Modeling of Liquid Magnesium Turbulent Convection in a Titanium Reduction Apparatus Using the RANS and LES Approaches

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Received September 4, 2019; revised November 18, 2019; accepted November 18, 2019

Abstract—This study focuses on turbulent convection of molten magnesium in a titanium reduction reactor. The reactor retort is a cylindrical vessel with a radius of 0.75 m and a height of 4 m, which contains liquid magnesium at a temperature of 850°C. During a process that lasts for more than 2 days, significant temperature gradients occur in the reduction apparatus due to an exothermic chemical reaction on the metal surface and simultaneous cooling of the side wall of the retort and heating of its bottom. Temperature gradients cause convective flows inside the reactor, which in turn significantly affect the formation of the titanium block. The mathematical model of convective flows in the reactor is based on the equations of thermogravitational convection for a single-phase medium in the Boussinesq approximation. We consider the possibility of modeling turbulent convective flows in a titanium reduction reactor using RANS (Reynolds-averaged Navier–Stokes equations) \( k-\varepsilon \) and \( k-\omega \) SST (Shear Stress Transport) models. The results of simulations performed with the \( k-\omega \) SST model on relatively coarse grids (0.825 million finite volumes) are shown to qualitatively and quantitatively agree with the results of LES simulations on fine grids (3.7 million finite volumes). However, the \( k-\varepsilon \) model does not always produce acceptable results. RANS simulations produce average velocity and temperature fields with averaging times much longer than those possible in LES simulations. Several different configurations of heating and cooling of the apparatus were examined, including those that were previously unstudied. It has been found that using the \( k-\omega \) SST model allows simulation of flow dynamics taking into account changes in the heating and cooling conditions of the apparatus during the entire process and identification of single- and double-vortex large-scale flows in the retort, as well as the transition between them, so the degree of convection influence on the reaction can be assessed.

Keywords: convection, turbulence, small Prandtl numbers, liquid metal, RANS, LES, numerical simulation, OpenFOAM
DOI: 10.1134/S0021894420070044

1. INTRODUCTION

Turbulent convection in liquids with a small Prandtl number \( \text{Pr} = \nu/\chi \) (where \( \nu \) is the kinematic viscosity and \( \chi \) is the thermal diffusivity), e.g., liquid metals, is actively studied both experimentally [1, 2] and numerically [3–5]. Liquids with \( \text{Pr} \ll 1 \) are characterized by a large value of the thickness ratio of thermal and dynamic boundary layers. Because of this, in the case of turbulent flow regimes (for large Grashof numbers \( \text{Gr} = \beta \Delta T h^3 / \nu^2 \)) the dynamic boundary layer is very thin (see, for example, review [6]). As a result, the properties of large-scale circulation in a developed turbulent flow and the integral characteristics of the flow differ significantly from those for large values of \( \text{Pr} \). Studying the features of convective flows in a metal is interesting both from a fundamental and from a practical point of view. Such flows are found in modern technical applications, for example, in nuclear energy. Liquid sodium is used as a coolant in cooling systems of fast-neutron nuclear reactors [7] and tokamaks [8].

Convective flows in liquid metals are also important for the metallurgical industry. In particular, the structure of convective flows can affect the behavior of metallothermal reduction of titanium using the Kroll process [9, 10]. During the process, titanium tetrachloride is fed from above into a cylindrical retort
with a radius of 0.75 m filled with liquid magnesium to a level \( H = 2.5 \) m at a temperature of 850°C. As a result, an exothermic reduction reaction occurs on the surface of magnesium, forming sponge titanium and magnesium dichloride [11, 12]:

\[
2\text{Mg} + \text{TiCl}_4 = \text{Ti} + 2\text{MgCl}_2 + Q,
\]
sinking to the bottom of the retort. The process takes over 2 days. The titanium block, which has a high porosity, gradually grows and occupies an increasing volume in the retort. The magnesium salt (\( \text{MgCl}_2 \)) that has accumulated in the lower part of the reactor is drained every several hours. The behavior of the process and the quality of the titanium sponge substantially depend on the temperature regime of the apparatus and the reaction rate and require constant monitoring of the latter. The large mass and size of the installation and extreme temperatures make direct control exceptionally difficult. Only the temperature of the outer surface of the retort is measured at several points, so the titanium recovery process remains largely a black box. Up to 5% of production cycles fail due to emergency situations associated with disruptions of magnesium chloride deposition, local overheating of the retort, or titanium sponge emerging on the magnesium surface. At times the so-called “nonseparation” mode may occur, in which the reaction by-product \( \text{MgCl}_2 \), whose density is close to the density of magnesium, ceases to sink to the bottom of the reactor, and the process is ruined.

