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Analysis and Suppression of Base Separation in the Casting of a Cylindrical Ingot

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This paper presents a comprehensive numerical investigation of the influence of cooling conditions on base separation, void formation and thermally induced stresses during the solidification of a high Prandtl number energetic melt in a cylindrical enclosure. Numerical models have been developed to simulate the heat and mass transfer processes in melt casting as well as to analyze the base separation and thermal stresses induced during solidification; the two models are dynamically coupled. The numerical predictions are validated against experiments. Based on the numerical analysis, modified cooling conditions are suggested which are shown to reduce base separation.

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INTRODUCTION

Casting is an established and widely used process for manufacturing complex shapes without the necessity of applying large forces. It is especially useful in processing energetic materials which cannot tolerate high forces. The ambient cooling conditions play an important role in determining the quality of the final cast product. One measure of quality is the nearness of the product to the final shape desired with little or no residual stresses. An example of deviation from the desired shape is base separation [1]. Well-designed cooling conditions could help avoid such deleterious effects.

In casting processes, the heat transfer, fluid flow, and phase change processes and the induced stresses are strongly coupled. The effects of natural convection in the melt induced by solidification are relatively well understood. Extensive analytical, experimental and numerical efforts have been reported on this topic [1-6].

Thermal stresses induced during the casting process are, in general, less well understood. Analytical solutions have been suggested under simpler conditions and geometries such as high-pressure die casting [7]. It is also challenging to experimentally visualize thermal stresses. Interesting approaches such as the use of X-ray diffraction [8] and neutron diffraction [9] have been suggested. However, these approaches require high-intensity emitters and can be prohibitively expensive. Moreover, transient development of the three-dimensional stress field is very difficult to map. Numerical simulation of thermal stresses also poses several challenges. The stress analysis must consider dynamic coupling between solidification heat transfer and the resulting stresses induced in order to predict the developing gap between mold and cast product. The governing equations for thermal transport and stress should be coupled to model the transient development of thermal stresses.

Finite element methods (FEM) have been widely used to numerically simulate casting problems. Thomas [10] reviewed in detail the various FEM thermal stress models and discussed difficulties in practical implementation. Contact conductance between the casting and the mold was modeled by Fackeldey et al. [11] as a simple function of pressure. But the separation of the casting from the mold, which has a detrimental effect on heat transfer, was neglected. Several models have been proposed to address this separation. Seetharamu et al. [12] considered loss of contact between the mold and the cast, and modeled the heat transfer as being across an air gap. Isaac et al. [13] predicted the size and distribution of the separation and modeled it as gap conductance.

Accurate materials characterization is also important for modeling thermal stresses as, in general, materials change from viscoelastic/viscoplastic in the liquid phase to elastic-plastic in the solid phase [14]. However, no generic constitutive relationships exist (other than for certain metals such as steel and aluminum), and experimental or empirical data [1, 15, 16] have to be relied upon.

Modeling of solidification and tracking of the solid front are also complicated by the steep jump in material properties across the front. In some stress analyses, simplified analytical solutions have been used to track the solid front location and stress development [17]. Stresses induced during the continuous casting of slabs were solved with a heat generation term in the steady-state heat conduction equation used to account for phase change [18]. Recently, a thermomechanical model for the continuous casting of steel was proposed by Li and Thomas [19]. Constitutive equations were formulated and the finite element method was used in the computations. The effect of melt convection has generally been neglected in these studies.

Integrated models incorporating fluid flow and solidification into residual stress analyses have also been attempted. In such cases, the temperature distribution was calculated using finite volume [20] or finite difference [21] methods, while the stress field was handled with finite difference [20] or FEM

[21] approaches. In one study [22], both phase change with melt convection and stresses were analyzed in the same solver.

