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THERMAL ANALYSIS OF HGFQ USING FIDAP™:
SOLIDIFICATION FRONT MOTION

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INTRODUCTION

The High Gradient Furnace with Quench (HGFQ) is being designed by NASA/MSFC for flight on the International Space Station. The furnace is being designed specifically for solidification experiments in metal and metallic alloy systems. The HGFQ Product development Team (PDT) has been active since January 1994 and their effort is now in early Phase B.

Thermal models have been developed both by NASA and Sverdrup (support contractor) to assist in the HGFQ design effort. Both these models use SINDA as a solution engine, but the NASA model was developed using PATRAN and includes more detail than the Sverdrup model. These models have been used to guide design decisions and have been validated through experimentation on a prototypical "Breadboard" furnace at MSFC.

One facet of the furnace operation of interest to the designers is the sensitivity of the solidification interface location to changes in the furnace setpoint. Specifically of interest is the motion (position and velocity) of the solidification front due to a small perturbation in the furnace temperature.

FIDAP™ is a commercially available finite element program for analysis of heat transfer and fluid flow processes. Its strength is in solution of the Navier-Stokes equations for incompressible flow, but among its capabilities is the analysis of transient processes involving radiation and solidification.

The models presently available from NASA and Sverdrup are steady-state models and are incapable of computing the motion of the solidification front. The objective of this investigation is to use FIDAP™ to compute the motion of the solidification interface due to a perturbation in the furnace setpoint.

ANALYTIC MODEL

A precursor to the numerical model is the development of a comparable analytic model. This model is not capable of providing information about solidification, but is useful for comparing numerically computed temperature distributions and gradients in a solid rod.

A Green's function approach [1] was used. It is assumed that heat is added uniformly over discrete sections along the length of the rod. Furthermore, it was assumed that the rod had constant thermal properties and had an axisymmetric temperature distribution. For a uniform heat addition over a zone from z_1 to z_2, the temperature at any point in the rod is

$$T^+(r^+, z^+, t^+) = 2\frac{q^+}{\gamma}\left\{\Delta z^+ t^+ + \gamma^2 \Delta z^+ \sum_{n=1}^{\infty}\frac{1}{\beta_n^2}\left[1 - e^{-\beta_n^2 t^+/\gamma^2}\right]\frac{J_0(\beta_n r^*)}{J_0(\beta_n)}\right.$$

$$+ \frac{2}{\pi^3}\sum_{m=1}^{\infty}\frac{1}{m^3}\left[1 - e^{-m^2\pi^2 t^+}\right]\cos(m\pi z^+)\left[\sin(m\pi z_2^+) - \sin(m\pi z_1^+)\right]$$

$$+ \frac{2}{\pi}\sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\frac{\gamma^2}{\beta_n^2 + \gamma^2 m^2\pi^2}\frac{1}{m}\left[1 - e^{-t^+(\beta_n^2 + \gamma^2 m^2\pi^2)/\gamma^2}\right]\frac{J_0(\beta_n r^*)}{J_0(\beta_n)}$$

$$\left.\times \cos(m\pi z^+)\left[\sin(m\pi z_2^+) - \sin(m\pi z_1^+)\right]\right\}$$

Here the characteristic values are the roots of $J_1(\beta_n)=0$, and the '+' notation denotes dimensionless quantities ($r^+ = r/L$, $z^+ = z/L$, $t^+ = \alpha t/L^2$, $r^*=r/r_0$, $\gamma=r_0/L$ and $q^+=q/q_{ref}$).

NUMERICAL MODEL

A schematic showing the relevant section of HGFQ to be modeled is shown in Figure 1. The FIDAP™ model is axisymmetric and includes the SACA detail but not the quench. The SACA representation includes the Aluminum sample, the graphite ampoule, the gas gap, and the stainless steel cartridge. Hot and cold loads are not modeled separately but are considered part of the sample. The baseline configuration is the SACA in a Helium atmosphere, with a furnace setpoint temperature of 1100 C.
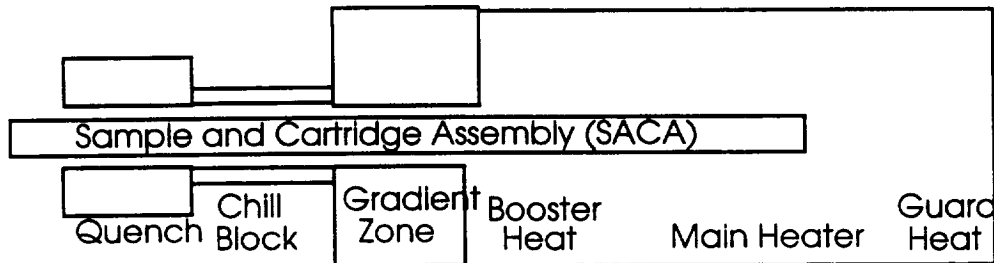

