Modeling of Transient Turbulent Natural Convection in a Melt Layer With Solidification

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Introduction

The process of natural convection in a volumetrically heated fluid has been investigated quite extensively in the past three decades or so, mainly because of its relevance to the cooling of core melt under severe accident conditions in a nuclear reactor [Theofanous et al., 1995]. Early studies by Roberts (1967), Tritton and Zarraga (1967), Thirby (1970), and Schwiderski and Schwab (1971) focused primarily on the post stability regime and the laminar natural convection flow patterns. Turbulent natural convection in a horizontal heat-generating layer under steady-state conditions was first investigated by Fielder and Wille (1970) and later by Kulacki and Emara (1977), Kulacki and Goldstein (1972), Kulacki and Nagle (1975), Mayinger et al. (1976), Cheung (1977, 1980a), Steinbemer and Reineke (1978), Cheung et al. (1992), Arpaci (1995), Nourgaliev and Dinh (1996), and Dinh and Nourgaliev (1997). Steady natural convection in a semicircular or hemispherical heat-generating melt pool was studied by Jahn and Reineke (1974), Min and Kulacki (1978), Gabr et al. (1980), Asfia and Dhir (1994), Tan et al. (1994), and Kymalainen et al. (1994). For the case of transient natural convection in a volumetrically heated layer, works were performed by Kulacki and Emara (1977), Cheung (1978, 1980b), and Keyhani and Kulacki (1983).

In all the above studies, solidification of the core melt at the cooled boundaries was not considered, and the volume occupied by the heat-generating fluid was assumed to remain unchanged. The effect of crust formation on the core melt heat transfer was completely ignored. Under severe accident conditions, a crust of core material is bound to form on the inner wall of the reactor lower head. This is because the inner wall temperature is well below the freezing temperature of the core melt. The formation of a crust layer at the cooled boundaries would affect the system behavior in three different ways. First, it would render the process of heat transfer in the system highly transient. Second, the growth of the crust represents a moving boundary at the solid-liquid interface. This would change the hydrodynamic boundary conditions for the melt pool which, in turn, would alter the natural convection heat transfer in the core melt. Third, as the crust grows thicker at the cooled boundaries, the depth of the melt pool would become smaller. This could considerably reduce the magnitude of the internal Rayleigh number which is proportional to the fifth power of the pool depth. Hence, the convective heat flux would decrease. Thus far, the crust dynamics and the crust effects on the core melt heat transfer have not been seriously explored by previous investigators.

In this work, the process of transient turbulent natural convection in a horizontal, heat-generating melt layer that is cooled from the top and bottom below its freezing temperature, is studied theoretically, taking full account of the crust formation at the lower and upper boundaries. The eddy heat transport model of Cheung (1977) is employed to describe the local turbulent heat transfer characteristics of the flow in the thermally unstable upper portion of the melt layer. An interface immobilization technique is used to transform the governing equations and the boundary conditions to immobilize the moving fronts of the lower and upper solid-liquid interfaces in the transformed space. In the meantime, a moving grid concept is applied to trace the unknown location between the thermally stable and unstable regions of the melt layer. The transient upper and lower surface heat fluxes are computed by solving the governing system using a fully implicit finite-difference scheme, whereas the instantaneous thicknesses of the lower and upper crusts are determined by integrating the interface energy balance equations using the fourth-order Runge-Kutta method. Special attention is given to the mutual interaction between the crust dynamics and the transient melt layer heat transfer.

Mathematical Formulation

The system under consideration is shown in Fig. 1. A horizontal layer with uniform volumetric heat sources is cooled from the upper and lower surfaces. Initially, no crust is present at the boundaries, and the liquid layer is at a steady state with the surface temperatures maintained at the freezing point of the liquid. At time zero, the temperatures at the upper and lower surfaces are suddenly lowered to a constant value below the freezing point of the liquid. The upper and lower crusts begin to grow at the cooled boundaries. While the rate of growth of the crusts depend on the heat transfer in the liquid layer, the latter, in turn, can be affected by the moving solid-liquid bound-
where $wT'$ is the turbulent eddy heat flux. This quantity can be expressed in terms of the eddy diffusivity for heat $\alpha$, by

$$wT' = -\alpha \frac{dT}{dz}. \quad (2)$$

Equation (1) becomes

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left( \alpha \frac{\partial T}{\partial z} \right) + \frac{S}{\rho C_p} \quad (3)$$

where

$$\alpha_{\text{eff}} = \alpha_i + \alpha_t \quad (4)$$

is the effective thermal diffusivity which includes the molecular and turbulent effects. The eddy heat transport model developed by Cheung (1977) will be employed to determine the local value of $\alpha_t$. This will be done in the next section.

**Lower Liquid Layer.** Conduction is the dominated heat transfer mechanism in the lower part of the liquid layer. The energy equation is similar to Eq. (3), but there is no advection effect in this region. That is

$$\frac{\partial T}{\partial t} = \frac{\partial}{\partial z} \left( \alpha_i \frac{\partial T}{\partial z} \right) + \frac{S}{\rho C_p}. \quad (5)$$