Solving the problem of controlling the reaction of titanium reduction requires working in two interrelated directions, that is, constructing a complete mathematical model of the reactor and searching for new methods of experimental measurement of the level of the magnesium surface in the retort on which the reaction occurs and recognizing whether it is in direct contact with \( \text{TiCl}_4 \) (in the normal course of the reaction) or its surface is covered by \( \text{MgCl}_2 \) (in the undesirable “nonseparation” mode).

Contactless induction methods have been proposed for measuring magnesium levels [13]. However, attempts to use them in actual production have shown that they work only for the initial stages of the reaction. Recently, an algorithm was proposed for restoring the level of liquid metal, based on measuring the characteristics of magnetic fields and taking the presence of a titanium sponge as a skull of various geometries and electrical conductivity into account. A mathematical model is used to interpret the results from the recording coils installed in the upper part of the retort, in which all possible combinations of the reduction process are calculated from the electrodynamic point of view (without convective motion of the medium). In total, several thousand combinations of parameters were considered. To determine the level of magnesium in a real process from the database that stores the parameters of various reduction process scenarios the ones that correspond to the scenario closest to the measurement results from the recording reel are selected [14].

During the process, significant temperature gradients arise in the recovery apparatus due to an exothermic chemical reaction on the metal surface \( Q = 1707 \) kJ per 1 kg of titanium tetrachloride [11, 12]) and simultaneous cooling of the side wall and heating of the bottom of the retort. Temperature gradients cause convective flows inside the reactor, which can affect the course of the reaction and the formation of the titanium block. One of the possible reasons for the “nonseparation” mode may be a change in the nature of the convective flow. Knowledge of the structure of the flows that occur in the reactor at various stages of the process may allow the formation of a metal flow in such a way as to ensure a stable reaction.

Developing a mathematical model that is capable of adequately describing the full cycle of a titanium sponge reduction reactor involves great difficulties in integrating physical chemistry, hydrodynamics, and computational mathematics. No software package exists with the functionality to study all the processes occurring inside the retort numerically.

The first attempts to estimate the intensity of convective flows in a reactor based on a numerical simulation of magnesium convection in a cylindrical vessel were made more than 40 years ago [15] for very underestimated Grashof numbers \( 10^5 \) instead of \( 10^{12} \). The convection of magnesium in a cylinder for realistic values of the control parameters was studied numerically in [16]; however, the problem had a stationary axisymmetric formulation.

The first simulation in a complete three-dimensional formulation for realistic Grashof and Rayleigh numbers was performed in [17]. It revealed the presence of intense turbulent flow. In [18], the convective flow of molten magnesium in a retort with 5-cm-thick steel walls was considered for three configurations of heating and cooling with and without a titanium block. It was discovered that unsteady turbulent flow modes arise in the retort at parameters that correspond to the real process. The structure of a convective flow has been shown to fundamentally differ at different stages of the process (that is, at different heating configurations). A two-phase flow, that is, the deposition of magnesium salt (\( \text{MgCl}_2 \)) on the surface of magnesium (\( \text{Mg} \)) in the reaction zone in the presence of a strong convective flow was discussed in [19].
The initial stages of the process were studied; therefore, the contribution from a porous medium (the titanium sponge) that also sinks to the bottom of the reactor was not taken into account. Equations for a two-phase flow of Mg and MgCl₂ are solved using a numerical code. A detailed analysis was carried out for configurations with and without taking the convective flow caused by furnace heaters and the chemical reaction into account. It was discovered that the magnesium salt sinks in drops with sizes from ≈3 to ≈10 cm. The droplet velocity (from ≈18 to ≈30 cm/s, depending on the mode) turned out to be greater than the velocity of the convective flow (up to 20 cm/s); however, it has been shown that a convective flow can entrain droplets and carry them along with the vortex.

