging made in the present work may be of help in designing facilities for melt purification. The corresponding numerical procedures may be used directly for prediction of purification of metal ingots from oxides and gas bubbles. The mathematical description supplemented by the mechanism of solubility of graphite impurity allows modeling of the complicated processes of practical importance in the manufacture of iron castings.

NOTATION

Dimensional quantities: r, x, cylindrical coordinates; τ_h and τ_e, time of the heater action and the process duration, respectively; ω, rotational speed; l and $r_0(x)$, crucible length and width; ϑ, temperature; $\hat{\vartheta}$, absolute temperature; $\vartheta_0 = \vartheta$ at $\tau = 0$; ϑ_f, melting point; ϑ_h, heater temperature; ρ_*, density of nonmetallic impurities; L, latent heat of phase transitions; q, heat or concentration flux density; v, velocity of floating up of the particle; A,

impurity size; d, diffusion coefficient. Dimensionless quantities: R, X, coordinates; t, time; T, temperature; H, enthalpy; Q, flux density; V, velocity; D, diffusion; K_ν, viscosity; Pe, Pr, Ko, K_ρ, K_a, similarity parameters.

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