Journal of Engineering Physics and Thermophysics, Vol. 67, No. 3-4, 1994

HEAT AND MASS TRANSFER IN A SOLIDIFYING BINARY MELT UNDER MIXED CONVECTION WITH ACCOUNT FOR TURBULENCE

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UDC 536.42

A generalized mathematical model has been developed for heat transfer and hydrodynamics with account for turbulence in the stages of pouring and subsequent formation of a steel ingot.

In the development of power- and resource-saving casting technologies, computer systems are being used more and more extensively. In particular, a promising trend is development of systems for computer-aided mathematical modeling of hydrodynamic and heat and mass transfer processes in forming ingots and castings. Such systems optimize operating conditions in the production of cast blanks. Moreover, their role cannot be overestimated in developing integrated expert systems of computer-aided technological preparation of casting processes.

A mathematical model that reflects adequately the controlling factors in the process of forming ingots and castings is an important unit of this system. The mathematical model suggested in the present work is a logical extension of the previous one [1]. It includes turbulent transfer of momentum, heat, and mass in a melt that takes place under commercial conditions in top-filling of the mold and in subsequent solidification of large steel ingots and castings.

1. The hydrodynamic, thermal, and diffusional parts of the problem are modeled within continuum thermal mechanics [1], and turbulence is described by the k-ε model [2]. The system of dimensionless equations has the following form:

the transfer equation for an averaged vortex of velocity ω:

$$\frac{\partial \omega}{\partial \mathrm{Fo}} + \frac{\partial}{\partial x}(V_1\omega) + \frac{\partial}{\partial y}(V_2\omega) = \mathrm{Pr}\,[\nabla(1+\nu_t)\nabla\omega] + \mathrm{Pr}^2\left(\mathrm{Gr}_T\frac{\partial\theta}{\partial x} + \mathrm{Gr}_D\frac{\partial S}{\partial x}\right); \quad (1)$$

the Poisson equation for the averaged stream function ψ:

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} = -\omega; \quad (2)$$

the heat transfer equation for the temperature θ

$$c_e\frac{\partial\theta}{\partial \mathrm{Fo}} + \frac{\partial}{\partial x}(V_1\theta) + \frac{\partial}{\partial y}(V_2\theta) = \nabla\lambda\nabla\theta; \quad (3)$$

the mass transfer equation for the concentration S

$$(1-(1-k_0)\xi)\frac{\partial S}{\partial \mathrm{Fo}} + \frac{\partial}{\partial x}(V_1S) + \frac{\partial}{\partial y}(V_2S) = \frac{1}{\mathrm{Lu}}\nabla D\nabla S + (1-k_0)S\frac{\partial\xi}{\partial \mathrm{Fo}}; \quad (4)$$

the transfer equation for the turbulent energy k

Donetsk State University, Donetsk, Ukraine. Translated from Inzhenerno-Fizicheskii Zhurnal, Vol. 67, Nos. 3-4, pp. 202-208, September-October, 1994. Original article submitted March 31, 1993.

1062-0125/94/6734-0859$12.50

$$\frac{\partial k}{\partial \mathrm{Fo}} + \frac{\partial}{\partial x}(V_1 k) + \frac{\partial}{\partial y}(V_2 k) = \mathrm{Pr}\left[\nabla\left(1 + \frac{\nu_t}{\sigma_k}\right)\nabla k\right] +$$

$$+ G - \mathrm{Pr}^3 \frac{\nu_t}{\sigma_T}\left(\mathrm{Gr}_T \frac{\partial \theta}{\partial y} \mathrm{Gr}_D \frac{\partial S}{\partial y}\right) - \varepsilon - 2\,\mathrm{Pr}\left[\left(\frac{\partial k^{1/2}}{\partial x}\right)^2 + \left(\frac{\partial k^{1/2}}{\partial y}\right)^2\right]; \tag{5}$$

the transfer equation for the dissipation rate ε of the turbulent energy

$$\frac{\partial \varepsilon}{\partial \mathrm{Fo}} + \frac{\partial}{\partial x}(V_1 \varepsilon) + \frac{\partial}{\partial y}(V_2 \varepsilon) = \mathrm{Pr}\left[\nabla\left(1 + \frac{\nu_t}{\sigma_\varepsilon}\right)\nabla \varepsilon\right] +$$