The thermal stress distribution has been shown to be closely related to cold cracks, hot tears and butt curl in aluminum casting [1,15]. Actual deformation from the desired shape in the form of butt curl was investigated by Barral and Quintela [1]. Hannart et al. [16] investigated the butt curl phenomenon in direct chill casting of aluminum slabs by assuming the metal to be elastic-plastic with strain rate-dependent behavior. A butt curl mechanism was proposed for sheet ingots (with a width to thickness ratio of 3) based on bending due to differential expansion [15]. Using finite volume and finite element methods, a preliminary study of both solidification heat transfer and residual stress during casting of high Prandtl number fluids was carried out by Sun et al. [4,23]. The effect of changing the cooling conditions on the resulting stresses was investigated. The stress analysis was decoupled from the flow and heat transfer analysis.

The objective of the present work is to develop an integrated finite volume-finite element computational model to analyze phase change heat transfer with melt convection and development of the stress field during the casting of a high Prandtl number fluid in a cylinder. User defined routines are developed to perform the computations with two commercial software packages (FLUENT [24] for the thermal analysis and ANSYS [25] for the stress analysis).

THE CASTING PROBLEM UNDER CONSIDERATION

A schematic diagram of the mold/riser assembly considered in this work is shown in Fig. 1. The mold and riser are made of stainless steel (AISI 302) and aluminum (Alloy 7075-T6), respectively. A steam heater is placed on top of the riser, and the sidewalls are cooled by natural convection. More information about the experimental setup is available in Sun et al. [4, 23]. The test specimen is

instrumented with 15 K-type thermocouples inside the casting. The black dots in Fig. 1 show three of the 15 internal thermocouple locations as well as those along the sidewall, top surface and bottom surface. A high Prandtl number material, Picatinny Arsenal Explosive (PAX) material, composed of 83%wt cyclo-trimethylene-trinitramine (RDX) particles and 17%wt carnauba wax, is considered in this work. Only the wax undergoes solid/liquid phase change during casting. Effective thermophysical properties of this material are listed in Table 1. These effective properties can be evaluated numerically using the microstructural RVE models developed by Annapragada et al. [26]. The Young's modulus for this material is shown in Fig. 2. The thermophysical properties for the mold and riser can be found in Table 2 [27,28].

Melt at 360 K is poured into the mold and riser assembly shown in Fig. 1. A steam heater is then placed on the top, to maintain the riser at higher temperature while the sides are exposed to natural convection by ambient air at 311 K, resulting in a natural convection coefficient of $6 \text{ W/m}^2\text{K}$. The heaters are switched off after 2.2 hours and then the whole assembly is cooled by natural convection. The total solidification process takes about 2.5 hours.

Temperature boundary conditions imposed in the experiment are measured using seven thermocouples mounted on the outer wall and four thermocouples on the top and bottom surfaces to obtain transient vertical and circumferential temperature variation as shown in Fig. 3; only selected locations along the sidewall are included in the figure for clarity. The transient cooling conditions, with the sidewall being at a lower temperature than the bottom surface from the beginning of the casting process, would be expected to lead to complex contraction/shrinkage patterns in the casting.

COMPUTATIONAL MODEL

As the rheological behavior of the high-viscosity, particle-laden (greater than 80% solid fraction of particles) energetic material considered in this work is not fully understood, the fluid is assumed to be incompressible and Newtonian. Although the model can account for temperature-dependence of thermophysical properties, the properties are assumed to remain constant over the range of temperatures investigated in this work. The governing mass, momentum and energy equations are:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = 0 \quad (1)$$

$$\left(\frac{\partial \rho u_i}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_j} \right) = -\frac{\partial p}{\partial x_i} + \frac{\partial}{\partial x_j} \left[\mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) \right] + \rho_\infty g_i \beta (T - T_\infty) + \frac{(1 - f_l)^2}{(f_l^3 + \varepsilon)} A_{mush} u_i \quad (2)$$

$$\frac{\partial \rho h}{\partial t} + \frac{\partial}{\partial x_j} (\rho u_j h) = \frac{\partial}{\partial x_i} \left(k \frac{\partial T}{\partial x_j} \right) \quad (3)$$

