Thermal convection of liquid metal in the titanium reduction reactor

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Abstract. The structure of the convective flow of molten magnesium in a metallothermic titanium reduction reactor has been studied numerically in a three-dimensional non-stationary formulation with conjugated heat transfer between liquid magnesium and solids (steel walls of the cavity and titanium block). A nonuniform computational mesh with a total of 3.7 million grid points was used. The Large Eddy Simulation technique was applied to take into account the turbulence in the liquid phase. The instantaneous and average characteristics of the process and the velocity and temperature pulsation fields are analyzed. The simulations have been performed for three specific heating regimes: with furnace heaters operating at full power, with furnace heaters switched on at the bottom of the vessel only, and with switched-off furnace heaters. It is shown that the localization of the cooling zone can completely reorganize the structure of the large-scale flow. Therefore, by changing heating regimes, it is possible to influence the flow structure for the purpose of creating the most favorable conditions for the reaction. It is also shown that the presence of the titanium block strongly affects the flow structure.

1. Introduction

Liquid metals are characterized by low Prandtl numbers, that is by low ratios of viscosity to thermal diffusivity. This implies, in general, a weak contribution of thermo-gravitational convection to heat transfer. However, recent studies have shown that convection can strongly affect turbulent heat transport in turbulent natural convective [1] or even forced flows [2] of liquid metals. Moreover, convective flows in metals can affect significantly technological processes in metallurgy. For example, the buoyancy force can influence the metallothermic reduction of titanium, as was shown in a simplified axisymmetric computation in [3]. The retort for titanium reduction is a cylindrical vessel with a diameter up to 2 m and a height up to 4 m containing liquid magnesium at a temperature of about 850°C. Titanium tetrachloride is supplied from the top to the magnesium surface. The chemical reaction of titanium reduction is highly exothermic and runs predominantly on the surface. It produces spongy titanium and magnesium dichloride that sink to the bottom of the retort. The fact that the large mass and dimensions of the vessel and the very high temperatures hamper any direct experimental measurements inside the reactor is one of the motivations for the numerical study of the process. A first fully three-dimensional numerical study of the structure of convective flows of molten magnesium at realistic Rayleigh numbers has revealed a strong turbulent flow [4].
The titanium reduction process takes more than two days during which the titanium sponge gradually occupies the retort. A stable reaction should be facilitated by controlling the supply of titanium tetrachloride, by draining the magnesium chloride, and by cooling and heating the furnace. At present, up to 5% of the production cycles are rejected due to contingencies associated with the disruption of the magnesium chloride settling process, the emergence of titanium sponge on the magnesium surface, and local retort overheating. Up to present, attempts to enhance the sponge production by local reactor cooling have ignored the flows inside the reactor [5].

In this paper we continue the numerical study of convective flows in the reactor for metallocthermic reduction of titanium for different configurations of reactor cooling and heating zones and different levels of titanium sponge. Our goal is to reveal how strongly the large-scale magnesium circulation in the reactor can be affected by the change of heating and by the growth of the titanium mass.

2. Formulation of the problem and the mathematical model

We consider a flow of liquid magnesium inside the cylindrical vessel made of steel with a wall thickness of 25 mm. During the process the combined effect of the furnace heaters in the lower part of the vessel, the exothermic chemical reaction on the top surface of the magnesium layer, and the cooling on the side walls in the reaction zone by airflow leads to substantial temperature gradients which generate a convective flow inside the reactor. The structure of this convective flow may have significant influence on the reaction process. The height of the vessel is $H = 2.5$ m, the radius $R = 0.8$ m. The height of the upper part of the side surface in the reaction zone, which is cooled by air, is varied from $h = 0.15$ m to 0.7 m. A scheme of the computational domain is shown in figure 1a. The simulations were done with and without a titanium block inside the vessel in its lower part. This titanium block is assumed to be a solid body (not a porous medium). The contribution of the second liquid phase, magnesium dichloride, is disregarded.

We used the software package OpenFoam Extend 3.2 [6], namely conjugateHeatFoam solver. It allows to simulate conjugate heat transfer between the incompressible fluid (liquid magnesium), the steel walls of the retort (heat conductivity $k = 26$ Wm$^{-1}$K$^{-1}$), and the solid titanium block ($k = 15$ Wm$^{-1}$K$^{-1}$). The convective parameters of the fluid, corresponding to molten magnesium at a temperature 850°C, are: Prandtl number $Pr = 0.0095$, [7], kinematic viscosity $4.17 \cdot 10^{-7}$ m$^2$s$^{-1}$, and thermal expansion coefficient $\beta = 1.69 \cdot 10^{-4}$ K$^{-1}$. 

