The Effect of Ultrahigh Magnetic Fields on Dopant Distribution in CZ Systems: A Modeling Study and Comparison with Asymptotic Solutions

O.J. ILEGBUSI and J. SZEKELY

A mathematical representation is developed to describe the velocity, temperature, and dopant concentration fields in a magnetically-damped axisymmetric Czochralski (CZ) crystal growing system. Particular attention is paid to the near-field conditions, that is, to the dopant concentration profiles in the vicinity of the crystal surface, to the transient dopant distribution, and to the effect of very high magnetic fields up to 80 kilogauss.

I. INTRODUCTION

The primary purpose of the work described in this paper is to represent the effect of high externally imposed magnetic fields on the behavior, and especially on the transient dopant distribution, in CZ systems. An additional objective is to compare the numerically computed velocity fields and transport rates with those predicted by analytical asymptotic methods and, thus, provide a direct validation of the computational approach developed here.

The magnetic damping of convection in CZ systems is being practiced in many instances, although a fully comprehensive understanding of the transport phenomena that occur in these systems is yet to emerge. As a result of interesting work reported in References 3 through 5 and 9 through 11, there is now emerging a semiquantitative appreciation of the role played by an axial field in modifying the velocity and the temperature fields. It is now understood that even moderate fields can suppress oscillatory motion and that heat transfer by convection in the melt can be reduced when the magnetic interaction parameter exceeds unity.

To date, the specific issue of radial dopant segregation has not been systematically addressed in the presence of a magnetic field nor has the question of ultrahigh fields been discussed. This latter point is of considerable practical interest because of the current interest in the possibility of producing CZ pullers with magnetic fields of the order of 30 or more kilogauss.

Simple order-of-magnitude arguments suggest that because of the high values of the Schmidt number, even small changes in fluid convection can have a profound effect on dopant transfer. There is, however, an as-yet unresolved question: how high a field would be required in order to reduce convection sufficiently so that the convective transport of the dopant to the crystal from the bounding surface would have a time scale comparable to, or larger than, the actual time scale of the operation. If such conditions can be achieved, there is a potential for growing "perfect" crystals of the type realized in Skylab. The present paper addresses this question explicitly.

II. FORMULATION

Let us consider a CZ growth system, such as that sketched in Figure 1, which is subjected to an axial magnetic field.

Fluid motion in the CZ system is a function of (1) forced convection caused by the crystal and crucible rotation; (2) buoyancy-driven flow resulting from temperature gradients; and (3) flow damping due to the imposed magnetic field.

The mathematical formulation of this problem is given in References 5 and 8 and will only be briefly highlighted here.*

*The formulation presented here is very similar to that given in Reference 5 except for the fact that in the present case we are considering steady-state fluid motion.

A. Momentum Conservation

\[ \nabla \cdot \nabla \mathbf{V} = -\frac{1}{\rho} \nabla \rho + \nu \nabla^2 \mathbf{V} + \frac{1}{\rho} \mathbf{E}_B + \frac{1}{\rho} \mathbf{E}_E \]  

[1]

In Eq. [1], \( \mathbf{E}_B \) and \( \mathbf{E}_E \) are the buoyancy force and the electromagnetic force, respectively, expressed as

\[ \mathbf{E}_B = \rho_0 [1 - \beta (T - T_0)] g \]  

[2]

and

\[ \mathbf{E}_E = \mathbf{j} \times \mathbf{B} \]  

[3]

where \( \mathbf{j} \) is the induced current density and \( \mathbf{B} \) the magnetic field.

By invoking Maxwell's equations, the components of \( \mathbf{E}_E \) for an axial magnetic field \( B_0 \) oriented parallel to the \( z \)-axis can be expressed as (see Appendix)

\[ F_r = -\frac{\sigma}{\rho} V_r B_0^2 \]  

[4]

\[ F_\theta = -\frac{\sigma}{\rho} V_\theta B_0^2 - \frac{\sigma}{\rho} E_r B_0 \]  

[5]

\[ F_z = 0 \]  

[6]
where \( E_r \) is the radial component of the electric field. A discussion on the calculation of \( E_r \) is also contained in the Appendix. As discussed in Reference 5 and also shown in detail in the Appendix, \( F_z \) is the logical consequence of the small value of the magnetic Reynolds number.