In [20] the convective flow over a circular heater in the upper part of a vertical cylinder filled with liquid sodium was considered experimentally and numerically. This flow was assumed to be a simplified model of the liquid magnesium flow in a titanium reduction reactor, although the typical Grashof number in the reactor is three orders of magnitude higher than in the experiment (10¹² instead of 10⁹).

Previous three-dimensional calculations [17–19] were performed using the large eddy simulation method (LES) and therefore required a very fine computational grid. However, the titanium reduction process takes more than 2 days. The global goal is to create a hydrodynamic model of the process in complete three-dimensional formulation, properly taking the features of turbulent flow into account and using it to study the features of convection in the reactor at different stages of the process, and to study the dynamics of the flow at changing conditions of heating and cooling of the apparatus over time. Describing the entire process requires such a significant amount of computational resources that it becomes impossible to use the DNS (direct numerical simulation) and LES (large eddy simulation) approaches. Therefore, the objective of this work was to simulate convection in a reactor using the RANS (Reynolds-averaged Navier–Stokes equations) approach, since it can significantly reduce the calculation cost.

2. THE STATEMENT OF THE PROBLEM AND THE MATHEMATICAL MODEL

The three-dimensional nonstationary mathematical model is based on the thermogravitational convection equations in the Boussinesq approximation. The heating and cooling configurations of the apparatus correspond to different stages of the process. The convective flow of only one phase, liquid magnesium, is considered (as in [17]). The contribution of the second liquid phase, magnesium chloride [19] and the porous medium, a titanium sponge [18] is not taken into account. Information on a single-phase flow (only on convection of liquid magnesium) is sufficient to test the RANS turbulence models and compare them with the results obtained using the LES approach.

The computational domain is the retort of a titanium reduction reactor; it is a cylinder of radius \( R = 0.75 \) m and height \( H = 2.5 \) m (Fig. 1a), filled entirely with liquid magnesium. Figure 1b shows the designations of the boundaries of the computational domain: \( B_t \) is the top surface of area \( S_t \); \( B_{ms} \) is the upper part of the side surface of height \( h_1 \) and area \( S_{ms} \); \( B_{ms} \) is the middle part of the side surface of area \( S_{ms} \); \( B_{ls} \) is the lower part of the side surface of area \( S_{ls} \) and \( B_b \) is the cylinder base surface of area \( S_b \).

The upper part of the side surface is blown with cold air; the height of the cooling zone \( h \) varies from 0.3 to 0.7 m. The retort is also heated on the side of the cylinder below the cooling zone. The power of the heaters in the furnace is 423 kW and is provided by heating from below, \( Q_{bs} = 94 \) kW and heating on the lower part of the side surface, \( Q_{B_{ms} \cup B_{ls}} = 329 \) kW. The thermal power of the reaction on the surface is \( Q_{r} = 205 \) kW. The convective parameters of the medium correspond to liquid magnesium at a temperature of 850°C; their values are given in Table 1. Under such conditions, the values of the control parameters are high (the characteristic Grashof numbers during the course of the process are on the order of 10¹²); therefore, the arising flows are unsteady and turbulent.

The general form of the system of equations of thermogravitational convection in the Boussinesq approximation using turbulence models is as follows:

\[
\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j} (u_i u_j) - \frac{\partial}{\partial x_j} \left( (\nu_0 + \nu_r) \left[ \frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right] \right) = -\frac{\partial}{\partial x_j} \left( \frac{p}{\rho_0} \right) + g_i \left[ 1 - \beta (T - T_0) \right], \tag{1}
\]

\[
\frac{\partial T}{\partial t} + \frac{\partial}{\partial x_j} (u_i T) - \frac{\partial}{\partial x_j} \left[ \left( \frac{\nu_0 + \nu_r}{Pr} \frac{\partial T}{\partial x_j} \right) \frac{\partial T}{\partial x_j} \right] = 0, \tag{2}
\]
Here, \( t \) is time; \( u_i \) is the velocity component; \( p \) is the pressure; \( T \) is the temperature; \( g_i \) is the gravity acceleration component; \( \beta \) is the temperature volumetric expansion coefficient; \( \nu_0 \) is the kinematic viscosity; \( \nu_t \) is the turbulent viscosity; and \( \text{Pr} \) is the turbulent Prandtl number.

