Analytical Modeling of Forced and Natural Convection in Molten Zones

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2019 PARADIM REU Intern @ Johns Hopkins

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Program: 2019 Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials Research Experience for Undergraduates Program at Johns Hopkins University

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Primary Source of JHU REU Funding: Support for PARADIM is provided under NSF Grant # DMR-1539918 as part of the Materials Innovation Platform Program

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Primary JHU PARADIM Tools Used: Laser Diode Floating Zone

Abstract:

A floating zone crystal growth procedure is utilized to grow large, bulk single crystals of interesting materials to further investigate properties such as electronic, magnetic or strength. This procedure is a direct melt process used to grow single crystals with two rods connected by a molten center. The molten zone is maintained when the feed, or top, rod is constantly melting and the seed, or bottom, rod is constantly solidifying via downward translation. The molten zone is a non-isothermal liquid bridge which causes natural convection and since the rods are moving by translation and rotation, there is forced convection component as well. The stability of the liquid bridge can be controlled based the speed of the rods and adjustments of heat. To more easily predict which settings will work best and provide the most stable molten zone for a given material, a dimensionless analytical model was developed, factoring in unexplored components such as, gravity, motion of the rods, wind driven shear force on the free surfaces of the melt, the complex geometry of the molten zone and, the effect of phase change temperature gradient. The proposed model accounts for the aforementioned assumptions which provides a more complete view of the fluid flow within the molten zone.

Summary of Research:

Geometry. The geometry of the molten zone can provide insight to what assumptions can and cannot be made. The molten zone is assumed to mimic the geometry of a liquid bridge between two spherical particles. This assumption is made, rather than a liquid bridge between parallel plates, because there is an external heating source in floating zone furnaces, since there is a temperature gradient in the radial and axial direction, the solid liquid interface will be curved since it will be colder in the center of the melt. The liquid bridge between two spherical particles is a simplifying assumption because the interface actually has an unknown geometry [1]. However, once this assumption is made many determinations about its overall geometry can be made. The schematic used to describe the geometry is shown in Figure 1.

Using the parameters shown in Figure 1, it can be proved that gravity has a non-negligible affect on the fluid flow. This is done using the modified bond number in equation 1[2].

$$V^*Bo = \frac{\pi H_{in}(\rho_{mz} - \rho_{air})g_z}{2\sigma_{liq-gas}(\frac{1}{\frac{1}{R_F}} - \frac{1}{\frac{1}{R_s}})} << 1 \tag{1}$$

One can also find the dimensionless radial and axial coordinates using equations 2-6.

$$\xi_r = |k_1|r \tag{2}$$

$$k_1 = \frac{P_c r_0^2}{2\sigma} \tag{3}$$

$$P_c = \sigma(\frac{1}{r_m} + \frac{1}{r_a}) \tag{4}$$

$$r_{a,intermediate} = r_c \tag{5}$$

$$\xi_z = \frac{z(\xi_r)}{|k_1|} \tag{6}$$

The expression for $z(\xi_r)$ varies depending on the type of capillary bridge [3]. Furthermore, this assumption allows the system to be described as a 2D axisymmetric flow rather than 3D, which will save computation time and complexity.

Governing Equations. Since this system is non-isothermal with a line heat source, [4] a continuity equation, equation of motion, and equation of thermal energy needs to be defined. These general equations, along with the boundary conditions will account for gravity, latent heat, radiation, rotation of the rods, and outside convective flux. The general equations have been non-dimensionalized, which will increase the accuracy and decrease the computation time of the model. A schematic showing relevant parameters for the governing equations is shown in Figure 2. The velocity is non-dimensionalized using $2r_c/\alpha_m$. Pressure is non-dimensionalized using $4r^2_c/\rho_m\alpha^2_m$ [5]. Enthalpy is non-dimensionalized by $1/\rho_m L$ [6]. The non-dimensionalized governing equations are shown in equations 7-9.

