Numerical simulations of convection in the titanium reduction reactor

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Abstract. We introduce a hydrodynamic model of convective flows in a titanium reduction reactor. The reactor retort is a cylindrical vessel with a radius of 0.75 m and a height up to 4 m, filled with liquid magnesium at a temperature of 850\degree C. The exothermic chemical reaction on the metal surface, cooling of the side wall and heating of the lower part of the retort cause strong temperature gradients in the reactor during the process. These temperature gradients cause intensive convective flows inside the reactor. As a result of the reaction, a block of titanium sponge grows at the retort bottom and the magnesium salt, whose density is close to the density of magnesium, settles down. The process of magnesium salt settling in a titanium reduction reactor was numerically studied in a two-dimensional (full size model) and three-dimensional (30\% size of the real model) non-stationary formulation. A detailed analysis was performed for configurations with and without presence of convective flow due to work of furnace heaters. It has been established that magnesium salt is settling in drops with sizes from $\approx 3$ cm to $\approx 10$ cm. It was shown that convective flow can entrain the drop and carry it with the vortex.

1. Introduction

Control of the reaction during the process of metallothermic reduction of titanium is one of the essential problems of its metallurgical production. 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\degree C. Titanium tetrachloride is supplied from the top to the magnesium surface. It produces spongy titanium and magnesium dichloride that sink to the bottom of the retort. The chemical reaction of titanium reduction is highly exothermic and runs predominantly on the surface:

$$2\text{Mg} + \text{TiCl}_4 = \text{Ti} + 2\text{MgCl}_2 + Q.$$  \hfill (1)

The 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.

In this work we introduce a hydrodynamic model of convective flows in a titanium reduction reactor. Large mass and dimensions of the apparatus as well as very high temperatures...
complicate the direct experimental measurements inside the reactor, which is one of the motivations for our numerical study of the process. Liquid magnesium is characterized by high thermal diffusivity (low Prandtl number), which implies a weak contribution of thermogravitational 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. The simplified axisymmetric computation in [3] showed that the buoyancy force can influence the metallothermic reduction of titanium. 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]. In the paper [5] we considered convective heat and mass transfer in the retort at different stages of the process under various cooling and heating regimes and demonstrated that the large-scale magnesium circulation in the reactor can be strongly affected by the change of heating and by the growth of the titanium mass. In the work [6] a convective flow of liquid metal generated nearby a hot round in the upper solid end face of a vertical cylinder has been studied experimentally and numerically. The considered flow is supposed to be a simplified model of the liquid magnesium flow in a reactor of metallothermic titanium reduction, although the typical Grashof number in the reactor is about three orders of magnitude higher than in the experiment ($10^{12}$ versus $10^9$).

Up to present all models considered only the convective flow of liquid magnesium, with and without presence of titanium sponge, and ignored the contribution of the second liquid phase – magnesium chloride. In the present paper we consider the flow of a two-phase system of immiscible fluids (liquid magnesium and magnesium salt) and analyze the settling of salt in the presence of strong convective flow inside the reactor.

2. Formulation of the problem and the mathematical model
The convective flow of liquid magnesium and magnesium chloride inside the cylindrical vessel is considered. We study early stages of the process, thus the contribution of the porous medium, titanium sponge, which sinks to the reactor bottom, is disregarded. The vessel is a cylinder with a diameter of $D = 1.55$ m and a height of $H = 2.5$ m. The height of the upper part of the side surface in the reaction zone, which is cooled by air, is $h = 0.7$ m. A scheme of the computational domain is shown in figure 1.

All the simulations were run using the free and open source finite volume code OpenFOAM 4.1. OpenFOAM includes the solver *multiphaseInterFoam* which relies on the Volume of Fluid
Table 1. Properties of Mg and MgCl$_2$.

| Property | Unit     | Mg     | MgCl$_2$ |
|----------|----------|--------|----------|
| $\nu$    | m$^2$/s  | 4.17 $\times$ 10$^{-7}$ | 9.9 $\times$ 10$^{-7}$ |
| $c_p$    | J kg$^{-1}$ K$^{-1}$ | 1344    | 971      |
| $\kappa$ | W m$^{-1}$ K$^{-1}$ | 90.7    | 1.7      |
| $\gamma$ | N/m     | 0.49    | 0.065    |
| $\rho$   | kg/m$^3$ | 1538    | 1637     |
| $\beta$  | K$^{-1}$ | 1.691 $\times$ 10$^{-4}$ | 1.845 $\times$ 10$^{-4}$ |
| Pr       |         | 9.5 $\times$ 10$^{-3}$ | 0.93      |

(VOF) method [7] and intends to solve problems with incompressible fluids, capturing the interfaces and including surface-tension and contact-angle effects for each phase [8], while not taking into account buoyancy effects. This solver is enhanced by the temperature equation using the Boussinesq approximation.