The RANS (Reynolds-averaged Navier–Stokes equations) and LES (large eddy simulation) approaches were used to take turbulence into account.

The first approach is based on the idea of dividing all of the quantities included in the Navier–Stokes equations into mean fields and pulsation fields. That makes it possible to write the equations of motion for mean fields, but an additional term appears in them, the Reynolds stress tensor, which characterizes the velocity pulsations and makes the system open. There are many models for completing the system [21]; all of them contain constants that have to be determined from experiment and are therefore called semi-empirical. Out of these, two-parameter models are the most popular.

This paper uses the \( k-\epsilon \) and \( k-\omega \) SST (Shear Stress Transport) turbulence models, in which two equations are added to close the system: in the \( k-\epsilon \) case these are equations for the kinetic energy of the velocity pulsations \( k \) and for the energy dissipation rate \( \epsilon \). Then, \( \nu_t = C_{\mu} k^2 / \epsilon \), where \( C_{\mu} \) is one of the empirical coefficients (this model has six in total). The \( k-\omega \) SST model uses the equation for specific turbulence dissipation rate \( \omega = \epsilon / k \) instead of an equation for \( \epsilon \). The \( k-\omega \) SST model is a hybrid of the \( k-\omega \)

Table 1. The physical parameters of magnesium at a temperature of \( T_0 = 850^\circ \text{C} \)

| Name                                | Designation | Units          | Value      |
|-------------------------------------|-------------|----------------|------------|
| Density                             | \( \rho_0 \) | kg/m\(^3\)     | 1538       |
| Temperature volumetric expansion coefficient | \( \beta \) | 1/K            | 1.69 \times 10^{-4} |
| Kinematic viscosity                 | \( \nu_0 \) | m\(^2\)/s       | 4.17 \times 10^{-7} |
| Thermal conductivity                | \( \chi_0 \) | m\(^2\)/s       | 4.39 \times 10^{-5} |
| Specific heat capacity              | \( C_p \)   | J/(kg K)        | 1344       |
| Coefficient of thermal conductivity | \( \lambda \) | W/(m K)        | 90.7       |
| Prandtl number                      | \( \text{Pr} \) | —              | 0.0095     |
and $k-\varepsilon$ models obtained by their superposition and by introducing an empirical function that allows the calculation of near-wall flows by the $k-\omega$ model and the core of the flow by the $k-\varepsilon$ model.

RANS requires validation and in each case it is necessary to ensure that the model and the chosen values of its constants correspond to the type of considered turbulent flow. Therefore, to compare the results and adjust the RANS parameters, calculations were performed taking the second, LES, approach into account. According to it, the division is not into mean fields and pulsations, but into “large” scales that are explicitly calculated on the accepted computational grid, and “small” scales, that are unresolvable by the computational grid. The contribution of these smaller vortices to the solution is taken into account using subgrid closure models. The finer the computational grid is, the less the turbulence model contributes, and the results tend closer to the results of direct numerical simulation (DNS).

This work uses the Smagorinsky LES model [22], which requires only one constant; its value is $C_s = 0.17$. Turbulent viscosity is defined as $\nu = \sqrt{2\varepsilon C_s^2 \Delta^2}$, where $[\Delta]$ is the norm of the strain rate tensor $S_{ij} = (1/2) (\partial u_i / \partial x_j + \partial u_j / \partial x_i)$, in which $\Delta = (h_x, h_y, h_z)$ is the grid step sizes along each of the coordinate axes, and the contribution from vortices smaller than $\Delta$ is taken into account using the accepted model. In the region of the viscous sublayer, in which the turbulent viscosity is set to zero, we apply the damping function proposed by Van Driest, which reduces the subgrid turbulent viscosity exponentially.