The initial and boundary conditions for the entire liquid region are

$$t = 0: \quad T_i = T_i(0, z)$$

$$t > 0: \quad T_i = T_i \quad \text{at} \quad z = \delta_1(t)$$

$$T_i = T_i \quad \text{at} \quad z = L - \delta_2(t) \quad (6)$$

where $\delta_1, \delta_2$ are given by the Stefan condition described below,

**Nomenclature**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$C_{Pi}, C_{Pr}$</td>
<td>Specific heats of the liquid layer and crust layer</td>
</tr>
<tr>
<td>$g$</td>
<td>Gravitational acceleration</td>
</tr>
<tr>
<td>$h$</td>
<td>Heat transfer coefficient</td>
</tr>
<tr>
<td>$k_{\text{eff}}$</td>
<td>Effective thermal conductivity of the melt layer</td>
</tr>
<tr>
<td>$k_i, k_s$</td>
<td>Thermal conductivities of the liquid layer and crust layer</td>
</tr>
<tr>
<td>$L$</td>
<td>Total layer thickness</td>
</tr>
<tr>
<td>$L_0$</td>
<td>Thickness of the thermally stable portion of the liquid layer</td>
</tr>
<tr>
<td>$N_u$</td>
<td>Nusselt number for heat transfer at the solid-liquid interface</td>
</tr>
<tr>
<td>$q_1, q_2$</td>
<td>Downward and upward heat fluxes at the boundaries</td>
</tr>
<tr>
<td>$Ra^*$</td>
<td>Local Rayleigh number</td>
</tr>
<tr>
<td>$R_q$</td>
<td>Internal Rayleigh number</td>
</tr>
<tr>
<td>$S$</td>
<td>Volumetric energy source</td>
</tr>
<tr>
<td>$St_e$</td>
<td>Stefan's number for internal energy source</td>
</tr>
<tr>
<td>$t$</td>
<td>Time</td>
</tr>
<tr>
<td>$T_0$</td>
<td>Wall temperature at the upper and lower surfaces</td>
</tr>
<tr>
<td>$T_f$</td>
<td>Freezing or melting temperature</td>
</tr>
<tr>
<td>$T_{\text{max}}$</td>
<td>Maximum temperature in the melt layer</td>
</tr>
<tr>
<td>$T_i, T_s$</td>
<td>Temperatures in the liquid layer and crust layer</td>
</tr>
<tr>
<td>$wT'$</td>
<td>Dimensionless eddy heat transport</td>
</tr>
<tr>
<td>$z$</td>
<td>Vertical coordinate</td>
</tr>
<tr>
<td>$\theta_w$</td>
<td>Dimensionless temperature at the upper and lower surfaces</td>
</tr>
<tr>
<td>$\theta_{\text{max}}$</td>
<td>Maximum dimensionless temperature in the melt layer</td>
</tr>
<tr>
<td>$\theta_i, \theta_s$</td>
<td>Dimensionless temperatures in the liquid layer and crust layer</td>
</tr>
<tr>
<td>$\theta_h$</td>
<td>Initial dimensionless temperature</td>
</tr>
<tr>
<td>$\nu$</td>
<td>Kinematic viscosity</td>
</tr>
<tr>
<td>$\rho_i, \rho_s$</td>
<td>Densities of the liquid layer and crust layer</td>
</tr>
<tr>
<td>$\delta_i, \delta_s$</td>
<td>Lower and upper crust thicknesses</td>
</tr>
<tr>
<td>$\delta_1, \delta_2$</td>
<td>Lower and upper crust thicknesses</td>
</tr>
<tr>
<td>$\Delta T^*$</td>
<td>Characteristic local temperature</td>
</tr>
<tr>
<td>$\Delta \tau$</td>
<td>Dimensionless time step</td>
</tr>
<tr>
<td>$\Delta H$</td>
<td>Latent heat of melting or solidification</td>
</tr>
<tr>
<td>$\eta_1, \eta_2$</td>
<td>Dimensionless spatial coordinates in the liquid layer</td>
</tr>
<tr>
<td>$\eta_{11}, \eta_{12}$</td>
<td>Dimensionless spatial coordinates in the lower and upper crust layers</td>
</tr>
<tr>
<td>$\eta_{0}$</td>
<td>Location of the thermal instability interface</td>
</tr>
</tbody>
</table>

**Greek Symbols**

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<tbody>
<tr>
<td>$\alpha_i, \alpha_s$</td>
<td>Thermal diffusivities of the liquid layer and crust layer</td>
</tr>
<tr>
<td>$\alpha_{\text{eff}}$</td>
<td>Effective thermal diffusivity of the melt layer</td>
</tr>
<tr>
<td>$\alpha_t$</td>
<td>Turbulent eddy diffusivity for heat</td>
</tr>
<tr>
<td>$\beta$</td>
<td>Coefficient of volumetric thermal expansion</td>
</tr>
<tr>
<td>$\Delta T^*$</td>
<td>Characteristic local temperature</td>
</tr>
<tr>
<td>$\Delta \tau$</td>
<td>Dimensionless time step</td>
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**Subscripts**

<table>
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<tr>
<th>Symbol</th>
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</tr>
</thead>
<tbody>
<tr>
<td>$i$</td>
<td>Internal heating</td>
</tr>
<tr>
<td>$l$</td>
<td>Liquid phase</td>
</tr>
<tr>
<td>$s$</td>
<td>Solid phase</td>
</tr>
</tbody>
</table>

**Superscripts**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\prime$</td>
<td>Fluctuating quantity</td>
</tr>
<tr>
<td>$-$</td>
<td>Dimensionless quantity</td>
</tr>
<tr>
<td>$-$</td>
<td>Ensemble average</td>
</tr>
<tr>
<td>$(\cdot)^*$</td>
<td>Correction value from grid point migration</td>
</tr>
<tr>
<td>$*$</td>
<td>Local variable</td>
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and the initial temperature distribution $T_i(0, z)$ is determined by the steady state solution for a volumetrically heated fluid layer without solidification.