where A_{mush} is the mushy zone constant, f_l the liquid fraction, $\varepsilon = 0.001$ is used to prevent division by zero, and $h = c_p T + f_l \Delta H$ the specific enthalpy of the melt [24]. The above equations were solved using FLUENT with custom User Defined Functions (UDFs) developed in this work. The enthalpy method [29] was employed to model solidification, which the SIMPLEX algorithm was used for pressure-velocity coupling. Second-order discretization schemes were used for both momentum and energy equations for improved accuracy and the pressure staggered option (PRESTO!) was adopted for discretizing the pressure term. The volume change during solidification was ignored. In view of the very thin thermal boundary layer and low velocities observed in high Prandtl number materials, regions near the boundaries in the computational domain were very finely resolved.

The solidifying melt was modeled as a single material with temperature-dependent thermal expansion coefficient and Young's modulus, with all other properties remaining the same in both solid and liquid

phases as shown in Table 1. In the absence of detailed visco-elastic-plastic material properties, the material was treated as an isotropic thermo-elastic material, defined by the following differential equation:

$$\frac{\partial}{\partial t} \left(\rho \frac{\partial \bar{w}}{\partial t} \right) = \nabla \cdot \left[\mu (\nabla \bar{w} + \nabla \bar{w}^T) \right] + \nabla (\lambda \nabla \cdot \bar{w} + (3\lambda + 2\mu) \beta_s T) - \left\{ \nabla \cdot \left[\frac{\sigma_{ij}^d \sigma_{kl}^d}{\bar{\sigma}^2} \left(\frac{9G^2}{H' + 3G} \right) \nabla \bar{w} \right] \right\} + \bar{b} \quad (4)$$

in which $\lambda = \frac{\nu E}{(1+\nu)(1-2\nu)}$. This equation is solved in ANSYS [25]. It should be noted that no relative displacement is allowed between the metal and the melt boundaries, implying perfect contact at this interface.

Coupling methodology

One-way coupling was implemented between FLUENT and ANSYS to solve for thermal stresses during the casting process. The coupling scheme is graphically illustrated in Fig. 4.

Identical grids are used for both FLUENT and ANSYS (grid-independence is discussed later in this paper). The thermal field predicted by FLUENT is fed into ANSYS as a “body load” to all the elements. The temperature body load is maintained constant for the whole time interval while calculating stress and displacement. Within each time interval, the transient stress and displacement fields are solved in a quasi-transient fashion in which the stress and displacement fields prevailing at the previous time step are used as initial values for the following time interval. The temperature load remains constant while stress and displacements fields are being solved. Deformation of the computational mesh due to stress-induced displacement is neglected in the current implementation, as is the resulting gap formation. The coupled model represents a convenient tool to model thermal stresses and displacement in the current casting problem.

RESULTS AND DISCUSSION

The coupled model is first benchmarked against results from the literature. It is then used to predict the stress and displacement fields in the casting of a high Prandtl number energetic material.

Coupled-model validation

The benchmark problem considered for validating the coupled model is the elastic-plastic stress development in an unconstrained solidifying plate [17], as shown in Fig. 5. The Neumann problem for solidification is studied, i.e., the left wall of a semi-infinite plate initially maintained at its melting point T_m is suddenly exposed to a temperature $T_w < T_m$ initiating solidification. Material properties and other related constants used in this validation are shown in Table 3 [19]. The yield stress of the material σ_0 is assumed to be a linear function of temperature, defined as:

$$\sigma_0(T) = \sigma_{0,w} \frac{T - T_m}{T_w - T_m} \quad (5)$$

where $\sigma_{0,w}$ is the yield stress at T_w .

The y-direction stress σ_{yy} is the significant stress component [17] in this problem. Temperature and σ_{yy} distributions along the x-direction can be solved analytically [30, 17]. The proposed coupled model is employed to solve this problem with a plane strain condition. It is evident from Eq. (5) that $\sigma_0 = 0$ at the melting temperature T_m ; however, to avoid numerical difficulties, a value of $\sigma_0 = 0.1$ MPa is used. Predictions from the model are compared to the analytical results for temperature and stress profiles at selected times in Fig. 6; the agreement is seen to be quite satisfactory.