B. Thermal Energy Balance

\[
V \cdot \nabla T = \alpha \nabla T^2
\]

where \( \alpha \) is the thermal diffusivity.

C. Concentration Balance

\[
\frac{\partial C}{\partial t} + V \cdot \nabla C = D \nabla^2 C
\]

in which \( D \) is the mass diffusivity.

D. Boundary Conditions

A “no-slip condition” is imposed on the velocity field on all solid walls. Symmetry and zero shear are allowed for along the central axis and at the free surface, respectively. The temperature is prescribed at the crystal and at the crucible surface, while the free surface is allowed to radiate heat to the environment.

In addition, thermocapillary convection is allowed for, such that the condition on the radial velocity components at the free surface is

\[
\frac{\partial V_r}{\partial z} = -\frac{1}{\mu} \frac{\partial \gamma}{\partial \Theta} \frac{\partial \Theta}{\partial t}
\]

where \( \gamma \) is the surface tension coefficient, and \( \mu \) is the dynamic viscosity.

In order to illustrate the effect of an ultrahigh magnetic field on convection, we shall consider the somewhat idealized case of transporting a dopant or impurity from the walls to the crystal. For the sake of mathematical convenience, we shall assume that the concentration of this transported species is unity at the wall and zero at the crystal surface, while a no-flux condition is being imposed at the free surface.

Figure 1 in the text depicts a more general case, where allowance is also made for dopant exchange with the environment. Such a situation may be readily represented with minimal complication, provided the exchange process can be defined.

The boundaries are assumed to be electrically insulated. The principal input parameters are summarized in Table I.

### III. SOLUTION PROCEDURE

In essence, the solution of the problem requires a numerical procedure for solving

1. the electromagnetic force field equations;
2. the Navier-Stokes equations, incorporating the effect of buoyancy and the electromagnetic (breaking) forces;
3. the differential thermal energy balance equation; and
4. the convection/diffusion equation for the dopant.

Of these, only the diffusion equation is uncoupled, because the electromagnetic forces will depend on the velocity field which, in turn, depends on both the electromagnetic force field and the temperature field within the system.

There are commercially available software packages for solving both the steady-state and the transient-transport equations; however, the coupling of the magnetic field does represent a significant additional undertaking.

In the present work, the PHOENICS code, supplemented by a “homemade” magnetic code, was used for solving the transport equations. To date, there has been little published experience with running this software package to represent rotating systems of this type. In carrying out the calculations, a good guess of the initial values of the flow variables was found to be critical for the stability of the numerical scheme, especially for the case when only the crystal was being rotated.

A \( 21 \times 18 \) nonuniform grid, identical to that described in Reference 15, was employed for the calculations. While

<table>
<thead>
<tr>
<th>Table 1. Principal Input Parameters</th>
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<tbody>
<tr>
<td>Crucible radius ( R_c = 0.127 ) m</td>
</tr>
<tr>
<td>Crystal radius ( R_x = 0.04125 ) m</td>
</tr>
<tr>
<td>Crucible rotation rate ( \omega_c = -15 ) rpm</td>
</tr>
<tr>
<td>Crystal rotation rate ( \omega_x = 60 ) rpm</td>
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<tr>
<td>Melt depth ( H = 0.12 ) m</td>
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<tr>
<td>Kinematic viscosity ( \nu = 3.5 \times 10^{-7} ) m(^2)/s</td>
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<tr>
<td>Thermal diffusivity ( \alpha = 1.25 \times 10^{-7} ) m(^2)/s</td>
</tr>
<tr>
<td>Volumetric expansion coefficient ( \beta = 1.41 \times 10^{-5} )</td>
</tr>
<tr>
<td>Reference density ( \rho_0 = 2.533 \times 10^3 ) kg/m(^3)</td>
</tr>
<tr>
<td>Temperature at crucible walls ( T_{cw} = 1498 ) °C</td>
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<tr>
<td>Temperature at crystal surface ( T_x = 1412 ) °C</td>
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<tr>
<td>Emissivity of melt surface ( \varepsilon = 0.3 )</td>
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<tr>
<td>Schmidt number of dopant transport ( \sigma = 1000 )</td>
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<tr>
<td>Surface tension constant ( \sigma = 0.15 ) m/K·s</td>
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<tr>
<td>Typical pulling rate ( v = 5 ) cm/h</td>
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