Figure 1. Scheme of the computational domain: (a) – general view with the coordinate system with the designated boundaries; (b) – computational mesh structure with solid (grey color) and fluid (blue color) regions.
Figure 2. Schemes of the heat flux distribution at the boundaries of the computational domain for various heating configurations: TBC-1 (a), TBC-2 (b), and TBC-3 (c).

Our numerical code solves the 3D equations of thermo-gravitational convection in the Boussinesq approximation for the fluid phase. We use the LES (Large Eddy Simulation) approach to take into account the turbulence, specifically the Smagorinsky-Lilly model model [8, 9] with the Smagorinsky constant $C_s = 0.14$ and turbulent Prandtl number $Pr_t = 0.9$. The mesh has a regular block structure with a total of 3.7 million nodes with additional mesh refinement near the boundaries (see figure 1b). The terms with time derivatives are discretised using an implicit Euler scheme. The convective terms are calculated by the TVD (Total Variation Diminishing) scheme [10]. The numerical simulations were performed on the Triton supercomputer of ICMM UB RAS.

Figure 1a designates the boundary faces: $\Gamma_U$ is the upper surface with area $S_U$, $\Gamma_{SU}$ is the part of the cooled side surface with area $S_{SU}$, $\Gamma_{SL}$ is the lower part of the side surface with area $S_{SL}$, and $\Gamma_L$ is the base with area $S_L$.

Three different variants of thermal boundary conditions (TBCs), which correspond to three possible heating configurations inside the reactor during the titanium production process, were considered. The first configuration, TBC-1 (figure 2a), combines the heating from above at the boundary $\Gamma_U$ with a constant heat flux $q_U$ resulting from the chemical reaction with a thermal power $Q_R = 205$ kW, the heating of the lower part of the side surface $\Gamma_{SL}$ with a heat flux $\Gamma_{SL}$ coming from the side heaters with the total power $Q_{SL} = 329$ kW, and the heating from below at the boundary $\Gamma_L$ with a heat flux $q_L$ from the lower heater with the power $Q_L = 94$ kW. All of this heat is removed from the retort by cooling the boundary $\Gamma_{SU}$ with height $h = 0.7$ m. Thus, the heat flux densities on the boundaries for TBC-1 are:

$$q_U = \frac{Q_R}{S_U}, \quad q_{SL} = \frac{Q_{SL}}{S_{SL}}, \quad q_L = \frac{Q_L}{S_L}, \quad q_{SU} = -\frac{(Q_R + Q_{SL} + Q_L)}{S_{SU}}.$$  

This heating regime corresponds to the situation with furnace heaters operating at full capacity and maximum air cooling efficiency. This case is most revealing for qualitative estimates of the maximum flow velocities inside the reactor, although it should be noted that during the real process also some specific sections of the furnace heater can be switched on simultaneously.

The second heating configuration, TBC-2 (figure 2b), is closer to the typical reactor operation and combines heating on $\Gamma_U$ by the chemical reaction with only the heaters on the bottom of the vessel being switched on, whereas heaters on the side surface $\Gamma_{SL}$ are switched off. Also note that the heat flux at the upper boundary $\Gamma_U$ is distributed not uniformly but with a parabolic law with a maximum at the center and a minimum on the periphery. Such a temperature non-uniformity can emerge in the reactor during the actual titanium reduction process due to
nonuniform titanium tetrachloride sputtering on the magnesium surface. The cooling zone has a height of \( h = 0.3 \) m in this case. Thus, the heat flux densities for TBC-2 are:

\[
q_U = \frac{2Q_R}{S_U} \left( 1 - \frac{x^2 + y^2}{R^2} \right); \quad q_{SL} = 0; \quad q_L = \frac{Q_L}{S_L}; \quad q_{SU} = -\frac{(Q_R + Q_L)}{S_{SU}}.
\]  