$$\nabla \cdot \boldsymbol{v}^* = 0 \tag{7}$$

$$\boldsymbol{v}^* \cdot \nabla \boldsymbol{v}^* = -\nabla P^* + Pr\nabla^2\, \boldsymbol{v}^* - PrRa_T(\Theta - 1)\boldsymbol{e_z} \tag{8}$$

$$Ste\frac{\delta\psi}{\delta\tau} + \boldsymbol{v}^* \cdot \nabla\psi = \nabla^2\psi - Ste\frac{\delta f_l}{\delta\tau} \tag{9}$$

where $\boldsymbol{v}^*$, P^*, Pr, Ra_T, Θ, Ste, ψ, f_l, τ is dimensionless velocity, dimensionless pressure, Prandtl number, Rayleigh number, dimensionless temperature, Stefan number, dimensionless enthalpy, fluid fraction, and dimensionless time, respectively.

Boundary Conditions. The boundary conditions were defined based on the schematic shown in Figure 3. When ξ_z = 1, -1 the boundary conditions for motion and thermal energy are very similar with the only changes being the parameters with respect to the feed rod or the seed rod.

$$\boldsymbol{v_r^*} = \frac{-2V_i r_c}{\alpha_m} \tag{10}$$

$$\boldsymbol{v_\theta^*} = \frac{2\Omega_i r_c}{\alpha_m}\frac{\xi_r}{2\pi} \tag{11}$$

$$Q_m - Q_i + \frac{\rho_{crystal}}{\rho_m}\frac{2r_c}{\alpha_m}[-V_i - \Omega_i\xi_r]Ste \cdot \boldsymbol{n} = 0 \tag{12}$$

Where V_i,α_m, Ω_i, and Q_i are the translating velocity of the feed or seed rod, the thermal diffusivity of the melt, the angular velocity of the feed or seed rod, and the heat flux either in the melt or the feed or seed rods. This heat flux accounts for radiation in the way that it is defined and calculated for all melts. This is especially important in semi-transparent melts [7].

On the free surface, when ξ_r = 1, there is a stress boundary condition for motion and a maximum temperature for the thermal energy boundary condition.

$$\boldsymbol{\tau : ns} = Gr\frac{\delta\Theta}{\delta s} + \boldsymbol{\tau_{wind}} \tag{13}$$

$$\boldsymbol{\tau : nn} = (2\boldsymbol{H}Bo) \tag{14}$$

$$\frac{\delta\Theta}{\delta\xi_r} = 0 \tag{15}$$

where equation 13 and equation 14 represent the tangential stress balance and normal stress balance, respectively.

Furthermore, τ, $\boldsymbol{n}$, $\boldsymbol{s}$, Gr, $\boldsymbol{H}$, Bo are the stress tensor, the vector normal to the surface of the melt, the vector tangential to the surface of the melt, the Grashof number, the principle curvature of the free surface, and the bond number, respectively.

Future Work:

The next phase of this work is to generate a computer model using COMSOL Multiphysics to better understand the convection within the molten zone. The model, both the previously mentioned equations and the computer model, can be verified with experiment. This verification would be done by growing silicon in the laser diode floating zone as the material properties of molten silicon are known.

Acknowledgements:

This material is based upon work supported by the NSF (Platform for the Accelerated Realization, Analysis, and Discovery of Interface Materials (PARADIM)) under Cooperative Agreement No. DMR-1539918 as part of the Materials Innovation Platform Program.

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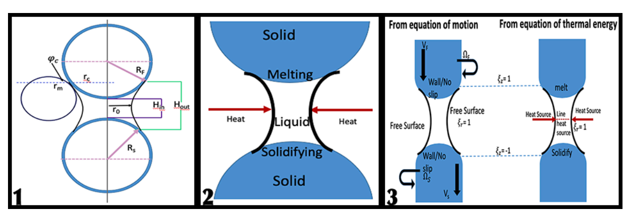

Figure 1, left: Parameters used to find geometric properties of the molten zone. rm, rc, φc *are the meridional radius, contact radius, and contact angle respectively.*

Figure 2, middle: Parameters that must be considered when defining governing equations.

Figure 3, right: Parameters that must be considered when defining motion and thermal boundary conditions.