**Solid Regions at the Top and Bottom.** The regions occupied by the lower and upper crusts are given by $0 \leq z < \delta_1$ and $L - \delta_2 < z \leq L$. The governing equations for the upper and lower crusts are the same by assuming constant properties for each, which can be written as

$$\frac{\partial T_i}{\partial t} = \alpha_r \frac{\partial^2 T_i}{\partial z^2} + \frac{S}{\rho_r C_p},$$

where $\alpha_r = \alpha_i = \alpha_t$ (7)

$t = 0$: $\delta_1(0) = \delta_2(0) = 0$

$t > 0$: $T_i = T_w < T_f$ at $z = 0$

$T_i = T_f$ at $z = \delta_1(t)$

$T_i = T_f$ at $z = L - \delta_2(t)$

$T_i = T_w < T_f$ at $z = L$.

(8)

**Stefan Condition at the Solid-Liquid Interfaces.** The lower and upper crust thicknesses $\delta_1(t)$ and $\delta_2(t)$ are determined by considering the Stefan condition (interface energy balance) at the solidification fronts, taking into account the density variation during phase change. From mass and energy conservation at the solid-liquid interfaces, a control volume analysis gives

$$\rho_s \Delta H \frac{d \delta_i(t)}{dt} = k_i \frac{\partial T_i}{\partial z} \bigg|_{z=\delta_i(t)^+} - k_i \frac{\partial T_i}{\partial z} \bigg|_{z=\delta_i(t)^-},$$

at $z = \delta_i(t)$

(9)

and

$$\rho_s \Delta H \frac{d \delta_i(t)}{dt} = k_i \frac{\partial T_i}{\partial z} \bigg|_{z=-(L-\delta_i(t))^-} - k_i \frac{\partial T_i}{\partial z} \bigg|_{z=-(L-\delta_i(t))^+},$$

at $z = L - \delta_2(t)$

(10)

where $\Delta H$ is the latent heat, and the crust density, $\rho_s$, is allowed to be different than the liquid density, $\rho_l$. The initial conditions are

$t = 0$: $\delta_1(0) = \delta_2(0) = 0$.

(11)

From Eqs. (9) to (11), the moving solidification fronts can be traced by integrating the instantaneous crust thicknesses with time.

**Numerical Model**

**Steady State Analysis (Initial Condition).** The initial condition corresponds to the steady-state solution for turbulent natural convection in a fluid layer with uniform volumetric energy sources. With cooling from the top and bottom, turbulent convection appears only in the upper portion of the liquid layer. The lower portion is dominated by conduction. Cheung (1977) developed an eddy heat transport model for high Rayleigh number thermal convection in a horizontal heated fluid layer with an adiabatic lower boundary and an isothermal upper wall. His model will be employed to the upper liquid layer in this study.

$$\frac{dT_i}{dz} = 0 \text{ at } z = L$$

(13)

where $T_f$ is the freezing temperature of the liquid and $L_0$ is the location of the thermal instability interface (see Fig. 1). To facilitate the task of computation, the following dimensionless variables are introduced:

$$\theta_0 = \frac{T_i(0, z) - T_f}{ST^{1/2}k_i}$$

$$\eta_i = \frac{z}{L} + 1$$

(14)

The dimensionless initial liquid temperature $\theta_0$ is a function of $\eta_i$. The quantity $\eta_0$ is the unknown location that separates the lower (stable) and upper (unstable) liquid layers. In dimensionless form, Eq. (12) becomes

$$\frac{d}{d\eta_i} \left( \frac{\alpha_{eff}}{\alpha_t} \frac{d \theta_0}{d\eta_i} \right) + 2 = 0 \text{ for } 1 \leq \eta_i \leq 2.$$

(15)

The boundary conditions are

$$\theta_0 = 0 \text{ at } \eta_i = 1$$

$$\theta_0 = 0 \text{ at } \eta_i = 2$$

(16)

where $\theta_0$ has a value bounded by $1 < \eta_0 < 2$.

**Eddy Heat Transport Model.** Cheung (1977) considered the eddy heat flux a function of the local Rayleigh number. The local Rayleigh number is defined in terms of a characteristic local length scale and a characteristic local buoyancy difference. Accordingly, the effective thermal diffusivity is given by

$$\frac{\alpha_{eff}}{\alpha_t} = 1 + a Ra_{*b}$$

(17)

where $a$ and $b$ are universal constants and $Ra_*$ is the local Rayleigh number given by

$$Ra_* = \frac{g \beta \Delta T^*(L - L_0)^3}{\alpha_{t\nu}} \left[ \frac{\eta_i(1 - \eta_i)}{3} \right]^{(1b)}$$

for $0 \leq \eta_i \leq 1$.

(18)

where $\eta_i = (z - L_0)/(L - L_0)$ is the dimensionless spatial coordinate in the thermally unstable region of the liquid layer for the case without solidification. It follows that $\alpha_{i}/\alpha_t$ would vary according to the third power of the distance from the solid boundaries, i.e.,

$$\frac{\alpha_{eff}}{\alpha_t} = 1 + a \left( \frac{g \beta \Delta T^*(L - L_0)^3}{\alpha_{t\nu}} \right) \left[ \frac{\eta_i(1 - \eta_i)}{3} \right]^{(1)}$$

(19)

for $0 \leq \eta_i \leq 1$.