Solidification in a cylindrical casting

The numerical model developed in this work is validated against experimental temperature measurements and the comparisons at representative locations are shown in Fig. 7. The good

agreement in this figure is an improvement over the predictions in [4, 23]. This is attributed to the more comprehensive experimental measurements obtained for this work, including temperature measurements during the first 10 minutes of the solidification process, after pouring. Data during this period are critical in setting the conditions for subsequent solidification. The minor deviations that can still be seen in the figure are in part due to the uncertainties in the thermophysical properties.

A grid-independence study was carried out in which three levels of successively refined meshes (Table 4) were evaluated; results with these grids at two different times are shown in Table 5. The times are chosen as those at which convective effects are strong. The temperatures listed in the table are at the location ($r = 0.01$ m, $z = 0.05$ m). The moderate mesh in Table 4 was used for the results in this study, and deviations in Table 5 are calculated as $\varphi\%_i = \frac{|\varphi_i - \varphi_m|}{|\varphi_m|}$ in which φ is the variable and $i = c$ or f represents coarse and fine mesh, respectively. From Table 5, it may be concluded that satisfactory grid-independence was achieved using the moderate mesh.

The transient development of the thermal and flow fields in the domain is shown in Fig. 8a-d. The solidification front develops from the side and bottom walls during the initial stages (Fig. 8a). Since the riser temperature is maintained above the melting temperature of 355.65 K by the heaters, no solid front emanates from the top surface of the melt until 2.2 hours into the process, at which time the heater above the riser is switched off. Initially, a long natural convection cell is formed in the narrow channel ($H_0/D \approx 6$). This long convection cell breaks up as solidification progresses and the solid front from the side reaches the vertical axis leaving behind pockets of melt in the lower region of the casting. One such liquid pocket can be seen in Fig. 8b. This could be a potential site for void formation due to shrinkage.

It may be noted that the maximum velocity induced by natural convection during the entire solidification process is 6.22×10^{-4} m/s ($Ra \approx 2200$), implying that natural convection effects are negligible under these conditions.

Once the heaters above the riser are switched off, the solid front develops from all sides including the top due to the presence of cold environment. As shown in Fig. 8d, the solidification process is completed in 2.25 hours. Additional discussion of the transient temperature and solid front development is available in [4, 23]. The temperature distribution at the end of the solidification process can lead to the induction of residual stresses and base separation, and this is the focus of the present work.

Displacement and stress fields

During the casting process, displacement fields and residual stresses are induced due to the combined effect of temperature distribution in the casting and the different thermal expansion coefficients between the steel metal mold ($\beta_{steel} = 1.24 \times 10^{-5}$) and the cast material ($\beta_{cast} = 8.754 \times 10^{-5}$). Fig. 9 shows the experimentally measured temperature variation along one vertical line in the cast at various times near the beginning of casting process. The non-monotonic temperature profile shown in the figure results in the shrinkage being inwards, towards the location of the lowest temperature. The vertical movement of the material near the sides is restricted by the steel mold which has a smaller thermal expansion coefficient. Hence the top and bottom surfaces of the material assume a concave surface due to greater unrestricted shrinkage near the axis as compared to the sides. This displacement of the bottom surface from the mold is termed base separation. Fig. 10 conceptually illustrates the mechanism of base separation.

Base separation may be avoided by imposing boundary conditions that result in a monotonic temperature profile along the vertical direction, with the lowest temperature being at the bottom.

Under these conditions, displacement of the solidified material would tend to be towards the bottom mold surface rather than away from it. The top open surface would still experience a concave shape due to shrinkage, but this is not of concern since the riser and the material inside is detached after casting and discarded.