FIGURE 1. Schematic of HGFQ

FIGURE 2. Depiction of Computational Mesh

Grid. Several computational meshes have been used in this study, but the latest one is depicted in Figure 2. This mesh has 2431 nodal points and contains 2682 elements and is identical to the one used previously except for the addition of a finer grid in the gradient zone. This fine grid is designed to capture the phase change interface to facilitate good resolution of its location at any time step.

Thermal Properties. The required thermal properties for Helium gas, 304 stainless steel, Graphite, and Aluminum were obtained from NASA [2]. These properties are consistent with those used in both the NASA and Sverdrup models.

Boundary Conditions. The only specified boundary conditions are the constant furnace wall temperature (taken as 1100 C in the baseline case) and a constant heat transfer coefficient and water temperature on the back of the chill block (take as h=750 W/m^2/K and 22 C). All other surfaces are assumed adiabatic. However, all surfaces in the cavity bounded by the SACA and the outer wall are assumed to participate in grey-body radiative exchange. Radiation within the SACA (between the cartridge and the ampoule) is neglected.

Modeling Solidification. FIDAP™ provides two means for accounting for phase change in a transient calculation. The first is an Explicit Front-Tracking method in which the location of the interface is added as an unknown in the system of equations. Once the location is determined, the mesh is regenerated so that a prespecified group of elements is always adjacent to the interface. The second technique is an Enthalpy-based method where the solidification is accounted for by a variable specific heat. In this case, the solidification front is found by locating the isotherm associated with the phase change temperature.

The enthalpy-based method was chosen for the computations for two reasons associated with the moving mesh. The mesh update algorithm is somewhat primitive and does not allow specification of "meshable" and "unmeshable" regions within the solid phase. This means that the ampoule, gas gap, and cartridge might be remeshed in the process. Secondly, the movement of nodes on the boundaries associated with remeshing will invalidate the previously computed radiation view factors.

Computations. The computational procedure is a two step process. First, FIDAP™ is used to solve the steady-state problem associated with the SACA at a fixed position (the 50% processed position was used). The output temperature field for this condition is saved in the output file. Second, a transient calculation is performed which uses the steady-state solution as initial condition data. The solution was obtained using a trapezoidal rule (Crank-Nicholson) integration with Δt = 1.0 second over a 120 second period.

Post-Processing: Position. Once the transient temperature field was obtained, the position and velocity of the interface were still to be determined. The basis for the location of the interface at any time was taken to be the intersection of the 660 C isotherm with the centerline of the sample. The history of this location was determined by using the "MOVIE" command of the FIDAP™ post processor, and relying on the fact that the data from any "LINE" plot is echoed to a file. By plotting the centerline temperature distribution at all times using the "MOVIE" feature, all the centerline $T(x)$ information at each time interval was captured in an ASCII file. This file was processed with a simple "C"-program which used linear interpolation to find the x-location of the 660 temperature level at each time step.

Post-Processing: Velocity. Once the $X_{front}(t)$ information is known, the velocity of the front is found as the derivative (slope) of this function. Unfortunately, the information is available discretely with finite precision, and the challenge of differentiating a "noisy" function is faced. The differentiation was achieved by three means: 1) finite-differencing on the $X_{front}(t)$ data, 2) differentiating a polynomial curve fit to the data, and 3) finite-differencing the 5-poii t average of the data.