In the above expressions, $\Delta T^*$ is the characteristic local temperature defined by

$$\Delta T^* = T_i - T_f.$$

(20)

The universal constants are given by $a = 0.051$ and $b = 0.87$. The eddy heat transport model is applied to the thermally unstable region where $L_0 \leq z \leq L$ or $\eta_0 \leq \eta_i \leq 2$. This is done by shifting the third order distance by algebra manipulation to maintain the same amplitude as the original one, i.e.,
where \( \eta_0 \) will be located using a shooting method as described in the next section. The coefficient \( G \) is based upon the same maximum amplitudes as

\[
G = 2 - \eta_0.
\]

(22)

Modifying the third order distance function in the local Rayleigh number, Eq. (18) becomes

\[
\text{Ra}^* = \frac{g \beta \Delta T^* (L - L_0)^3}{\alpha_1 \nu} (2 - \eta_0)^{-1.0} \left( (\eta_1 - \eta_0)(2 - \eta_1) \right)^{1.0}
\]

for \( \eta_0 \leq \eta_1 \leq 2 \).  

(23)

Combining Eqs. (14), (20), and (23), the local Rayleigh number can be expressed by

\[
\text{Ra}^* = \text{Ra}\theta_1 (2 - \eta_1)^{1.0} \left( (\eta_1 - \eta_0)(2 - \eta_1) \right)^{1.0}
\]

where \( \text{Ra}\theta_1 \) is the internal Rayleigh number given by

\[
\text{Ra}\theta_1 = \frac{g \beta S L^2}{2 \kappa_1 \nu}.
\]

(25)

In the lower liquid layer \( 1 \leq \eta_1 \leq \eta_0 \) where there is no turbulent convection, the ratio \( \alpha_1/\alpha_1 \) in Eq. (15) is equal to unity.

**Numerical Analysis.** Integrating Eq. (15) once using the boundary condition at \( \eta_0 \), the following equation is obtained for the upper liquid layer:

\[
\frac{d \theta_1}{d \eta} = \frac{2(\eta_0 - \eta_1)}{1 + 0.05 L \text{Ra}^{1/3} \theta_1 (2 - \eta_0)^{-0.5} (\eta_1 - \eta_0)(2 - \eta_1)}
\]

for \( \eta_0 \leq \eta_1 \leq 2 \).  

(26)

Similarly, the governing equation for the lower liquid layer is:

\[
\frac{d \theta_2}{d \eta} = \frac{2(\eta_0 - \eta_2)}{1 + \eta_2 (2 - \eta_2)}
\]

for \( \eta_1 \leq \eta_2 \leq \eta_0 \)

(27)

To determine the unknown location \( \eta_0 \) at which the liquid temperature is maximum, the coupled problem represented by Eqs. (26) and (27) are solved numerically by using the fourth-order Runge-Kutta integration and bisection shooting methods.

**Steady State Temperature Profiles.** The calculated steady state dimensionless temperature distributions at different internal Rayleigh numbers are shown in Fig. 2. The solid lines represent the result from numerical prediction; the data points are from the work of Kulacki and Goldstein (1972). Overall, the calculated results compare quite well with the experimental data, especially near the top and bottom surfaces. The differences between the predicted and the measured values in the core region could be due to the fact that the flow is not highly turbulent for a Rayleigh number on the order of 10^6. Note that as the internal Rayleigh number is increased, the temperature distributions become relatively flat in the upper liquid layer except in a region near the upper surface. Considerably smaller differences between the predicted and the measured values are obtained for the case of \( \text{Ra}\theta_1 = 8.76 \times 10^6 \), relative to the case of \( \text{Ra}\theta_1 = 2.02 \times 10^6 \). Due to the intensive turbulent mixing in the core, the thermal boundary layer is restricted to a very thin region at the upper surface where the temperature gradients are large. The location \( \eta_0 \) tends to shift toward the bottom with increasing internal Rayleigh number. This alters the upward and downward heat fluxes through the upper and lower surfaces accordingly. The estimated steady-state results will be used to specify the initial conditions for the transient problem.

**Transient Analysis.** To alleviate the need for tracking the moving fronts at the upper and lower solid-liquid interfaces, the governing differential equations along with the initial and boundary conditions are transformed into dimensionless forms.

**Liquid Region.** \( \delta_1(\tau) < z < L - \delta_2(\tau) \) or \( 1 < \tau < 2 \).

The following dimensionless variables are introduced

\[
\tau = \frac{T_i - T_f}{\ell}, \quad \eta = 1 + \frac{z - \delta_1(\tau)}{L - \delta_1(\tau) - \delta_2(\tau)}
\]

(28)

where the dimensionless temperature \( \theta_1 \) is function of the dimensionless time \( \tau \), and the dimensionless spatial variable \( \eta \). Transforming Eq. (3) in terms of the dimensionless variables, the following equation can be obtained:

\[
\frac{\partial \theta_1}{\partial \tau} + \frac{1}{1 - \delta_1 - \delta_2} \left[ (\eta_2 - 2) \frac{d \delta_1}{d \tau} + (\eta_1 - 1) \frac{d \delta_2}{d \tau} \right] \frac{\partial \theta_1}{\partial \eta} = 2 + \frac{1}{(1 - \delta_1 - \delta_2)^2} \frac{\partial}{\partial \eta} \left[ \frac{\alpha_1}{\alpha_i} \frac{\partial \theta_1}{\partial \eta} \right]
\]

(29)

where \( \delta_1, \delta_2 \) are dimensionless lower and upper crust thicknesses defined by

\[
\delta_1(\tau) = \frac{\delta_1(\tau)}{L}, \quad \delta_2(\tau) = \frac{\delta_2(\tau)}{L}
\]