The simulations consider three different configurations of heating and cooling that occur in the reactor at various stages of the process (Fig. 2). In all cases, a constant heat flux $q_B$ is set at the upper boundary of the computational domain $B$, which simulates the heat generation in a chemical reaction of power $Q_B = 205 \text{ kW}$. At the bottom $B_b$, a heat flux $q_{B_b}$ is set that is due to constantly working lower heaters of power $Q_{B_b} = 94 \text{ kW}$. The boundary conditions for the temperature on these surfaces are as follows ($\partial T/\partial n$ is the derivative along the normal directed inside the chamber):

$$q_B = -\lambda_{mg} \frac{\partial T}{\partial n} \bigg|_{B} = \frac{Q_B}{S_B}, \quad q_{B_b} = -\lambda_{mg} \frac{\partial T}{\partial n} \bigg|_{B_b} = \frac{Q_{B_b}}{S_{B_b}}.$$

In this case, the upper part of the side surface $B_{us}$ of the retort is cooled by air.

The first configurations (Fig. 2a) corresponds to the situation where all the heaters in the furnace along the side surface of the retort are at full power $Q_{B_{us} \cup B_b} = 329 \text{ kW}$. To maintain the energy balance, a heat flux is removed from the cooling zone of height $h = 0.7 \text{ m}$, which is numerically equal to the sum of all heat fluxes created by the heaters and the heat generated in the exothermic reaction. This setup corresponds to the most extreme operating mode of the reduction reactor; considering it makes it...
possible to estimate the values of the maximum rates and temperatures. We note, however, that
during a real process not all heaters in the furnace are turned on most of the time. The temperature
boundary conditions have the form (TBC-1):

\[ q_{B_{ms} \cup B_{us}} = -\lambda_{mg} \frac{\partial T}{\partial n} \bigg|_{B_{ms} \cup B_{us}} = \frac{Q_{B_{ms} \cup B_{us}}}{S_{B_{ms} \cup B_{us}}}, \quad q_{B_{us}} = -\lambda_{mg} \frac{\partial T}{\partial n} \bigg|_{B_{us}} = -\left( \frac{Q_{B_{us}} + Q_{B_{ms} \cup B_{us}}}{S_{B_{us}}} \right). \]

The second configuration (Fig. 2b) is closer to the typical operating mode of the reactor and differs
from the first in that several heating elements within the B_{ms} zone are turned off; this boundary is consid-
ered thermally insulated. This regime can be called transitional between the intensive operation of the
entire heating system and the complete shutdown of the side heaters. The height of the cooling zone is
h_{c} = 0.3 \text{ m} and the height of the heated part of the side surface B_{us} is h_{c} = 0.3 \text{ m}. In this case, the tempera-
ture boundary conditions are as follows (TBC-2):

\[ q_{B_{us}} = -\lambda_{mg} \frac{\partial T}{\partial n} \bigg|_{B_{us}} = 0, \quad q_{B_{ms}} = -\lambda_{mg} \frac{\partial T}{\partial n} \bigg|_{B_{ms}} = \frac{Q_{B_{ms}}}{S_{B_{ms}}}, \quad q_{B_{us}} = -\lambda_{mg} \frac{\partial T}{\partial n} \bigg|_{B_{us}} = -\left( \frac{Q_{B_{us}} + Q_{B_{ms} \cup B_{us}}}{S_{B_{us}}} \right). \]

The third configuration, TBC-3 (Fig. 2c), corresponds to the “gentle” operating mode of the reactor,
when only the lower pair of heaters located in the B_{us} zone is switched on to maintain the reaction and pre-
vent the cooling of magnesium. Thus, the boundary conditions for temperature have the form:

\[ q_{B_{ms}} = -\lambda_{mg} \frac{\partial T}{\partial n} \bigg|_{B_{ms}} = q_{B_{us}} = -\lambda_{mg} \frac{\partial T}{\partial n} \bigg|_{B_{us}} = 0, \quad q_{B_{us}} = -\lambda_{mg} \frac{\partial T}{\partial n} \bigg|_{B_{us}} = -\left( \frac{Q_{B_{us}} + Q_{B_{ms} \cup B_{us}}}{S_{B_{us}}} \right). \]

Within the framework of the LES approach, a configuration close to TBC-1 was previously studied in
[17, 18], and one similar to TBC-3 was studied in [18], while the TBC-2 configuration has never been con-
sidered.

