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Numerical modelling of thermoelectric magnetic effects in solidification

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Abstract

Since several years experiments performed on solidification of alloys with application of a static magnetic field show a significant effect of the latter on the solidified structure and segregation. A hypothesis suggests that these modifications are related to a thermoelectric magnetic force. Serious efforts were made to reproduce observed phenomena with numerical modeling, yet, they faced significant difficulties. In the paper we discuss some numerical issues using a model magneto-thermoelectric problem coupled with hydrodynamics with finite volume and a finite element method.

Key words: thermoelectric effect, finite element method, finite volume method, magnetohydrodynamics

Introduction

Experiments on solidification with static magnetic field revealed numerous results: motion of dendrites [1], shift of columnar to equiaxed transition conditions [2], spiral segregation [3] and others. It is supposed that thermoelectric magnetic forces which appear in conductive media with variable electric properties subjected to a temperature gradient may be responsible for observed phenomena. For qualitative and quantitative proof of this hypothesis the numerical modelling is ultimately needed. Yet, one can cite only a limited number of simulations of magneto-thermoelectric effect which were performed either with a simplified treatment of the electric problem [4] or for simplified domains [5]. The aim of the present paper is to discuss issues related to the simulations of thermoelectric problem coupled with hydrodynamic one using various numerical methods. Our presentation is based on a model problem which consists of an immovable spherical solid grain immersed into a liquid metal subjected to a thermal gradient as shown in fig.1. A vertical magnetic field is imposed over the domain parallel to the thermal gradient. In this system an electric current appears due to a different electric response of the system to the temperature, i.e. to a so-called thermoelectric effect. Further Lorentz force acting both on the liquid and on the solid appears due to the interaction between the thermoelectric current and the magnetic field. It creates convection in the liquid and makes a particle move. The thermoelectric part of the problem can be solved analytically if an infinite domain around the sphere is considered [6]. Analytically obtained distributions of the density of the electric current along a vertical and a horizontal line which passed through the center of the sphere are presented in fig. 2, properties correspond to those given in Table 1.

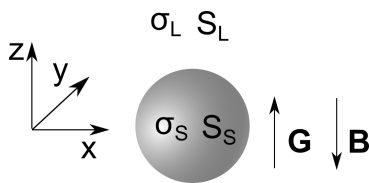


Fig. 1: A model problem for a sphere immersed into a liquid. A thermal gradient $G = 6 \cdot 10^3 \text{ K/m}$ and a static magnetic field $B = 1 \text{ T}$ are imposed on the system along the z-axis

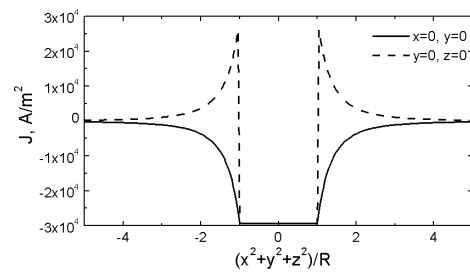


Fig. 2: Distribution of the density of the thermoelectric current along the vertical (solid) and a horizontal (dashed) line passing through the center of the sphere placed in an infinite media

Table 1. Properties used in analytical calculations and in simulations.

Property	Units	Solid	Liquid
Thermoelectric power, S	V/K	$1.1 \cdot 10^{-6}$	$1.0 \cdot 10^{-7}$
Electrical conductivity, σ	$(\Omega \cdot \text{m})^{-1}$	$1.37 \cdot 10^7$	$3.8 \cdot 10^6$
Dynamic viscosity, η	Pa·s	-	0.00115

A remarkable fact about the solution is that the maximal value of the electric current does not depend on the size of a particle, but is related only to the properties of the media and to the thermal gradient near the interface.