$$+ C_1\,\mathrm{Pr} G - C_3\,\mathrm{Pr}^2 \frac{\varepsilon \nu_t}{k \sigma_T}\left(\mathrm{Gr}_T \frac{\partial \theta}{\partial y} + \mathrm{Gr}_D \frac{\partial S}{\partial y}\right) - C_2 \frac{\varepsilon^2}{k}(1 - 0.3 \exp(-\mathrm{Re}_t)) +$$

$$+ 2\,\mathrm{Pr}\left[\left(\frac{\partial^2 V_1}{\partial x^2}\right)^2 + \left(\frac{\partial^2 V_1}{\partial y^2}\right)^2 + \left(\frac{\partial^2 V_2}{\partial x^2}\right)^2 + \left(\frac{\partial^2 V_2}{\partial y^2}\right)^2\right]; \tag{6}$$

the kinetic process of crystal growth is described by Kolmogorov's equation for the solid-phase fraction ξ:

$$\xi = 1 - \exp\left\{-a \int \alpha(\Delta\theta)\, V(\Delta\theta)\, d\theta\right\}. \tag{7}$$

The system of equations (1)-(6) is completed by the initial conditions

$$\mathrm{Fo} = 0: \quad \omega = \varphi = k = \varepsilon = \xi = 0; \quad \theta_m = \theta_{\mathrm{in.m}}; \quad \theta_{md} = \theta_{\mathrm{in.md}}. \tag{8}$$

The boundary conditions include the vertical symmetry of the region. Ideal contact is assumed on the metalingot interface. The boundary conditions for the stream function are written as

$$\varphi_{\Gamma_2} = 0; \quad \varphi_{\Gamma_3} = 0; \quad \varphi_{\Gamma_4} = \begin{cases} V_m x, & [0, R], \\ V_m R x/(L_1 - R)], & [R, L_1]. \end{cases} \tag{9}$$

The boundary conditions for the temperature are

$$\partial\theta/\partial r_{\Gamma_2\Gamma_3} = K(\theta - \theta_{\mathrm{ave}}). \tag{10}$$

On the interface of the melt and the mold wall conjugation conditions are used. The boundary conditions for ω are formed in the stage of the finite-difference approximation.

An inadequate description of turbulence in the near-wall region is a drawback of the k-ε model. This drawback is eliminated by the effects of nonisotropic dissipation and molecular viscosity. The modification of the model recommended in [2, 3] consists in inclusion of the elimination term

$$2\,\mathrm{Pr}\left[\left(\frac{\partial k^{1/2}}{\partial x}\right)^2 + \left(\frac{\partial k^{1/2}}{\partial y}\right)^2\right]$$