(30)
Eddy Heat Transfer Model—Application to the Transient Problem. Based upon the concept of the eddy heat transport model, a transient local Rayleigh number can be introduced as follows:

\[
Ra^* = \frac{g \beta \Delta T^*[L - \delta_1(\tau) - \delta_2(\tau) - L_0(\tau)]^{1/3}}{\alpha_1 \nu} \\
	imes [2 - \eta_0(\tau)]^{-6/3\delta} \left[ (\eta_i - \eta_0(\tau))[2 - \eta_i] \right]^{3/6}
\]

for \( \eta_0 < \eta_i < 2 \) \( \eta_i = \frac{z}{\delta_1(\tau)} \) for \( 0 \leq \tau < \delta_1(\tau) \) \( 0 \leq \eta_i < 1 \),

\[ \eta_i = 3 - \frac{L - z}{\delta_2(\tau)} \] for \( L - \delta_2(\tau) < z \leq L \) \( 2 \leq \eta_i < 3 \),

where \( \eta_0(\tau) = 1 + \frac{L_0(\tau)}{L - \delta_1(\tau) - \delta_2(\tau)}. \)

From Eqs. (20), (28), (30), and (31), the local Rayleigh number is given by

\[
Ra^* = Ra_0 \left[ 1 - \frac{1}{\delta_1(\tau)} - \frac{1}{\delta_2(\tau)} \right] \left[ 2 - \eta_0(\tau) \right]^{3/6} \times \left[ (\eta_i - \eta_0(\tau))[2 - \eta_i] \right]^{3/6} \tag{33}
\]

The effective thermal diffusivity in the upper (unstable) liquid layer is

\[
\frac{\alpha_{\text{eff}}}{\alpha_i} = 1 + 0.051 \frac{Ra_{0.87} \theta_i}{1.87 \theta_i} \left[ 1 - \frac{1}{\delta_1(\tau)} - \frac{1}{\delta_2(\tau)} \right]^{0.61} \times [2 - \eta_0(\tau)]^{-3.39} \left[ (\eta_i - \eta_0(\tau))[2 - \eta_i] \right]^{3} \tag{34}
\]

for \( \eta_0 < \eta_i < 2 \).

On the other hand, the effective thermal diffusivity in the lower (stable) liquid portion is

\[
\frac{\alpha_{\text{eff}}}{\alpha_i} = 1 \quad \text{for} \quad 1 < \eta_i = \eta_0. \tag{35}
\]

Substituting Eqs. (34) and (35) into Eq. (29), the following governing equations can be derived:

### Thermally unstable upper liquid layer, \( \eta_0 < \eta_i < 2 \)

\[
\frac{\partial \theta_i}{\partial \tau} + \frac{1}{1 - \delta_1 - \delta_2} \left[ (\eta_i - 2) \frac{\partial \delta_1}{\partial \tau} + (\eta_i - 1) \frac{\partial \delta_2}{\partial \tau} \right] \frac{\partial \theta_i}{\partial \eta_i} = 2 + \frac{1}{(1 - \delta_1 - \delta_2)^2} \frac{\partial^2 \theta_i}{\partial \eta_i^2}
\]

\[
+ 0.051 \frac{Ra_{0.87}}{1.87} (1 - \frac{1}{\delta_1} - \frac{1}{\delta_2})^{0.61} (2 - \eta_0)^{-3.39} \times \left\{3((\eta_i - \eta_0)(2 - \eta_i))^{2}(2 + \eta_0 - 2\eta_i) \frac{\partial (\theta_i^{0.87})}{\partial \eta_i} + \left[ (\eta_i - \eta_0)(2 - \eta_i)^3 \frac{\partial^2 (\theta_i^{0.87})}{\partial \eta_i^2} \right] \right\} \tag{36}
\]

### Thermally stable lower liquid layer, \( 1 < \eta_i = \eta_0 \)

\[
\frac{\partial \theta_i}{\partial \tau} + \frac{1}{1 - \delta_1 - \delta_2} \left[ (\eta_i - 2) \frac{\partial \delta_1}{\partial \tau} + (\eta_i - 1) \frac{\partial \delta_2}{\partial \tau} \right] \frac{\partial \theta_i}{\partial \eta_i} = 2 + \frac{1}{(1 - \delta_1 - \delta_2)^2} \frac{\partial^2 \theta_i}{\partial \eta_i^2} \tag{37}
\]

The boundary conditions are the same as those given in the steady state analysis, i.e., Eq. (16), with \( \eta_0 \) being a function of time in the transient problem.

### Solid Regions (Lower and Upper Crust Layers). A coordinate transformation is applied to immobilize the solid-liquid interfaces at the spatial locations of \( \eta_i = 1 \) and \( \eta_i = 2 \). This is done by invoking the following dimensionless spatial variables and dimensionless temperature

\[
\eta_i = \frac{z}{\delta_1(\tau)} \quad \text{for} \quad 0 \leq \eta_i < 1,
\]

\[
\eta_i = 3 - \frac{L - z}{\delta_2(\tau)} \quad \text{for} \quad L - \delta_2(\tau) < z \leq L \quad \text{or} \quad 2 \leq \eta_i < 3,
\]

where \( \theta_i \) is function of \( \tau \) and \( \eta_i \). Performing the coordinate transformation, Eq. (7) becomes