The third heating configuration, TBC-3 (figure 2c), implies a nonuniform heat flux \( q_U \) with parabolic law specified at the upper boundary \( \Gamma_U \) of the cylinder. A constant heat flux \( q_{SU} \) is removed from the side surface \( \Gamma_{SL} \) with height \( h = 0.15 \) m. The lower part of the side surface \( \Gamma_{SL} \) and the base \( \Gamma_L \) are assumed to be thermally insulated. In this case the solid titanium block occupies the lower half part of the vessel, which corresponds to later stages of the process. Consequently, the heat flux densities on the outer boundaries for TBC-3 are:

\[
q_U = \frac{2Q_R}{S_U} \left( 1 - \frac{x^2 + y^2}{R^2} \right); \quad q_{SL} = q_L = 0; \quad q_{SU} = -\frac{Q_R}{S_{SU}}.
\]  

Free-slip conditions are specified for the velocity at the upper boundary \( \Gamma_U \). This is in contrast to the no-slip boundary condition which was used in [4]. It is known that films emerge on a free surface in liquid metals, and it is often assumed in simulations that there is some sticking on that boundary. However, in the case of a chemical reaction on the surface the use of free-slip velocity boundary condition seems to be more reasonable. The no-slip conditions are specified for the velocity at all other boundaries which are “fluid to steel walls” and “fluid to titanium block” boundaries.

3. Results
All simulations were performed in dimensional form, with the governing parameters values corresponding to the actual titanium reduction process. The only parameter which is not exactly known is the intensity (heat transfer coefficient) of air cooling in the reaction zone. It is also known that there are several types of reactors with different heights \( h \) of the cooling zone and varying intensities of the cooling. In the real reactor the separate zone heaters in the furnace are switched on and off dynamically, depending on the temperature values measured at certain control points on the outer sidewall of the retort. In our simulations we assume that the integral thermal balance in the reactor is guaranteed, i.e. for every considered TBCs the amount of heat which goes into the vessel (by chemical reaction and furnace heaters) is equal to the amount of heat which is removed from the reactor (by air cooling).

Figure 3 presents the results of the simulations with the TBC-1 heating configuration (figure 2a). The snapshot of the instantaneous velocity field (figure 3a) shows that the turbulent flow occupies the entire volume of the liquid metal. The maximum instantaneous velocity \( V_{max} \) near the boundary reaches 18 cm s\(^{-1}\). The time-averaged velocity field (figure 3b) demonstrates a two-vortex structure of the convective flow, with one ring vortex in the upper part of the retort and one in its lower part. A maximum mean velocity \( < V >_{max} \approx 12 \) cm s\(^{-1}\) is observed near the boundaries. The temperature field (figure 3d) reflects the unsteady pattern of the motion caused by the near-wall ascending from the heated lower part of the reactor and by the descending flow arising in the cooled part of the retort. The intensity of turbulence can be characterised by the distribution of the energy of turbulent pulsations or by the standard deviation (SD). Figures 3c,d show the velocity and temperature SD fields. The most pronounced pulsations are observed in the region near the interface between heated and cooled parts of the sidewall. Strong temperature pulsations also exist in the upper part of the retort in the reaction zone.

It should be noted that in our previous paper [4] a similar heating configuration was studied. In this work we made the following changes: (a) – more accurate physical properties of liquid
Figure 3. Results for the TBC-1 heating configuration in the $yOz$ plane: (a) – instant velocity field, (b) – time-averaged velocity field, (c) – standard deviation of velocity field, (d) – instant temperature field, (e) – time-averaged temperature field, (f) – standard deviation of temperature field.

Figure 4. Results for the TBC-1 heating configuration: (a) – instant temperature field on the walls of the steel cavity, (b) – time series for variations of the temperature for the points at a distance of 10 mm from side wall (dashed lines) and for the points on the steel sidewall. Black line – $z = 0.3$ m, red line – $z = 1.8$ m, blue line – $z = 2.3$ m.
magnesium according to [7]; (b) – use of free-slip boundary condition for the velocity on the top surface instead of no-slip boundary condition; (c) – taking into account the influence of steel walls of the vessel.

Although the steel walls of the vessel with thickness 25 mm are not expected to strongly influence the heat transfer and flow structure, they should be taken into account for two reasons. First, applying heat fluxes to steel walls instead of applying it directly to the liquid metal leads to a more accurate imposition of temperature BCs. Figure 4a demonstrates the instant temperature field on the walls of the steel cavity. It can be seen that the temperature drop near the interface between the cooled and heated parts of the lateral surface of the vessel and becomes essentially less pronounced on the inner surface. Second, the temperature evolution at several points on the outer sidewall surface of the retort are the only temperature measurements which are available during the real process of titanium production. The conjugate heat transfer simulations allow us to obtain temperature distributions on the outer sidewall of the retort, which can be compared with real data. Figure 4b shows the time series for variations of the temperature for the points on the the steel sidewall (solid lines) and inside the vessel at a distance of 10 mm from the wall (dashed lines).