To better illustrate the effects of experimental cooling conditions on residual stresses, the displacement and von Mises stress fields from the numerical simulations are shown in Fig. 11; the vertical displacement is shown on the right in each panel and the von Mises stress on the left. Since the liquid is assumed to be stress-free in this work, the stress development in the solidified layer plays the determining role in the predicted displacement, i.e., separation. Since $\sigma \sim E\beta\Delta T$, a qualitative comparison of stresses in the mold and casting can be written as

$$\frac{\sigma_m}{\sigma_c} = \frac{(E\beta\Delta T)_m}{(E\beta\Delta T)_c} \approx \frac{(E\beta)_m}{(E\beta)_c} \approx 150 \quad (6)$$

Hence, much higher residual stresses were found in the mold and the riser compared with the cast. Also, since the mold and riser have lower expansion coefficients than the casting (Table 1, Table 2), the differential contraction induces compressive stresses in the mold and tensile stresses in the solidified melt in all directions. This explains the high stresses observed along the outer surface of the casting. Due to the combined vertical and radial stresses, the stress contours reunite at various locations on the vertical axis.

The maximum base separation of 0.081 mm predicted from the coupled numerical model developed, which occurs at the lowest point on the vertical axis, is comparable to the experimentally measured value of 0.061 mm.

Reduction of base separation through control of boundary conditions

An analysis of the results from the numerical model suggests modified boundary conditions that would lead to a more monotonic temperature profile in the vertical direction, and therefore, reduced base separation. The calculations shown thus far for the experimental cooling conditions (termed “original” case below) were repeated with modified conditions in which the top and bottom surfaces were assumed to be at 360 K and 343 K, respectively (instead of the experimentally measured conditions shown in Fig. 3), for the first two hours, after which the top heaters are switched off and the top surface exposed to the ambient. The sides are exposed to the ambient at 311 K throughout the casting period, with a natural convection coefficient as before of $6 \text{ W/m}^2\text{K}$. It is noted that only numerical results were obtained for the “modified” case, with no corresponding experiments.

Fig. 12 shows a comparison of the displacements at the bottom surface of the specimens 3 hours into the casting process, obtained with the original and modified cooling conditions. A 25% reduction in the base separation is seen to result from the new cooling conditions. The new boundary conditions pin the displacement at the base such that all the shrinkage is directed towards the base and allows reduced shrinkage. However, the natural air cooling along the side walls does not control the vertical temperature distribution to the extent desired, which contributes to the fact that even under the modified conditions, base separation is observed. It is expected that with more carefully controlled temperature boundary conditions, base separation may be further reduced or even eliminated; this is being done in ongoing work.

It is also noted that the modified cooling conditions increase the solidification time, as seen from Fig. 13. It takes 2.25 hours for the casting to reach total solidification under the original conditions, while 2.55 hours are required using the modified condition. More of the material is held above the melting

temperature during the first 2 hours under the modified conditions, leading to a solidification time that is longer by approximately 0.3 hours.

CONCLUSIONS

A comprehensive numerical investigation was conducted of the influence of cooling conditions on base separation, void formation and thermally induced stresses during the solidification of a high Prandtl number melt in a cylindrical enclosure. A dynamically coupled model was developed to compute the heat and mass transfer processes in melt casting as well as thermal stresses induced during solidification. Improved cooling conditions were suggested based on the predicted results obtained under the experimental conditions, which were found to suppress the extent of based separation by 25%.

Ongoing enhancements to the coupled model developed in this work include an explicit consideration of mold-material separation as well as heat transfer through the gap. The particle-laden energetic material melt will also be treated as a visco-elastic-plastic material in future work.