\[
\frac{\partial \theta_i}{\partial \tau} + \frac{3 - \eta_1 - \frac{\partial \delta_1}{\partial \tau}}{(\delta_1) \frac{\partial \theta_i}{\partial \eta_1}} = \left( \frac{\alpha_1}{\alpha_i \delta_1^2} \frac{\partial^2 \theta_i}{\partial \eta_1^2} + 2 \frac{\alpha_i}{\alpha_i} \right) \tag{39}
\]

for \( 0 \leq \tau < \delta_1(\tau) \) \( 0 \leq \eta_i < 1 \),

\[
\frac{\partial \theta_i}{\partial \tau} + \frac{(3 - \eta_2 - \frac{\partial \delta_2}{\partial \tau})}{(\delta_2) \frac{\partial \theta_i}{\partial \eta_2}} = \left( \frac{\alpha_1}{\alpha_i \delta_2^2} \frac{\partial^2 \theta_i}{\partial \eta_2^2} + 2 \frac{\alpha_i}{\alpha_i} \right) \tag{40}
\]

for \( L - \delta_2(\tau) < z \leq L \) \( 2 \leq \eta_i < 3 \),

The initial and boundary conditions are

\[
\tau = 0, \quad \delta_1(\tau) = 0, \quad \delta_2(\tau) = 0
\]

\[
\tau > 0, \quad \theta_i = -\theta_w \quad \text{at} \ \eta_i = 0
\]

\[
\theta_i = 0 \quad \text{at} \ \eta_i = 1
\]

\[
\theta_i = 0 \quad \text{at} \ \eta_i = 2
\]

\[
\theta_i = -\theta_w \quad \text{at} \ \eta_i = 3 \tag{41}
\]

where

\[
\theta_w = \frac{T_e - T_c}{SL^2/2k_i} \tag{42}
\]

is the dimensionless wall temperature at the upper and lower surfaces.

### Stefan Condition at the Solid-Liquid Interfaces. The Stefan condition at the lower and upper solid-liquid interfaces are given by Eqs. (9) and (10) which can be transformed into the following forms:

\[
\frac{d \delta_1}{d \tau} = Ste_1 \left( \frac{1}{\delta_1 \frac{\partial \theta_i}{\partial \eta_1 |_{\eta_i = 1}} - \frac{1}{\delta_1 - \delta_2 \frac{\partial \theta_i}{\partial \eta_1 |_{\eta_i = 1}}} \right) \tag{43}
\]

at \( \eta_i = \eta_1 = 1 \)

\[
\frac{d \delta_2}{d \tau} = Ste_2 \left( \frac{1}{\delta_1 - \delta_2 \frac{\partial \theta_i}{\partial \eta_2 |_{\eta_i = 2}}} - \frac{1}{\delta_2 \frac{\partial \theta_i}{\partial \eta_2 |_{\eta_i = 2}}} \right) \tag{44}
\]

at \( \eta_i = \eta_2 = 2 \)

where \( Ste_i \) is the internal Stefan number defined by

\[
Ste_i = \frac{C_p \Delta H}{SL^2/2k_i} \tag{45}
\]

Equations (43) and (44) are coupled first order nonlinear ordinary differential equations, which can be solved by the fourth-order Runge-Kutta time integration method. To handle the ini-
tial jump and to avoid the singularity points from zero crust thickness, Eq. (43) is multiplied by \( \delta_1 \) on both sides whereas Eq. (44) is multiplied by \( \delta_2 \). In so doing, the singularity points are removed from the right hand side of the equations whereas the left hand side becomes the time derivative of \( \delta^{3/2} \).

**Tracing of the Thermal Instability Interface.** To trace the imaginary interface between the thermally stable and unstable liquid regions, it is assumed that the interface location corresponds to the maximum temperature location. A one-dimensional moving grid method is employed to account for the moving interface, where the grid point is fixed on the physical boundary and moving along with the migrating interface.

The grid point redistribution depends on the same dimensionless temperature profile. A correction can be made by simply using a Lagrangian polynomial formula expressed as

\[
(\theta_j') = \theta_1 \left[ \frac{(n_j') - n_j}{(n_j' - n_j)(\eta_j' - n_j)} \right] + \theta_2 \left[ \frac{(n_j') - n_j}{(n_j' - n_j)(n_j - n_j)} \right] + \theta_3 \left[ \frac{(n_j') - n_j}{(n_j' - n_j)(\eta_j - n_j)} \right] + \theta_4 \left[ \frac{(n_j') - n_j}{(n_j' - n_j)(n_j - n_j)} \right]
\]

(46)

where (\( \cdot ' \)) indicates the new nodal values, and the subscripts 1, 2, 3, 4 are the four grid points which have the nearest locations about the grid point \( t \). Note that the subscript \( t \) is ignored since only the liquid region is being considered.

**Computational Procedure.** To discretize the governing equations, a fully implicit scheme with a first-order forward difference in time and a second-order central difference in space is developed. The finite difference form of Eq. (36) is algebraically nonlinear due to the differential term involving \( \theta \) at the unknown time level. The Newton linearization procedure is used so that the system can be rearranged for the TDMA solver. Using the moving grid method to trace the location of \( n_{\eta} \), the grid spacings in the upper and lower liquid portions are adjustable, and a nonuniform finite difference form is used for the location of thermally unstable interface.

