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CYCLIC PHASE CHANGE WITH FLUID FLOW

V.R. VOLLER†, P. FELIX‡ AND C.R. SWAMINATHAN††

†*St Anthony Falls Hydraulics Research Laboratory, Civil Engineering, University of Minnesota, Minneapolis, Mn 55455, USA*

‡*Fluent Inc, 10 Cavendish Court, Lebanon, NH, USA*

††*Deceased*

ABSTRACT

Cyclic phase change involves the successive freezing and melting of a region driven by a boundary temperature that cycles above and below the solid/liquid phase change temperature. In this paper, a recently proposed fixed grid phase change enthalpy method is modified and applied to cyclic solid/liquid phase change problems. The basic approach is demonstrated on application to a one-dimensional, heat conduction controlled phase change. Then the method is used to investigate a cyclic phase change problem that involves fluid flow. The interaction of the melting and freezing with the phase change leads to some interesting predictions for the location and shape of the solid/liquid interface. The results also indicate that melting cycles are more effective than freezing cycles.

KEY WORDS Enthalpy Fluid flow Phase change

INTRODUCTION

Cyclic phase change involves the successive freezing and melting of a region driven by a boundary temperature that cycles above and below the solid/liquid phase change temperature. Examples of this type of behaviour can be found in thermal storage, freeze-linings in pyrometallurgical processes[1], and freeze/thaw cycles in soils[2]. The key element in a cyclic phase change problem is the tracking of the multiple freezing and melting fronts as they move through the domain of interest. Recent examples of solving cyclic phase problems include the works of Choi and Hsieh[3] who use a moving heat source method, Hasan[4] who uses deforming front tracking grids, Gong *et al.*[5] who use a fixed grid enhanced heat capacity approach, and Ho and Chu[6] who use a combination of fixed grid and front tracking methods.

This paper focuses on the development of a fixed grid scheme for the tracking of the solid/liquid fronts during a cyclic phase change. This approach is based on an enthalpy formulation and uses the highly efficient enthalpy scheme recently proposed by Swaminathan and Voller[7]. A key feature in this work is the inclusion of cyclic phase change problems that involve fluid flow and convection, in addition to heat conduction. In this respect, the work is similar to the recent cyclic melting study reported by Ho and Chu[6]. In the work of Ho and Chu, although a fixed grid enthalpy is used to initially locate the solid/liquid fronts, subsequent movements are tracked on explicitly satisfying the interface heat balance (i.e., the Stefan condition). In contrast, in the current work, a fixed grid enthalpy method is used throughout and explicit tracking of the solid/liquid fronts is not required: in fact, the creation and movement of the fronts can be reconstructed after the fact from the predicted transient liquid fraction fields.

In the first instance the basic mechanisms of the approach are outlined in the context of a one-dimensional heat conduction controlled phase change problem in a semi-infinite slab with a cyclic

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Dirichlet boundary condition applied at $x = 0$, $T(0, t)$. This is followed by the application to a problem involving the melting and freezing of gallium in a two-dimensional cavity insulated on three sides with a cyclic Dirichlet boundary condition, $T(0, t)$, applied on the right hand vertical wall. This cyclic problem is essentially a modification of the well known Galljura melting problem introduced by Gau and Viskanta[8].

A HEAT CONDUCTION PROBLEM

The problem

In order to present the basic approach, the one-dimensional heat conduction problem involving the cyclic solidification/melting of aluminum, investigated by Choi and Hsieh[3], will be used as a test problem. Initially pure aluminum, in the solid phase, is held at its phase change temperature, T_m, in the region $x \geq 0$. For time $t \geq 0$ the surface temperature at $x = 0$ is cycled according to[3]:

$$T_o(t) = T_m + 200 \sin\left(\frac{\pi}{10} t\right) \quad [K]. \tag{1}$$

With this cycle the aluminum will first melt ($t \leq 10\ s$) and then freeze ($10s \leq t \leq 20s$). During the time interval between 10 and 20 seconds both a melting and freezing front will coexist in the region $x \geq 0$.