The slip condition is specified for the velocity at the upper boundary. All other boundaries of the region
are considered to be solid and adhere to the no-slip condition \( \mathbf{v} = 0 \).

The free open-source software package OpenFOAM 4.1 is used for simulations. Discretization is per-
formed using the finite volume method. The \textit{buoyantBoussinesqPimpleFoam} solver is used, in which the
PISO (Pressure Implicit with Splitting of Operators) algorithm [23] based on the pressure correction pro-
cEDURE is used for the Navier–Stokes equations. The terms with time derivatives are discretized according
to the implicit Euler scheme and the diffusion terms are discretized according to the central difference
scheme. The latter, in the case of the finite volume method, implies a linear interpolation of the variable
values from the centers on the edge of neighboring volumes; therefore, the scheme is called \textit{linear}. Con-
vective terms are calculated according to the \textit{limitedLinear} scheme, which provides a good balance
between accuracy and stability of calculations. The system of linear algebraic equations is solved at each
step of the pressure correction algorithm using the Preconditioned Conjugate Gradient (PCG) method
with DIC (incomplete Cholesky factorization) preconditioner. The velocity and temperature fields were
determined using the Preconditioned Biconjugate Gradient (PBiCG) method with the DILU precondi-
tioner (diagonal incomplete LU decomposition) and a system of linear algebraic equations for \( k, \epsilon, \) and \( \omega \) was solved using smoothSolver with Gaussian–Seidel smoothing. During the calculations the Courant
number did not exceed 0.9.

All simulations used a block nonuniform mesh refined near the boundaries of the domain (Fig. 1c). For LES calculations, the mesh had 3.7 million finite volumes in total. One advantage of the RANS
approach for describing turbulence is that it allows one to adequately represent the mean fields of turbu-
 lent flows on much coarser grids than are required for LES calculations. While the result is closer to DNS
the finer the mesh is using the LES, this is not so in the case of the RANS approach; it makes no sense to
refine the mesh more than is necessary to resolve mean fields, since the entire contribution from flow tur-
bulence is taken into account using additional, closing, equations of the model. In RANS simulations, the
grids had different densities of finite volumes (3.7; 1.5; 0.825; and 0.6 mln), since the goal was to find the
coarsest grid that would allow qualitative and quantitative agreement with the data of much more expen-
sive LES calculations.

Numerical experiments have shown that a grid with 0.825 million finite volumes is sufficient for RANS
modeling (a comparison of the results on different grids is given in the next section). Figure 3 shows code
scalability on the Triton computing cluster of the Institute of Continuous Media Mechanics in Perm, Rus-
sia. The Triton supercomputer is based on Intel Xeon E5450 processors (Harpertown generation, 256 pro-
When using Harpertown processors on a grid of 3.7 million finite volumes, a acceleration of 112 times is observed during the transition from 1 to 240 computing cores. Using the more efficient Broadwell generation processors allows acceleration up to 94 times during the transition from 1 to 224 processor cores. We note that the parallelization efficiency also depends on the design features of a particular cluster. As an example, each computing node of the Triton Harpertown partition contains 16 processor cores, while Triton Broadwell has 28 cores on each node. RANS calculations require slightly more time than LES calculations on the same grid, since in the first case two additional equations for turbulent fields of $k$ and $\omega$ have to be solved; this drawback is compensated by the possibility of using coarser grids than those required for LES. Compared to LES calculations on a grid of 3.7 million finite volumes, RANS calculations on a grid of 0.825 million finite volumes using 56 Broadwell cores take 17.5 times less time. It should be noted that it is impractical to use a very large number of cores for calculations on relatively coarse grids. As an example, on a grid of 0.825 million finite volumes the computation parallelization efficiency decreases at the number of cores greater than 100, since each core has too little data.