Due to the strong coupling of the governing equations for each liquid portion with the two solid-liquid interface energy balance equations, iterations between the fully implicit and Runge-Kutta schemes are necessary in each time step. However, if the time step is small enough, using one iteration at each time step is acceptable but not encouraged, especially for the calculation near the initial jump. At the first time step, the crust thicknesses and solidification front velocities are computed before the temperature distributions, so that the singular points from zero crust thicknesses will only appear on the interface energy balance equations. On the other hand, there is no singular point once solidification has begun. As mentioned above, the singularity points in the first time step are conveniently removed by multiplying \( \delta_1, \delta_2 \) on both sides of Eqs. (43) and (44), respectively.

The transient heat transfer characteristics including the solid-liquid interface heat transfer coefficient, transient Nusselt number, melt layer turbulent intensity, and boundary heat fluxes are determined at the end of each time step along with the interface locations.

**Results and Discussion**

There are three major dimensionless parameters that control the transient behavior of the melt pool heat transfer and the crust dynamics. These are the internal Rayleigh number, \( R_a \), the dimensionless wall cooling temperature, \( \theta_w \), and the internal Stefan number, \( \alpha \). Under steady-state conditions, however, the Stefan number is irrelevant. A value of \( \alpha = 0.9 \) is used for the thermal diffusivity ratio of the reactor fuel, and the other thermal properties are treated constant in each phase. In addition, the solid and liquid densities are assumed to be equal in the numerical computation.

The optimized dimensionless time step \( \Delta \tau \) and the grid point distribution depend on the magnitude of the internal Rayleigh number. At a moderate internal Rayleigh number of \( 1 \times 10^6 \), a total of 111 grid points is applied for the entire computational domain with 30, 51, and 30 nodes for the lower crust, melt layer, and upper crust, respectively. A very small time step equal to \( 1 \times 10^{-3} \) is used in order that the transient phenomena are clearly understood even around the initial jump condition. A much finer melt layer grid distribution is needed at very high internal Rayleigh numbers. Nevertheless, the order of magnitude of the characteristic time \( \tau_c \) for a steady state transition is roughly equal to unity in all cases. To assure the accuracy of the numerical results, a global convergence criterion with a relative error of \( 1 \times 10^{-9} \) is used. Numerical Experiments have been performed and the results have been found to be independent of the grid size. Further decrease in the grid size used in the present study would not improve the accuracy of the results (see Fan, 1996).

The idea of combining the Lagrangian and Eulerian approaches is successfully applied in this study. The solid-liquid interfaces are immobilized at the dimensionless locations \( \eta = 1 \) and \( \eta = 2 \) in order to trace the solidification fronts (fixed grids). Meanwhile, the thermal instability interface is traced by the maximum dimensionless temperature at location \( \eta = \eta_0 \). The grid spacings are adjustable in the liquid region (moving grids). The grid point migration is restricted to a small amount at each time step compared with the grid spacing in order to prevent wavy solutions due to numerical oscillation.

Before presenting the numerical results, it is necessary to justify the transient model (i.e., the eddy heat transport model) employed for the unstable melt region. Kulacki and Emara (1977), Cheung (1978, 1980b), and Keyhani and Kulacki (1983) studied the case of transient natural convection in a volumetrically heated horizontal fluid layer without solidification. In particular, they investigated the nature of developing and decaying turbulent convection in an internally heated fluid layer following a step change in volumetric energy generation. They found that the turbulent heat transport maintains its steady-state behavior during turbulent-to-turbulent transients despite any restructuring of the flow in the transient process. This quasi-steady behavior of the turbulent heat transport is due to the fact that the time scale of the turbulent natural convection flow is much smaller than the total time scale of the developing or decaying flow process. Thus, it is appropriate to extend the eddy heat transport model of Cheung (1977), which has been shown to correctly predict the steady turbulent natural convection behavior, to the case of transient flows. This is particular true for the case of solidification as the time scale of the turbulent natural convection flow is much smaller than the time scale of solidification. To further demonstrate this point, i.e., the validity of the eddy heat transport model, numerical calculations have been performed to simulate the turbulent decaying flow investigated in the experimental work of Kulacki and Emara (1977). Results for a decaying flow from an initial Rayleigh number of \( 8.55 \times 10^5 \) are shown in Fig. 3. In this figure, the data points are from the work of Kulacki and Emara (1977) whereas the solid lines are the predictions of the present transient model without solidification. Overall, the agreement is quite satisfactory in spite of the fact that some deviation does exist. The present transient model correctly predicts not only the transient temperature distribution of the fluid layer but also the time scale of the decaying flow process.
Figure 4 presents the transient temperature variation at a moderate internal Rayleigh number, $5 \times 10^3$, with a relatively strong cooling effect, $\theta_w = 0.2$. The internal Stefan number is fixed at 1.0. To show the advancing fronts of the upper and lower solid-liquid interfaces, the physical distance along the vertical direction is plotted against the dimensionless temperatures at different time instants. The dashed line at zero-dimensionless temperature is the freezing interface which separates the solid and the liquid phases. Very large temperature gradients are present in the crust regions at small times. The initial temperature distribution is very close to the one given by Curve 1 and would not show any difference on the scale presented in the figure. Since the heat generated is removed instantly from the cooling boundaries, the crusts grow rapidly by releasing the latent heat in early stages. Due to the intensive turbulent mixing effect, the liquid temperature profile is relatively flat in the upper liquid layer where the temperature stratification is unstable. The initial Rayleigh number decreases with time due to decrease in the local characteristic length. The thermal instability interface moves upward to a higher location in the melt layer region as time proceeds. Once a steady state is attained, the upper and lower crusts assume their maximum thicknesses. No additional latent heat is released in the system. It should be noted that the nonlinear temperature profiles in the crust regions are generated by the energy sources. The nonsymmetric temperature profiles in the crust regions imply different heat fluxes across the cooling boundaries. At steady state, the upper and lower heat flux ratio is the same as the ratio of the upper and lower layer thicknesses determined by the location $\eta_0$. The numerical data have been presented in tables by Fan (1996).