On assuming that conduction is the major heat transport mechanism the governing equation can be written as[7]:

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T - \frac{L}{c} \frac{\partial f}{\partial t}. \tag{2}$$

where α is the thermal diffusivity, L is the latent heat, c is the specific heat and

$$f = \begin{matrix} 1 & if\ T > T_m \\ 0 & if\ T < T_m \end{matrix} \tag{3}$$

is the local liquid fraction which ensures a correct accounting of the phase change in the solid and liquid regions. The boundary condition at $x = 0$ is given by (1) and as $x \to \infty$, $T \to T_m$. The initial conditions are $T(x, 0) = T_m$ and $f(x, 0) = 0$.

For consistency with the work of Choi and Hsieh[3] the following thermal data for pure aluminum are used

$$\alpha = 6.15 \quad 10^{-5} \left[\frac{m^2}{s}\right]; \quad \frac{L}{c} = 313.8 \ [K]. \tag{4}$$

Note that the melting point of pure aluminum is $T_m = 932\ K$[3]; for convenience in the current work, however, a temperature translation will be used such that $T_m = 0$.

The discretization

A fully implicit finite difference discretization of (2) on a grid with a fixed space step, Δx, results in the general equation, at node point P

$$T_P = T_P^{old} + Fo\,[T_w - 2T_P + T_E] + \frac{L}{c} f_P^{old} - \frac{L}{c} f_P \tag{5}$$

where $Fo = \alpha \Delta t / \Delta x^2$, the superscript $[\ ]^{old}$ denotes previous time values, the subscript $[\ ]_P$ denotes evaluation at node P and the subscripts $[\ ]_W$ and $[\ ]_E$ denote evaluation at the neighbouring nodes. At the first node adjacent to the surface $x = 0$ the discrete equation takes the form

$$T_1 = T_1^{old} + Fo\,[T_0 - 2T_1 + T_2] + \frac{L}{c} f_1^{old} - \frac{L}{c} f_1 \tag{6}$$

where the nodal temperature T_0 will take the prescribed values given by the cyclic melting freezing boundary condition, (1). On solution of the non-linear system given by (5) the location and movement of the cyclic phase change fronts can be tracked from the predicted nodal liquid fraction field, f. It is important to recognize that the location of the phase fronts is not required during the numerical solution. As such, if desired, the phase front locations can be obtained after the solution from the stored transient liquid fraction fields.

The numerical solution

In solving (5) an efficient version of the predictor corrector, fixed grid, implicit method proposed by Swaminathan and Voller[7] will be used. For the given problem (with phase change temperature $T_m = 0$) this can be implemented in the following manner:

(1) In a given time step, (5) is written in iterative form

$$a_P^m\, T_P^{m+1} = T_P^{old} + Fo\,[T_W^{m+1} - 2T_P^{m+1} + T_E^{m+1}] + \frac{L}{c} f_P^{old} - \frac{L}{c} f_P^m \tag{7}$$

where the superscript $[\ ]^m$ indicates the iterative level. Equation (7) is linear in T^{m+1} since the liquid fraction f and the coefficient a_P are only defined at the known level m. The system of equations can be solved using a tri-diagonal matrix algorithm (TDMA) solver.

(2) The iteration in (7) is initiated on setting $f^0 = f^{old}$.

(3) A key feature in the solution is the evaluation of the coefficient a_P. Given the m^{th} level liquid fraction field this coefficient is calculated as

$$a_P^m = \begin{cases} 10^{20} & \text{if } 0 < f_P^m < 1 \\ 1 & \text{otherwise.} \end{cases} \tag{8}$$

(4) In order to illustrate the role of the a_P coefficient consider the case where the control volume associated with the P^{th} node is undergoing the phase change. In this case $0 < f_P^m < 1$ and (8) will set a_P^m to a large value. This forces the solution of (7) to return a value of T_P^{m+1} very close to 0 which is the correct nodal temperature value. Further, since the predicted phase change nodal temperatures are correct, the predicted temperatures at the non-phase change nodes (i. e., nodes at which $[f_i^{old} - f_i^m] = 0$) will also be correct. The updated liquid fraction field then follows on rearrangement of equation (5), i.e.:

$$f_P^{m+1} = \frac{c}{L}\left(T_P^{old} + Fo\,[T_W^{m+1} + T_E^{m+1}]\right) + f_P^{old} \tag{9}$$

where it is assumed that $T_P = 0$.