RESULTS

The results were obtained for a +2 C step in the furnace temperature. Although this is larger than a perturbation that likely will be seen on the furnace, it will demonstrate the effect. The position and velocity results are shown in Figures 3 and 4, respectively.
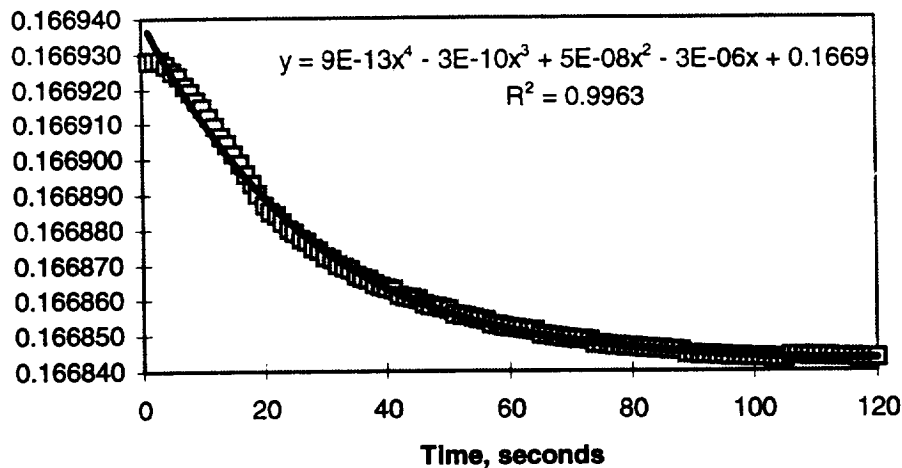

Figure 3. Front location versus time for +2 C furnace step

A more typical variation in furnace temperature is a +0.2 C step. The results for this case (both position and velocity) are seen in Figure 5. The effects of limited precision, associated primarily with the 5-digit accuracy from the FIDAP™ post processor printout, is evident.

Conclusions

Based on the present results, it is clear that front velocities of 2-3 μm/s may be possible due to a furnace instability of +2 C. It is less certain but apparent that for a +0.2 C furnace step that front velocities of 0.2-0.3 μm/s may be possible. For each of these cases, the present analysis indicates a transient associated with the front motion lasting at least 2 minutes.
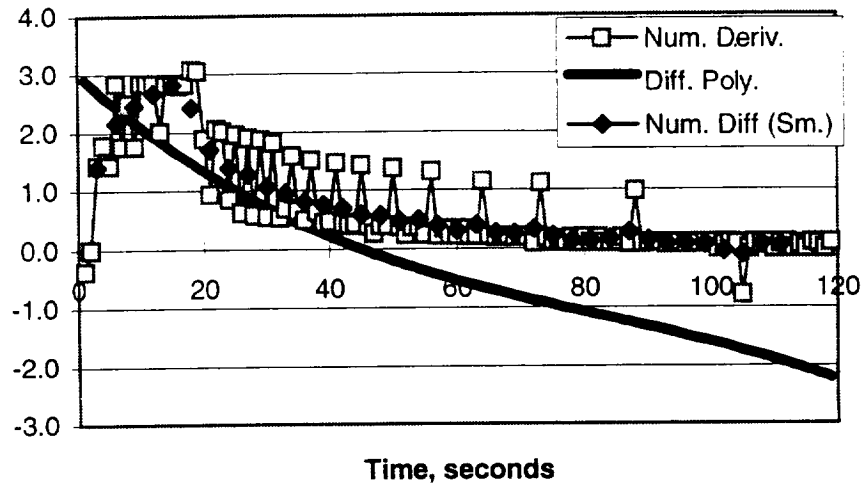
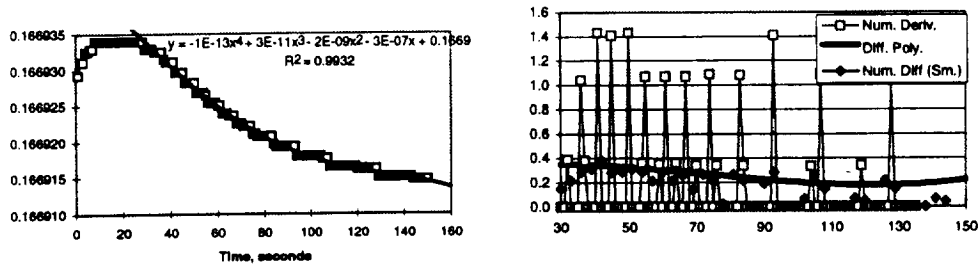Figure 4. Front velocity versus time for +2 C furnace step

Figure 5. Position(left) and velocity (right) for +0.2 C furnace step

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[1] Beck, J. V., Cole, K. D., Haji-Sheikh, A., and Litkouhi, B., *Heat Conduction Using Green's Functions*, Hemisphere Publishing Co., 1992.

[2] Westra, D., ED63 Branch MSFC, Private Communication, July, 1995.

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