The numerical code solves equations for the two-phase fluid (liquid magnesium and magnesium salt). The properties of magnesium [9] and magnesium salt [10] at working temperature 850$^\circ$C are assumed to be constant and are shown in table 1. The interface tension can be estimated using the surface tensions using the method of Girifalco [11] as

$$\gamma = \gamma_1 + \gamma_2 - 2\phi\sqrt{\gamma_1\gamma_2}. \quad (2)$$

The parameter $\phi$ is not exactly known; it is 0.41 for Al|cryolith [12] or 0.51 for Al|NaCl-KCl [13]. We may therefore assume $\phi = 0.5$ and find $\gamma = 0.38$ N/m.

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 $S_L$.

The process of magnesium salt settling from the top surface to the bottom is considered. Initially, the vessel is filled with Mg, but with a layer of MgCl$_2$ on the bottom with thickness $0.3$ m. During the process the chemical reaction produces 442 kg of MgCl$_2$ per hour on the top boundary. The boundary $\Gamma_U$ is therefore considered as an inlet with uniform salt supply with constant velocity $4 \times 10^{-5}$ m/s. The salt is assumed to be drained through the hole on the bottom, thus the boundary $\Gamma_{LO}$ is considered as an outlet with diameter $d = 0.1$ m. All other boundaries are solid walls.

The simulations were done with and without heating. The heating configuration 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 $q_{SL}$ 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 (see figure 1d). All of this heat is removed from the retort by cooling the boundary $\Gamma_{SU}$. Thus, the heat flux densities on the boundaries are:

$$q_U = \frac{Q_R}{S_U}; \quad q_{SL} = \frac{Q_{SL}}{S_{SL}}; \quad q_L = \frac{Q_L}{S_L}; \quad q_{SU} = -\frac{(Q_R + Q_{SL} + Q_L)}{S_{SU}}. \quad (3)$$

The VOF method for multiphase flows implies that the numerical grid resolution should be high enough in order to resolve the regions of each phase as well as the boundaries between them. Therefore, we first utilize a two-dimensional (2D) formulation of the problem in order
to determine the typical sizes and forms of the droplets. The structure of the 2D mesh is shown in figure 1b. In that case the vertical cross section of the vessel is considered, and the heat fluxes \( q \) from the heaters at the boundaries are equal to the heat fluxes for the three dimensional cylindrical apparatus. The 2D mesh has 0.95 million grid points. A three-dimensional (3D) formulation of the problem is also considered, but due to restrictions on computational resources the model is only 30\% size of the real retort. These 3D simulations of the smaller model, using 1.5 million nodes, allow to study the salt settling with required spatial resolution. Again, the heat fluxes \( q \) from the heaters on the boundaries are equal to heat fluxes for three dimensional cylindrical apparatus. For 3D simulations we additionally use the LES (Large Eddy Simulation) approach, specifically the Smagorinsky-Lilly model [14, 15] with the Smagorinsky constant \( C_s = 0.17 \) and turbulent Prandtl number \( Pr_t = 0.9 \). The terms with time derivatives are discretised using an implicit Euler scheme. The convective terms are computed by the “limitedlinear” TVD (Total Variation Diminishing) scheme. The numerical simulations were performed using the supercomputer Triton of ICMM UB RAS.

3. Results

Figure 2 demonstrates results of 2D simulations for the real retort’s size without heating. The field of volume fraction function \( \alpha \) shows that the MgCl\(_2\) is settling in drops (figure 2b), which are indicated by white circles in all figures. During their fall, the drops produce vortex trails (figure 2a) with maximum instantaneous velocities of \( \approx 25 \text{ cm/s} \). The shape of the drops changes during the fall, their sizes vary from 3 cm to 10 cm. The enlarged parts of the instant phase fraction field (figure 2c) demonstrate the typical shape of drops. From the grid in that picture, which denotes the volumes of numerical mesh, one can see that the drops are well resolved.