Statement of the problem

The governing equations for the thermoelectric problem presented in fig.1 are the following [7]:

$$\mathbf{J} = -\sigma \nabla \varphi - \sigma S \nabla T + \sigma (\mathbf{V} \times \mathbf{B}) \quad (1)$$

$$\nabla \cdot \mathbf{J} = 0 \quad (2)$$

Here \mathbf{J} is the density of the electric current, φ is the electrical potential, \mathbf{V} is the velocity in the liquid, \mathbf{B} is the magnetic field, other symbols and values used in simulations are given in the table 1. The boundary conditions presume no electric current through the walls of the calculation domain. Because of the axial symmetry of the problem, the electric current is developed in meridional plane (r, z) and the resulting electromagnetic force given by eq.3 has only the tangential component:

$$\mathbf{F} = F \cdot \mathbf{e}_\theta = \mathbf{J} \times \mathbf{B} \quad (3)$$

This force is to be introduced into momentum equations related to a hydrodynamic problem. However, the latter was treated differently with respect to software and is discussed in appropriate sections.

Results obtained with a finite volume method

A modeling with FVM approach was made in Fluent using user-defined functions and with an axisymmetric swirl model. A governing equation which was solved for the electric potential is obtained from the eq.(1)-(2):

$$\nabla(\sigma \nabla \varphi) = -\nabla(\sigma S \nabla T) + \nabla(\sigma (\mathbf{V} \times \mathbf{B})) \quad (4)$$

A natural way for treatment of the model is to use two domains separated with a sharp boundary. Another approach with utilization of a "phase function" is presented in this proceeding [8]. Since the temperature gradient is imposed and each of the domains has constant properties, the first term in the right-hand part turns to be zero. Because of restriction of an axisymmetric model in Fluent the eddy current in the liquid phase could not be taken into account in the liquid phase. Therefore, an equation to be solved for the φ was Laplace equation. A continuity of the electric current at the interface between the domains should be assured via an appropriate boundary condition. Consequently, for the electric potential at the interface one obtains:

$$\varphi_S = \varphi_L \quad (5a)$$

$$-\sigma_L \left(\frac{\partial \varphi}{\partial n} \right)_L - \sigma_L S_L G = -\sigma_S \left(\frac{\partial \varphi}{\partial n} \right)_S - \sigma_S S_S G \quad (5b)$$

Here indices S and L stay for the solid and the liquid phase, respectively. Eqs.(5a)-(5b) can be reduced to a single Dirichlet condition using a discretised form of the governing equation. For the present case a first-order discretisation scheme was used with a correction for a non-orthogonal mesh.

For the hydrodynamics only the tangential component of the velocity was calculated with the eq.(6) where V_θ and η denotes the tangential component of the velocity field and dynamic viscosity, respectively. No-slip conditions were imposed at all boundaries including the solid/liquid interface.

$$\eta \nabla^2 V_\theta + (\mathbf{J} \times \mathbf{B})_\theta = 0 \quad (6)$$

In calculations the radius of the particle was $100 \cdot 10^{-6}$ m and the size of the domain was $1 \cdot 10^{-3}$ m by $5 \cdot 10^{-4}$ m. Results of simulations are shown in fig.3. The maximal calculated value of the thermoelectric currents is equal to the one from analytical solution (fig. 2). The current is indeed uniform inside the sphere and decreases rapidly in the liquid, i.e. for the thermoelectric problem the domain can be considered as an infinite one. The Lorentz force tends to create two vortices under and over the sphere with different direction of their rotation. However, because of walls the secondary flow should appear in the liquid. The values for the angular velocity are quite high and it can be supposed that the eddy current has an important impact on the resulting electric current.