Figure 5 shows the transient dimensionless turbulent heat flux in the thermally unstable upper liquid layer where the dimensionless turbulent heat flux is defined by

$$\frac{\overline{W \theta'_f(\tau, \eta)}}{\frac{\overline{\alpha(T_{\max} - T_f)}}{L}}.$$ (47)

Physically, this dimensionless quantity represents the ratio of the turbulent heat flux to the conduction heat flux. The peak value is concentrated at the location just outside the upper thermal boundary layer. The mixing intensity decreases very rapidly due to the wall cooling effect. Throughout the transient, the turbulent mixing core is shrinking due to the inward growth of the two solidification fronts. The transient Rayleigh number decreases continuously with decreasing liquid layer thickness. At steady state, the peak turbulence intensity is about half of the initial value.

Figure 6 shows the upper and lower crust thicknesses at different cooling temperatures. The two solidification fronts move rapidly in the early stage. They eventually slow down and approach their steady-state thicknesses at large times. During the entire transient stage, the upper crust is thinner than the lower crust. This is because of a higher heat flux through the upper solid-liquid interface due to turbulent convection, which suppresses the latent heat release and the crust growth. In general, both the upper and lower crusts become thicker at a larger value of $\theta_w$.

Due to the presence of turbulent thermal convection in the upper liquid layer, a higher heat flux is obtained at the upper solid-liquid interface. The transient Nusselt number at the upper surface is defined by

$$\text{Nu}(t) = \frac{h(t)[L - \delta_1(t)]}{k_i}$$ (48)

where $h$ is the heat transfer coefficient at the upper solid-liquid interface given by

$$h = \frac{1}{T_{\max} - T_f} \left( -k_i \frac{\partial T_f}{\partial z} \right)_{z=L-L_i}.$$ (49)
In dimensionless form, Eq. (48) becomes

$$\frac{Nu(\tau)}{\theta_{\infty}(\tau)} = -\left[ \frac{2 - \eta_{\infty}(\tau)}{\theta_{\text{max}}(\tau)} \right] \frac{\partial \theta_{j}(\tau, \eta)}{\partial \eta} \bigg|_{\eta=\infty}. \quad (50)$$

The transient Nusselt number at the upper solid-liquid interface normalized by the initial steady-state value, $Nu_0$, is presented in Fig. 7. During the early stage, $Nu/Nu_0$ is larger than unity. This early transient is a classical time-lag effect. It takes certain time for the inward movement of the cold upper solid-liquid interface to penetrate the entire length of the boundary layer, as clearly shown in Fig. 4. After the early stage of growth, the thickness of the thermally unstable upper liquid layer gradually decreases. This results in a lower Rayleigh number, leading to a decrease in the transient Nusselt number.

The internal Stefan number effect (i.e., the latent heat effect) is depicted in Figs. 8 and 9. In order to keep the same magnitudes of $Ra$ and $\theta_{\infty}$, all physical properties, initial liquid layer thickness, and energy sources are fixed at the same values. The Stefan number is varied mainly with the inverse of the latent heat. An increase in the internal Stefan number corresponds to a decrease in the latent heat which results in a rapid growth of crusts at the top and bottom boundaries. This in turn induces a higher convective heat transfer in the early stage of transient. As can be seen from Eqs. (43) and (44), the Stefan number only affects the transient solutions and the characteristic time $\tau_{\infty}$. As the new steady state is attained, all three cases have
the same final steady-state values, independent of the Stefan number.

Conclusions

A numerical model has been successfully developed to investigate the transient phenomenon of turbulent natural convection in a volumetrically heated horizontal melt layer, with solidification taking place at the cooled boundaries. Based upon the results obtained in this study, the following conclusions can be made:

1. The heat transfer in the melt layer is strongly coupled to the crust dynamics throughout the entire transient process. While the rate of solidification (i.e., crust growth) depends strongly on the boundary heat fluxes from the melt layer, the turbulent natural convection in the melt layer is strongly affected by the crust.

2. In the early stage of the transient process, the growth of the crust at the upper surface induces a wall suction effect on the melt layer which enhances the convective heat transfer at the upper solid-liquid interface. However, as the upper and lower crusts grow thicker in the later stage of the transient process, the depth of the liquid layer becomes smaller. This results in a large reduction in the magnitude of the transient Rayleigh number and thus the convective heat flux at the upper solid-liquid interface.

3. The presence of turbulent natural convection in the upper portion of the melt layer tends to suppress the crust growth at the upper boundary. As a result, the upper crust is considerably thinner than the lower crust. The difference in thickness between the upper and lower crusts becomes more pronounced as the internal Rayleigh number defined in terms of the initial depth of the melt layer is increased.

4. The transient thermal behavior of the system is controlled not only by the internal Rayleigh number but also by the internal Stefan number and the dimensionless surface cooling temperature. Higher rates of growth of the crusts are obtained as the Stefan number or the dimensionless cooling temperature is increased. The steady state upper and lower crust thicknesses, however, are dictated by the internal Rayleigh number and the dimensionless cooling temperature, independent of the Stefan number.

5. The crust dynamics, which has an important effect on the transient turbulent natural convection in the melt layer, needs to be taken into account in predicting the transient boundary heat fluxes from the heat-generating melt layer.

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