in the k-equation and the generation term

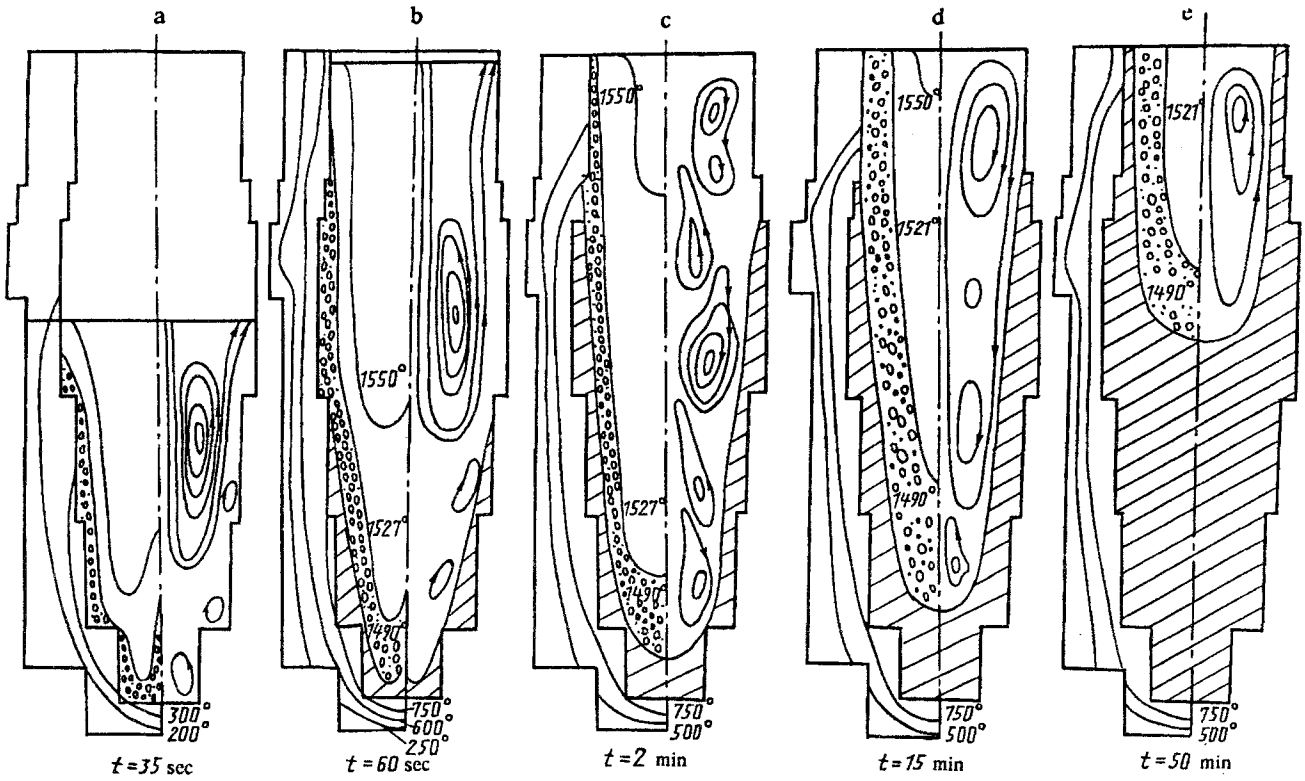

Fig. 1. Isotherms and lines of stream functions during pouring of steel into a mold (a, b) and solidification of the steel ingot (c, d, e).

$$2\,\mathrm{Pr}\left[\left(\frac{\partial^2 V_2}{\partial x^2}\right)^2+\left(\frac{\partial^2 V_2}{\partial y^2}\right)^2+\left(\frac{\partial^2 V_2}{\partial x^2}\right)^2+\left(\frac{\partial^2 V_2}{\partial y^2}\right)^2\right],$$

in the ε-equation and replacement of the turbulence constants C_μ and C_2 by

$$C_\mu \exp\left[-2.5/(1+\mathrm{Re_t}/50)\right];\quad C_2\frac{\varepsilon^2}{k}\left(1-0.3\exp\left(-\mathrm{Re_t^2}\right)\right).$$

The quantities k and ε are assumed to be zero on the walls, and the boundary conditions at the inlet are as follows:

$$k_{\Gamma_4}=1.5\,\mathrm{Tu}\,V_{\mathrm{m}}^2;\quad \varepsilon_{\Gamma_4}=C_\mu^{3/4}k^{3/2}/l;\quad [0,R]. \tag{11}$$

On the axis the fluxes of kinetic energy and the rates of its dissipation are 0, and on all the other boundaries, $k=\varepsilon=0$. For the diffusional part of the problem no admixture flows are assumed on all boundaries. In solidification, on the upper boundary, conditions of adhesion and impermeability are realized for the velocity, conditions of ideal insulation are realized for the temperature, and $k=0$, $\varepsilon=0$ for turbulence.

The model suggested allows momentum, heat, and mass transfer to be considered for various methods of pouring into molds of arbitrary configuration.

2. For construction of a computational algorithm, a finite difference method is used with application of methods of "disturbed coefficients," balance, and variable directions, which allows the problem to be reduced to Samarskii's monotonic scheme. The computational algorithm is implemented on a nonuniform spatial net of dimensions 38 × 45. A complicated configuration of the region is prescribed by stepwise approximation of the boundary conditions [4].