Next we consider the salt settlement for the case with the heaters switched on at full power, with the heating configuration shown in figure 1d. The snapshot of the instantaneous velocity field (figure 3a) shows that the convective flow occupies the entire volume of the liquid metal. There are two large scale vortices in the bulk and a few weak vortices in the bottom layer of MgCl\(_2\). The temperature field reflects the unsteady pattern of the motion caused by the near-wall ascending flow from the heated lower part of the reactor and by the descending flow arising in the cooled part of the retort. The hot droplets cool down during its fall to the bottom (compare the temperature of drops with different positions in figure 3c).
Figure 3. 2D simulations, real size model, heaters are switched on, $yOz$ plane: (a) – instant velocity field; (b) – instant phase fraction $\alpha$ field; (c) – instant temperature field.

Figure 4. 3D simulations, 30% size of the real model: (a),(b) – no heating. (c)-(f) – heaters are switched on. (a),(d) – instant velocity field; (b),(c),(e) – instant phase fraction $\alpha$ field; (f) – instant temperature field.
While the 2D simulations allow us to estimate the form and velocity of drops and the requirements on the mesh resolution to resolve them, the turbulence cannot be properly modelled. Hence, the structure of the convective flow in the cylindrical geometry should be different from the flow structure obtained using 2D Cartesian grid. As a first attempt, the 3D simulations were done with a smaller model, which is only 30% size of the vessel. Figure 4 presents the results of the 3D simulations using an LES model for small-scale turbulence. Figures 4a,b show the salt settling without heating. Note that the size and velocity of drops are similar to those in the 2D case. In case of switched on heaters (figures 4c-f) one can see that the situation is very different in comparison to the previous case. The convective flow occupies the whole cavity (figures 4d,f), the average velocity field shows 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 (as shown in [4, 5]). The motion exhibits a distinct boundary-layer pattern. Evidently, the convective flow can entrain the drops and carry them with the vortex. The drops then tend to fall along the walls and not in the bulk (see figures 4c,e).

4. Conclusions
The process of magnesium salt settling in a titanium reduction reactor was numerically studied in a 2D (full size model) and 3D (30% size of the real model) non-stationary formulation. The numerical code solves the equations for two-phase fluid (liquid magnesium and magnesium salt). A detailed analysis was performed for configurations with and without presence of convective flow due to work of furnace heaters. It was shown that magnesium salt is settling in drops with sizes from $\approx 3$ cm to $\approx 10$ cm. The velocity of drops (from $\approx 18$ cm/s to $\approx 30$ cm/s, depending on regime) is higher than the velocity of the convective flow (up to 20 cm/s), but it was shown that convective flow can entrain the drop and carry it with the vortex.

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References
[1] Frick P, Khalilov R, Kolesnichenko I, Mamykin A, Pakhollkov V, Pavlinov A and Rogozhkin S 2015 Europhys. Lett. 109 14002
[2] Zikanov O, Listratov Y I and Svirdov V G 2013 J. Fluid Mech. 720 486–516
[3] Tsaplin A I and Nechaev V N 2013 Computational continuum mechanics 6 483–490
[4] Teimurazov A S and Frick P G 2016 J. Appl. Mech. Tech. Phys. 57 1264–1275
[5] Teimurazov A, Frick P and Stefani F 2017 IOP Conference Series: Materials Science and Engineering 208 012041
[6] Khalilov R, Kolesnichenko I, Teimurazov A, Mamykin A and Frick P 2017 IOP Conference Series: Materials Science and Engineering 208 012044
[7] Hirt C and Nichols B 1981 J. Comput. Phys. 39 201 – 225
[8] Weber N, Beckstein P, Herreman W, Horstmann G M, Nore C, Stefani F and Weier T 2017 Phys. Fluids 29 054101
[9] Smithells C J, Gale W F and Totemeier T C 2004 Smithells Metals Reference Book 8th ed (Elsevier Butterworth-Heinemann)
[10] Janz G J, Allen C B, Bansal N P, Murphy R M and Tomkins R P T 1979 Physical Properties Data Compilations Relevant to Energy Storage. II. Molten Salts: Data on Single and Multi-Component Salt Systems (U. S. Department of Commerce)
[11] Girifalco L A and Good R J 1957 J. Phys. Chem. 61 904–909
[12] Roy R and Utitgard T A 1998 Metall. Trans. B 29B 821–827
[13] Roy R and Sahai Y 1997 Mater. Trans. 38 546–552
[14] Smagorinsky J 1963 Mon. Weather Rev. 91 99
[15] Deardorff J W 1970 J. Fluid Mech. 41 453–480