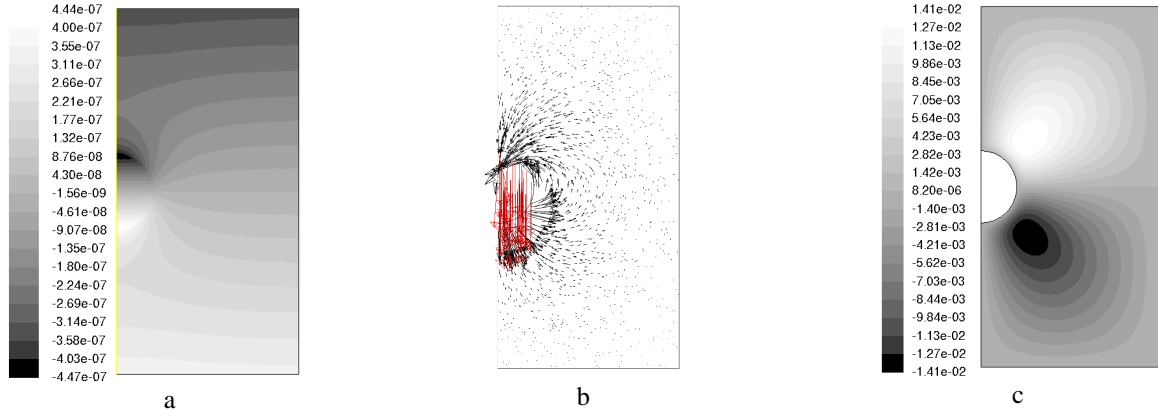


Fig. 3: Results obtained with finite volume method realized in Fluent: electric potential (a); vector field for the density of the thermoelectric current, $|\mathbf{J}|_{\max} = 29112 \text{ A/m}^2$ (b); contours of tangential velocity (c)

Results obtained in Flux Expert with a finite element method

In calculations made with Flux Expert the size of the particle was the same as in the previous case, but the size of the domain was two times larger. Similar to the simulation performed in Fluent, only the tangential component of the velocity was calculated for the hydrodynamic problem. However, the eddy current which appears due to the motion of conductive liquid in this direction was taken into account according to eq.(1). To solve the coupled problem a Galerkin projective method was used. The equations (2) and (6) are projected on the basis functions α_i , the continuity of the electric current at the interface is taken into account at this step. Further, the electric current is replaced with the eq.(1) which leads to the following weak finite element formulation :

$$\iint_{\Omega} \sigma \nabla \alpha_i \nabla \varphi r dr dz - \iint_{\Omega} \sigma \nabla \alpha_i (\mathbf{V} \times \mathbf{B}) r dr dz = - \iint_{\Omega} \sigma \nabla \alpha_i \nabla T r dr dz \quad (7a)$$

$$\iint_{\Omega} \eta \nabla \alpha_i \nabla V_{\theta} r dr dz + \iint_{\Omega} \alpha_i \sigma V_{\theta} B^2 r dr dz + \iint_{\Omega} \alpha_i \sigma \nabla \varphi \times \mathbf{B} r dr dz = - \iint_{\Omega} \alpha_i \sigma S \nabla T \times \mathbf{B} r dr dz \quad (7b)$$

Here Ω is the whole domain and because of this the FEM methods does not require a special treatment of the conditions at the interface since they are satisfied naturally. Also, in this formulation strong interaction between the two phenomena – electrical one and hydrodynamic – are taken into account.