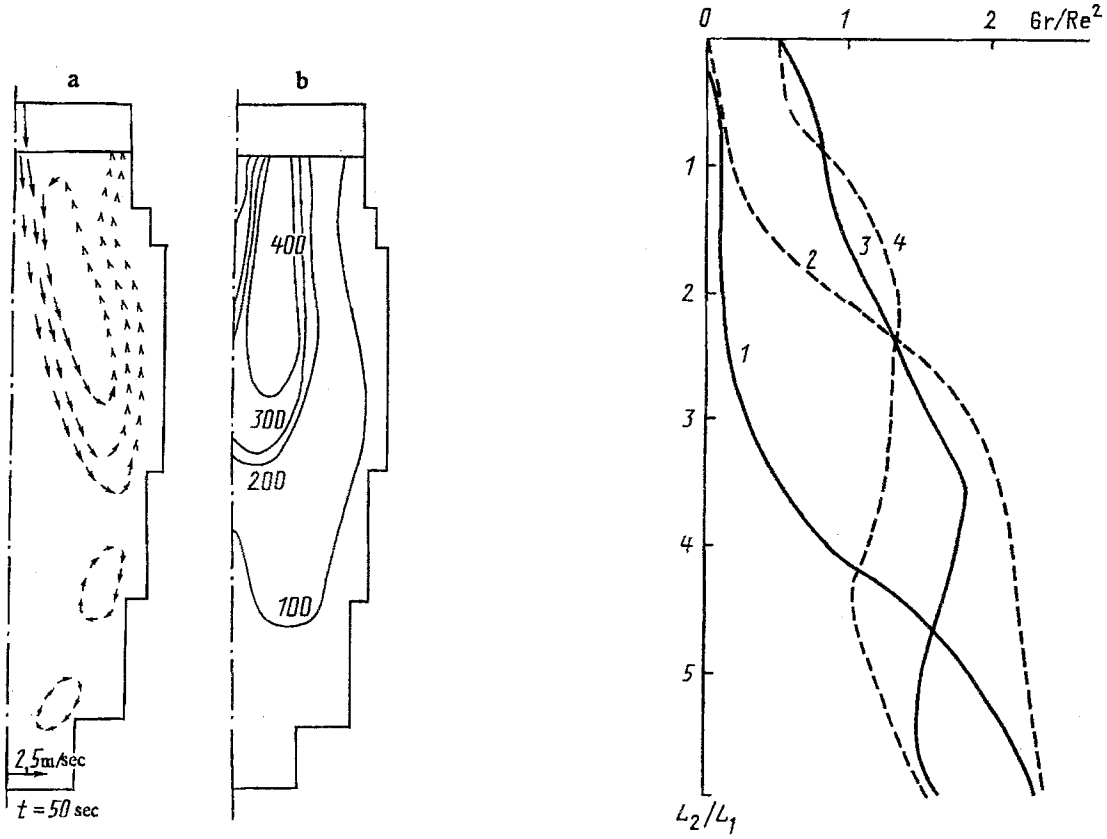

Fig. 2. Fields of the velocity vector (a) and lines of turbulent viscosity (b) during pouring of steel into a mold.

Fig. 3. Distribution of the criterion Gr/Re^2 over the height of an ingot: 1, 2) during pouring; 3, 4) 4 min after completion of pouring (solid lines, calculations in the laminar statement; dashed lines, calculations in the turbulent statement).

In the stage of pouring, characterized by the highest Reynolds numbers, a locally one-dimensional scheme proved to be efficient. A nonuniform space-time net is used because of substantial unsteadiness of momentum, heat, and mass transfer and developing inhomogeneity of the fields of ω, ψ, θ, V_1, V_2, ε, and k in the region of the submerged jet and at the walls of the mold.

The algorithm for the model suggested is as follows. Equation (1) is solved for ω, and then Eq. (2) is iterated for ψ using the method of variable directions. After the velocity fields were found from Eqs. (5) and (6), k and ε are calculated and then used for determination of the turbulent viscosity and thermal conductivity at all points of the melt. The time cycle is completed by solution of Eqs. (3), (4), and (7), because of which it is possible to determine θ, S, and ξ. Then, this calculation process is repeated in the following time step with account for the values obtained. Solution of the Poisson equation is carried out within 0.1% with 20 iterations.

The program is implemented in TURBO PASCAL in application to a PC. A structural feature of the program is addition of the stand-alone module REGION, which allows approximation of an arbitrary configuration of the region of study and generation of a spatial net as well as introduction of an object with required thermophysical properties into the calculation. Because of this, the software developed can be used as a component of an expert system in the CAD of casting processes.