3. RESULTS

We consider three qualitatively different flow regimes that occur under the TBC-1, TBC-2, and TBC-3 heating configurations. The results are presented for LES calculations on a grid with 3.7 million finite vol-
umes and RANS calculations using the $k-\varepsilon$ and $k-\omega$ SST models with standard wall functions on a grid of 0.825 million finite volumes.

Figure 4 shows the time-averaged velocity fields of liquid magnesium for TBC-1 (Fig. 2a), as determined using different models of turbulent flow. This regime corresponds to the most intensive mode of the reactor operation. The general structure of the averaged flow has a double-vortex form. A stagnation zone with a height of approximately 20 cm is observed in the upper part of the retort.

The most intense convective motion is caused by a temperature drop near the interface between the cooled and heated parts of the side surface of the cylinder. Since the vortices are toroidal in this regime, the orientation of the vertical section plane for presenting the results can be arbitrary. In this case, the flow has a pronounced boundary-layer character. From Fig. 4 it follows that the structures of the mean flow found using the LES approach and $k-\omega$ SST models coincide qualitatively, while the shape and size of the vortices obtained using the $k-\varepsilon$ model differ significantly.

Time averaging of the velocity and temperature fields for TBC-1 and TBC-2 lasted 3500 s; this time was sufficient for the mean flow to stabilise. A further increase in the averaging time did not lead to a structural change of the fields.

To compare the data quantitatively, Fig. 5 shows the average velocity profiles along horizontal lines at various heights. The greatest intensity of the flow is observed in the wall layer near the side surface of the retort. Estimates of the maximum velocity obtained using the $k-\omega$ SST model are close to the values provided by the LES calculation, while the $k-\varepsilon$ model shows an underestimated flow intensity.

The greatest difficulty for RANS modeling using wall functions is to calculate the heat transfer at the upper boundary, where the chemical reaction takes place and the temperature gradients are max-
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The LES simulation shows a “warmed” stagnant region with large temperature values in the upper part of the retort, while in simulations based on the RANS approach with standard coefficient values (turbulent Prandtl number $Pr_t = 0.9$) the stagnant heated zone in the upper part is absent and convective vortices reach the free surface.

Typically, a value of 0.9 is selected for $Pr_t$, which is suitable for liquids with relatively large Prandtl numbers (e.g., water) and gases. However, according to different models, in convective flows of liquid metals $Pr_t$ can take large values \cite{24, 25}. Experiments in round tubes to determine the $Pr_t$ value show that it depends on the molecular Prandtl number, the Reynolds number, and the distance from the wall. Higher values of $Pr_t$ result in lesser contribution to the solution by the turbulent heat transfer, which is calculated using LES or RANS approaches. Additional calculations were performed to estimate the effect of the $Pr_t$ value on the results. For RANS models the values of 4.1 and 24 were considered in addition to 0.9, as well as a variable $Pr_t$ with a value of 4.1 everywhere inside the domain \cite{24}, but increasing linearly up to 100 in the upper part (from 2.3 to 2.5 m) of the retort, so that the contribution from turbulent heat transfer in this stagnant zone is excluded. This corresponds to the fact that in the stagnant zone the motion is slow and turbulence is absent, while the turbulence models used by RANS imply turbulence in the entire region. Figure 6a demonstrates that an increase in the turbulent Prandtl number makes it possible to bring the RANS results closer to the LES results (Fig. 6a). Therefore, all RANS calculations presented in this article use a variable $Pr_t$ (the bold solid line in Fig. 6a).

It should be noted that LES models are much less sensitive to the $Pr_t$ value at the parameters of the problems considered in this paper. In the case of LES for a grid of 3.7 million finite volumes and specified heat fluxes even at a standard value $Pr_t = 0.9$ the contribution from the “subgrid” turbulent heat transfer is small compared to that calculated explicitly. Therefore increasing the $Pr_t$ value in LES simulations does not lead to significant changes in temperature and velocity fields. Figure 6b presents time-average temperature profiles along the vertical axis of the cylinder for the chosen parameters for the LES, $k-\omega$ SST, and $k-\epsilon$ models; they all exhibit similar behavior.