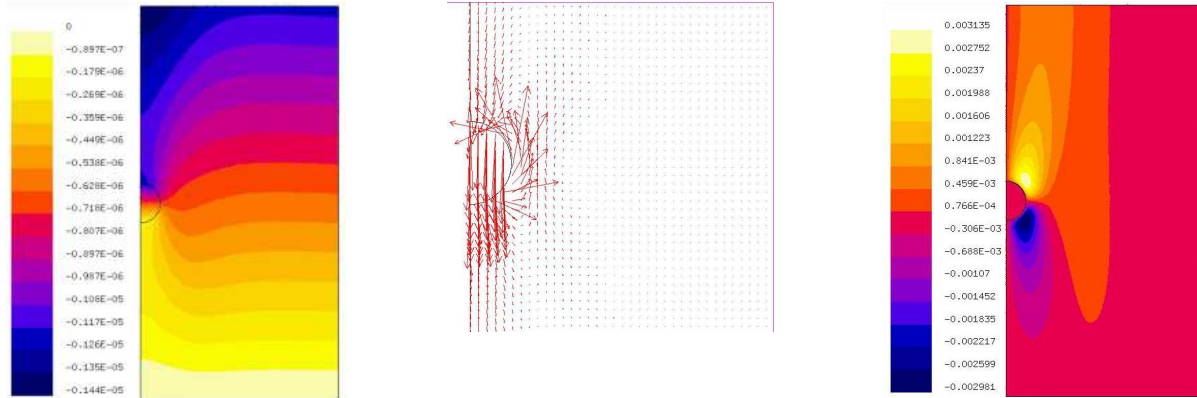


Fig. 4: Results obtained with finite element method realized in Flux-Expert: electric potential (a); vector field for the density of the thermoelectric current, $|\mathbf{J}|_{\max} = 17390 \text{ A/m}^2$ (b); tangential velocity (c)

Qualitatively the distribution of the electric potential in Fig. 4a is similar to the one obtained with Fluent, however, its maximal difference is larger and potential isolines are “pushed” toward the vertical axis. The first effect is related to the size of the domain which is two times larger compared with previous calculation. The second effect may be attributed to the influence of the eddy current which is given by the product $\sigma(\mathbf{V} \times \mathbf{B})$ and is directed along the radius toward the z-axis. It should be stressed that the eddy current influences both potential and the resulting current according to eq.(1)-(2). Consequently, the maximal value of the electric current differs from the analytical one: 17390 A/m^2 vs 29112 A/m^2 . The angular velocity is also lower and the vortices are displaced toward the axis of symmetry.

Finite element method: realization with AEQUATIO

Presented results shows that the problem is extremely sensitive to the mesh size and a fine mesh is needed near the interface between the two media where properties of media varies. At the same time to treat the convection properly an actual size of the experimental domain should be considered, otherwise boundaries alter both the thermoelectric current and convective flow. One of the ways to overcome these difficulties is the use of multiple meshes for treatment of different phenomena. This approach was realized with a numerical toolbox AEQUATIO based on the finite element method [9]. Coupled equations for the energy and electric current are projected over two meshes: the one which is constructed for the whole domain and which is coarse and a significantly finer mesh for a sub-domain around the particle as shown in fig. 5. The boundary conditions for the sub-domain are obtained via interpolation of data from the coarse mesh and only one system of linear equations is constructed for all meshes. Simulation performed with AEQUATIO without convective flows gives results similar to the analytical ones (fig. 6) and obtained with Fluent, detailed discussion can be found elsewhere [10]. The further step is to introduce the calculation of Naviers-Stokes equation into the AEQUATIO.

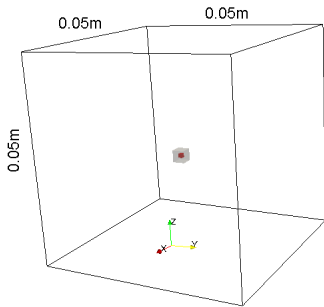


Fig. 5: Illustration of a multi-domain structure used in AEQUATIO, the sphere is seen as a central point

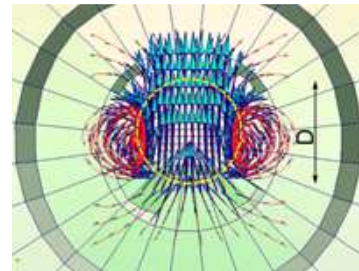


Fig. 6: A zoom on the subdomain with a particle with a calculated density of the thermoelectric current

Conclusion

The treatment of the thermoelectric problem with a FVM requires special treatment of the boundary conditions at the interface between two media whereas with FEM the continuity of the electric current satisfies naturally. Both methods are sensitive to mesh size near the interface and use of multiple meshes or adaptive meshes are required for a good treatment of a coupled thermoelectric hydrodynamic problem. The eddy current which appears due to the convection in the liquid may affect strongly the thermoelectric current.

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