3. The studies were carried out with an 8-ton hot-topped killed big-end-up ingot.

Steel was poured into a mold at $V_m = 5$ m/sec (Figs. 1a, b and 2). The flow structure consisted mainly of one vortex. However, in the lower part of the mold an additional vortex of low intensity arises as a result of temperature nonuniformity and development of heat convection. In this region velocities are an order of magnitude higher than those in the jet region (Fig. 2a). Inclusion of turbulent viscosity results in a decrease in the depth of

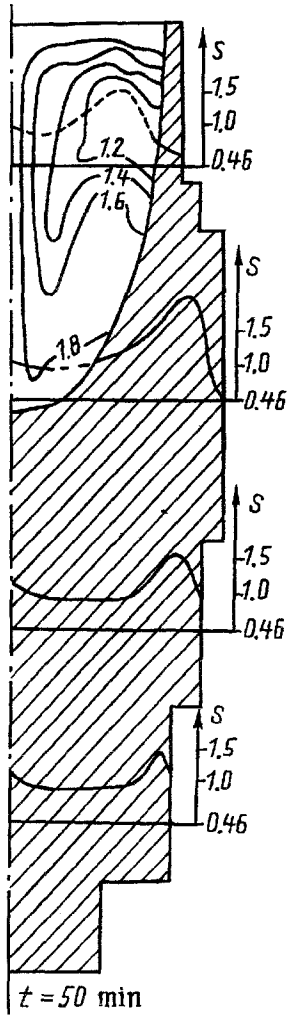

Fig. 4. Distribution of a carbon admixture in the solid and liquid phases of a solidifying ingot.

penetration of the jet into the bulk of the metal compared to calculations carried out with the assumption of a laminar flow [5]. This can probably be attributed to the character of the distribution of the turbulent viscosity in the submerged space and to a general increase in the total viscosity of the melt (Fig. 2b). This is confirmed by estimation of the contributions of the forced and natural convection components, which was carried out in terms of the criterion Gr_x/Re_x^2 [5]. As can be seen from Fig. 3, in the upper part of the mold, forced convective motion prevails ($Gr_x/Re_x^2 \ll 1$), whereas the contribution of natural convection is insignificant. Downstream the situation becomes the opposite. In the flange part of the ingot the contribution of forced convection is almost absent ($Gr_x/ Re_x^2 \gg 1$). The difference in results for pouring in the laminar and turbulent statements is appreciable. In the former case the zone with prevailing forced convection is more extensive, which is caused by the deeper penetration of the jet into the bulk of the metal in the problem in the laminar statement.

The results of the numerical experiments agree satisfactorily with those of other authors [6], which testifies to the adequacy of the mathematical model and the efficiency of the computational algorithm. The difference is 23% for the starting length of the submerged jet and 10% for viscosity.

The thermal "core" follows the shape of the vortex induced by the jet. The pouring is so rapid that no redistribution of the carbon admixture occurs in the melt. From an analysis of the streamlines, isotherms, and diagrams of the components of the velocity and the turbulent viscosity, it has been concluded that account for turbulence in the period of pouring of this ingot will change the hydrodynamic situation in the melt substantially. However, because the process of pouring is very short, its effect on the transfer processes and the kinetics of solidification is insignificant.

The hydrodynamic, thermal, and concentration fields that remained after pouring of the melt into the mold are the initial conditions for solution of the second part of the problem, i.e., solidification of the melt. In this period the motion of the melt due to the mechanical action of the jet is attenuated, and thermal convection represented by a multijet structure develops simultaneously (see Fig. 1c). The opposite direction of the thermal relaxation, on the one hand, and the dissipating effect of the viscosity, on the other, lead to a rapid decrease in the rate of motion of the melt.

An analysis of mixed convection after pouring in terms of the ratio Gr_x/Re_x^2 (Fig. 3, curve 2) indicates that, first, the contribution of the mechanical factor is insignificant compared to natural convection and, second, the conductive and turbulent mechanisms of momentum transfer are commensurable.

In the stage of "thermal convection," the rate of mixed convection changes from 0.6 to 0.1 m/sec. At the end of the stage when the superheat is removed (the stage lasts for 15 min), the effect of turbulence is almost absent. Therefore, in what follows, to save computer time, it is reasonable not to calculate the k-ε equations.

The next stage is "transient" and the effects of the thermal and diffusion gradients are commensurable here (Fig. 1d). The mixing rate falls to 0.04 m/sec. In this stage a diffusion boundary layer develops.