Figure 7 contains examples of the dependences of temperature and the vertical velocity component $U_z$ on time at individual points of the retort. The amplitude of the temperature and velocity pulsations is close in LES and RANS simulations using the $k-\omega$ SST model, although LES simulations, as expected, reproduce high-frequency pulsations better.

Figure 8 shows the time-averaged velocity fields of liquid magnesium calculated using different representations of the turbulent flow for the case of TBC-2 (Fig. 2b), in which part of the heaters along the side
wall of the retort are disabled. Again, a double-vortex flow is observed, as in the case of TBC-1, but its intensity is generally lower and the size ratio of the upper and lower vortices is different: now the upper vortex is larger than the lower. The field structures obtained using the LES and \( k-\omega \) SST models coincide qualitatively, while the \( k-\varepsilon \) model again fails to reproduce the ratio of the vortex sizes.

Figure 9 contains average velocity profiles along horizontal lines at various heights for TBC-2. Again, the greatest intensity of the flow is observed in the wall layer near the side walls of the retort. The maximum velocity estimates obtained in the LES and \( k-\omega \) SST calculations are similar and the \( k-\varepsilon \) model gives underestimated values.

Figure 10 presents the results for the TBC-3 configuration (Fig. 2c). In this regime, all heaters along the side surface of the retort are turned off and only those located at the bottom are active. The flow structure is significantly different from that observed with TBC-1 and TBC-2: now a large-scale circulation occurs in the cylinder, accompanied by two small rolls rotating in the opposite direction. The large-scale circulation orients randomly and exhibits complex dynamics during the evolution of the flow. Such a flow structure is well known in Rayleigh–Benard convection problems, when inversions of large-scale circulation can be observed as well as its twisting and sloshing [2, 5, 6]. In the present work, these effects have not been studied in detail. The sections for presenting the results in Fig. 10 were not chosen arbitrarily, but in accordance with the orientation of large-scale circulation in these simulations. For TBC-3 all three turbulence models give similar results; even the \( k-\varepsilon \) model underestimates the velocity but reproduces the general structure of the flow.
Figure 11 shows examples of the time dependences of the temperature and the vertical velocity component at individual points of the retort during a successive change in heating configurations: TBC1 → TBC2 → TBC3. The vertical lines separate the regimes, for each of which we present the evolution over 4000 s. Performing LES simulations of this duration was not possible; however, by using the RANS approach it was possible to conduct them on a relatively coarse grid. The results of numerical experiments show that the values and distributions of the pulsations of temperature and velocity at different points in the chamber change significantly with a change in the flow regime.

Since in a real reactor it is only possible to measure the temporal evolution of the temperature of the outer retort surface at several points, only long-term calculations will allow the comparison and adjustment of the model taking these experimental data into account.

4. CONCLUSIONS

Turbulent convective flows in a titanium reduction reactor were simulated by RANS (using the $k-\omega$ and $k-\epsilon$ SST models) and LES (the Smagorinsky model) approaches.

It has been shown that simulations using the $k-\omega$ SST model on relatively coarse grids (0.825 mln finite volumes) produce results that are qualitatively and quantitatively consistent with the results of LES.
simulations on fine grids (3.7 mln finite volumes). However, the $k-\varepsilon$ model does not always produce acceptable results.

RANS simulations using the $k – \omega$ SST model produce average velocity and temperature fields with an averaging time significantly longer than is possible for LES simulations. This is especially important since the real process lasts more than 2 days.

Several different heating and cooling configurations of the apparatus are considered, for which the structure and intensity of convective flows differ significantly. Depending on the operational mode, either a large-scale circulation with complex dynamics (as in the Rayleigh–Benard problem [2, 5, 6]), or toroidal vortices appear in the retort.

It has been shown that the developed mathematical model makes it possible to describe the dynamics during the entire titanium reduction process with a dynamic change in the heating and cooling conditions of the apparatus and to identify single- and double-vortex large-scale flows in the retort, as well as transitional regimes. This makes it possible to assess the degree of influence of convection on the course of the reaction.

ACKNOWLEDGMENTS

The simulations were carried out on the Triton supercomputer at the Institute of Continuous Media Mechanics in Perm, Russia.

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Translated by L. Trubitsyna