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NOMENCLATURE

A_{mush} mushy zone constant

$\mathbf{b}$ body force

c_p specific heat, J/kg-K

E Young's modulus, Pa

g	acceleration due to gravity, m/s^2
G	shear modulus, Pa
h	specific enthalpy, J/kg
H_0	height of the tube and riser in cylinder casting
ΔH	latent heat, kJ/kg
k	thermal conductivity, W/m-K
p	pressure, Pa
Pr	Prandtl number, $Pr = \nu/\alpha$
R	thermal resistance
Ra	Rayleigh number, $Ra = g\beta\Delta T r^3/(\nu\alpha)$
Re	Reynolds number, $Re = UD/\nu = 1/Pr$
t	time, s
T	temperature, K
$\bar{u}$	velocity, m/s
$\bar{w}$	displacement vector, m

Greek Symbols

α	thermal diffusivity, m^2/s
β	volume expansion coefficient, $1/\text{K}$
ε	solid/ liquid interface thickness, discretization, m
ϕ	particle volume fraction
φ	deviation
λ	Lame's coefficient
μ	Lame's coefficient, dynamic viscosity
ν	Poisson's ratio, kinematic viscosity
ρ	density, kg/m^3
σ	stress, Pa
σ_o	yield stress, Pa
σ_R	Stefan-Boltzmann constant, $5.67 \times 10^{-8} \text{ W/m}^2\text{-K}^4$

Subscripts

eff effective

f fluid

i cartesian component, inner, initial

l liquid

m melting, mold

o outer

p particle

s solid

w wall, water

∞ ambient

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Table 1. Thermophysical properties of the high Prandtl-number energetic material being cast.

Density, ρ	1562 kg/m ³
Thermal conductivity, k_{eff}	0.428 W/(m·K)
Specific heat, c_p	1524 J/(kg·K)
Viscosity, μ	3.11 Pa·s
Melting temperature, T_m	355.65 K
Latent heat, ΔH	14.83 kJ/kg
Poisson ratio, ν	0.22
Liquid thermal expansion coeff, β_l	1.11×10^{-4} 1/K
Solid thermal expansion coeff, β_s	8.754×10^{-5} 1/K

Table 2. Thermophysical properties of the mold and riser.

	Mold	Riser
Density, ρ (kg/m ³)	8030	2719
Thermal conductivity, k	16.27	202.4
Specific heat, c_p (J/(kg·K))	502.48	871
Young's modulus (Pa)	2.1×10^{11}	7.2×10^{10}
Poisson ratio	0.3	0.345
Thermal expansion coefficient, β (1/K)	1.24×10^{-5}	2.36×10^{-5}

Table 3. Thermophysical properties and other constants used in the validation exercise [19].

Density, ρ (kg/m ³)	7500
Thermal conductivity, k (W/m-K)	33
Specific heat, c_p (J/kg-K)	661
Elastic modulus of solid, E_s (GPa)	40
Elastic modulus of liquid, E_l (GPa)	14
Poisson's ratio, ν	0.3
Thermal expansion coefficient, β (1/K)	2×10^{-5}
Melting temperature, T_m (°C)	1494.4
Latent heat, ΔH (kJ/kg)	272.0
Wall temperature, T_w (°C)	1000
Yield stress at T_w , $\sigma_{0,w}$ (MPa)	20

Table 4. Meshes in the grid-independence study.

	Coarse	Intermediate	Fine
Riser	20×2	40×4	80×8
Mold	40×4	80×8	160×16
Casting	60×20	80×40	160×80

Table 5. Results obtained with different grids; deviations are with respect to the intermediate grid.

Grid	f_l	$ \mathbf{u} _{\max}$ (m/s)	$\Psi_{\max}$ (m ² /s)	T (K)
t = 600 s				
Coarse	0.402	1.824×10^{-4}	4.631×10^{-6}	353.02
% Deviation	3.60	6.63	2.62	0.90
Intermediate	0.388	1.954×10^{-4}	4.513×10^{-6}	356.23
Fine	0.386	1.964×10^{-4}	4.503×10^{-6}	356.48
% Deviation	0.51	0.50	0.23	0.07
t = 1200 s				
Coarse	0.2581	6.541×10^{-5}	4.126×10^{-5}	350.21
% Deviation	10.58	2.34	1.72	0.72
Intermediate	0.2334	6.698×10^{-5}	4.198×10^{-5}	352.74
Fine	0.2302	6.702×10^{-5}	4.204×10^{-5}	352.86
% Deviation	1.38	0.06	0.14	0.03

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