The stage of "concentration convection" starts about 50 min after completion of the pouring. The mixing rate falls to 0.001 m/sec (Fig. 1e) and the molecular and convective transfers become commensurable.

In the solid phase of the solidified ingot the followng pattern of the distribution of the soluble admixture is observed. On the periphery and in the bottom part of the ingot there are admixture-depleted areas (Fig. 4). They are formed in the stage of "thermal convection" and depend on its duration. Then, an area of increased content of the admixture occurs and the time for forming this area corresponds to the "transient" stage of convection. In the stage of "concentration convection" areas with a homogeneous distribution of the admixture appear. Since the test volume is limited, in the axial and upper parts of the ingot a zone of an increased amount of the admixture is formed.

Computational experiments carried out for a series of ingots of various weights have revealed that inclusion of turbulence in the mathematical model for the second part of the problem (after pouring) is necessary for ingots with $m > 20$ ton. Therefore, when studying the formation of steel ingots with $m < 20$ ton, it is recommended that a simplified mathematical model of hydrodynamic and heat transfer processes in the laminar statement [1] be used. Meanwhile, in the stage of filling the mold, modeling of mixed convection should be carried out in the turbulent statement, using Eqs. (5) and (6) of the k-ε model, irrespective of the weight of ingots.

NOTATION

ω, velocity vortex; x, y, dimensionless current coordinates; φ, stream function; $\theta = T/T_0$, dimensionless instantaneous temperature; T, T_0, dimensional current and initial temperatures; $S = C/C_0$, dimensionless concentration of the admixture; C, C_0, instantaneous and initial concentrations of the admixture; $G = \nu_t[2(\partial V_1/\partial x)^2 + 2(\partial V_2/\partial y)^2 + (\partial V_2/\partial x + \partial V_1/\partial y)^2]$, dissipative function arising in a flow of viscous liquid due to irreversible work of internal friction forces; $\nu_t = C_\mu k^2 \exp[-0.5/(1 + Re_t/50)]/\varepsilon$, turbulent viscosity; $Re_t = k^2/\nu\varepsilon$, turbulent Reynolds number; $\sigma_T = 1$, $\sigma_k = 1$, $\sigma_\varepsilon = 1.3$, $\sigma_D = 1$, turbulent Prandtl numbers for θ, k, ε, and S, respectively [2]; $C_1 = 1.44$; $C_2 = 1.92$; $C_3 = 1.44$; $C_\mu = 0.09$ [2]; $V_1 = (1 - \xi)(\partial\psi/\partial y)$; $V_2 = (\xi - 1)(\partial\psi/\partial x)$; $\lambda = (1 - \xi)(1 + \nu\rho c_e/\sigma_T) + \xi\lambda_t$; λ_t, turbulent thermal conductivity; $D = (1 - \xi)(1 + \nu_t/\sigma_D) + \xi D_t$, D_t, turbulent diffusivity; $c_e = 1 - W/(c_{liq}T_0)\partial\xi/\partial\theta$, effective heat capacity; W, latent heat of crystallization; c_{liq}, heat capacity of the liquid phase; a, a coefficient that depends on N_0, the number of ready crystallization centers; α, the law of generation of crystallization centers; V, crystallization parameter [7]; Fo, Pr, Gr_T, Gr_D, Lu, Fourier, Prandtl, Grashof (thermal and diffusive), and Lewis numbers [8]; subscripts m and md refer to the melt and the mold, respectively; $\theta_{in.m}$, $\theta_{in.md}$, initial temperatures of the melt and the mold, respectively; Γ_1, Γ_2, Γ_3, Γ_4, Γ_5, Γ_6, boundaries of the region of calculation (Fig. 1a); V_m, flow rate of the melt to the mold; R, radius of the jet coming into the melt; L_1, halfwidth of the melt surface, which is a function of the height of filling of the mold; K, heat transfer coefficient obtained from the formula $C(Gr_T Pr)^n$ [9]; Tu = 0.1, initial turbulence level (this value of Tu

can be explained by substantial turbulization in the nozzle and in air by the falling jet); $l = 0.1r_0$, turbulence scale; $\mathrm{Gr}_x = g\beta\Delta T_x L_1^2/\nu^2$, $\mathrm{Re}_x = V_x L_1/\nu$, local Grashof and Reynolds numbers.

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