Next, we consider the heat flux configuration TBC-2 (figure 2b), which is representative for most of the process. It combines the nonuniform heating from the top due to the reaction with the heating from below due to bottom heaters. Figure 5 shows that the flow structure in this case is very different from the TBC-1 regime. A large-scale circulation (LSC) with two small

![Figure 5](image-url)
counter-rotating vortexes in the topmost and bottommost cylinder parts can be clearly seen on the instant and time-averaged velocity fields (figures 5a,b). It is well known that in the classical Rayleigh-Bénard problem (convection in a vessel heated from bottom) a large-scale circulation appears on the background of fully developed turbulence [11]. This LSC can reveal a variety of dynamical regimes (see, i.e. [12] for a cylinder with unit aspect ratio, or [13] for cubic geometry). The intensity of the velocity field is lower than in the case TBC-1, the maximum instant velocity \( V_{\text{max}} \approx 14 \text{ cm s}^{-1} \) and the average velocity is \( < V >_{\text{max}} \approx 9 \text{ cm s}^{-1} \). The most intense velocity pulsations are observed in the regions with interaction of the LSC with the counter-rotating rolls (figure 5c), the strongest temperature pulsations are located near the top of the cavity in the “reaction zone” (figure 5f).

Figure 6. Same as figure 3 for the TBC-3 heating configuration. The grey domain in the lower part of the cylinder corresponds to the titanium block.

Note that in previous simulations [4] we had argued that if the cooling intensity on the sidewall were not strong enough a uniform vertical temperature gradient would establish in the upper part of the retort (see figure 6 in [4]). In a real reactor this would lead to overheating, given that the temperature on the vessel walls should not exceed 950°C. Since the performance of the cooling system is not exactly known we varied the height of the cooling zone \( h \) (and thus the heat flux density on the boundary \( \Gamma_{SU} \)) in order to maintain thermal balance and to prevent overheating. For TBC-2 the height of the cooling zone is \( h = 0.3 \text{ m} \), which guarantees that there is no uniform vertical temperature gradient in the upper part of the retort (figure 5d).

The configuration TBC-3 (figure 2c) models the flow structure in the presence of a titanium
block in the lower part of the vessel. This corresponds to the middle stages of the process when the titanium occupies approximately half of the vessel volume. The furnace heaters are switched off and we have only the nonuniform heating from above. The velocity fields demonstrate one ring vortex structure flow in the liquid magnesium (figures 6a,b). The vortex intensity reaches its maximum (4.5 cm s\(^{-1}\)) near the boundaries, which is much lower than in the cases TBC-1,2. The distribution of velocity pulsations against a background of the mean flow (figure 6c) shows that the strongest pulsations appear in the regions where the descending flow along the boundaries collides with the surface of the solid block.

Note that in reality the titanium block is a porous medium, and magnesium trickles through the titanium sponge to the bottom of the retort. Yet, as was shown in [3], the flow intensity inside the titanium block is four orders of magnitude lower than the magnesium flow in the vessel. Therefore, in the present work the titanium block is assumed to be solid.

The temperature field in this heating configuration is almost stationary (figures 6d,e), the temperature pulsations are very weak and concentrated in the layer close to the upper part of the retort (figure 6f).

4. Conclusions

The structure of the convective flow of molten magnesium in a titanium reduction reactor was numerically studied in a three-dimensional non-stationary formulation with conjugated heat transfer between liquid magnesium and solids (steel walls of the cavity and titanium block), for different heating and cooling regimes. A detailed analysis was performed for three configurations of the heating rate control: with furnace heaters operating at full power, with furnace heaters switched on at the bottom of the vessel only, and with switched-off furnace heaters.

The most important finding of our study concerns the fact that the localization of the cooling zone can completely reorganize the structure of the large-scale flow. Therefore, by changing heating regimes, it is possible to influence the flow structure for the purpose of creating the most favorable conditions for the reaction. It was also shown that the presence of the titanium block strongly affects the flow structure.

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