(5) In practice, for computational convenience, the liquid fraction update, (9), is applied at every node (regardless of its phase change status). To avoid un-physical results from this step the following under/overshoot correction is applied:

$$\begin{aligned} &f_P^{m+1} < 0 \text{ then set } f_P^{m+1} = 0 \\ &f_P^{m+1} > 1 \text{ then set } f_P^{m+1} = 1. \end{aligned} \tag{10}$$

Note that use of this correction will also take account of cases where a control volume initiates or completes its phase change during a time step.

(6) In cases where the phase change status of a control volume remains unchanged in a time step, the above solution procedure will require only one iterative sweep. If a control volume changes its status, a common occurrence in a cyclic problem, additional iterations are

required to obtain consistency between the nodal temperature and liquid fraction fields. In the one-dimensional conduction problems reported here, at most three iterative sweeps were required to reach a consistent solution.

Results

In solving a cyclic phase change problem the above numerical scheme is implemented directly with the cyclic boundary condition. As previously noted the relative positions of the melt and solid phase fronts are not required as part of the solution. The appropriate movement of these fronts is reconstructed from the liquid fraction field. This can be achieved in one of two ways.

(1) After the complete solution, a post processing operation on the stored transient nodal liquid fraction fields can be carried out.

(2) Alternatively, to save storage, the predicted nodal liquid fraction field can be "interrogated" after each time step.

In this work the second of these two approaches will be employed. In the first instance two additional, "phase maker", nodal field variables, f^{free} and f^{melt} (initialized to zero), are introduced. Following each time step the phase maker variables, at each node $P = i \ldots n$, are updated as

$$\begin{aligned} &\text{if } f_P^{old} < f_P \text{ then } f_P^{melt} = f_P \\ &\text{if } f_P^{old} > f_P \text{ then } f_P^{free} = f_P. \end{aligned} \tag{11}$$

On performing a sequential search through the nodes ($P = i \ldots n$), the nodal location, of the freezing front nearest the heating/cooling surface ($x = 0$), I_{free}, is identified as the first node I where $f_I^{free} > 0$ and the nodal location of the melt front nearest $x = 0$, I_{melt} is identified as the first node I where $f_{I-1}^{melt} - 1$ and $f_I^{melt} < 1$. From these nodal locations, the positions of the freeze and melt fronts are calculated as

$$P_{melt} = [I_{melt} - 0.5 + f_{I_{melt}}^{melt}]\,\Delta x \tag{12}$$

$$P_{free} = [I_{free} - 0.5 + f_{I_{melt}}^{melt} - f_{I_{free}}^{free}]\,\Delta x \tag{13}$$

respectively, where, in keeping with the current problem, it is assumed that the melt front proceeds the freeze front. In this way, with appropriate storing of the front positions, the movements of the solidification and melt fronts over a number of cycles can be obtained.

The predicted movements of the melting and freezing fronts, over one cycle, using 20 space steps of $\delta x = 0.0025$m, a time step of $\delta t = 0.05$s and the thermal data in Eq. (4) are shown in *Figure 1*. These predictions are in very close agreement with the results presented by Choi and Hsieh[3] (*Figure 5*) and Ho and Chu[6] (*Figure 2*); in particular the lagging of the freezing front due to the residual super heat remaining after the melting step[3] is evident. The CPU time (Fortran 77 running on an Intel 90 MHz Pentium processor) for the calculation in *Figure 1* is less than 1 second.

CYCLIC PHASE CHANGE WITH FLUID FLOW

The cyclic phase change algorithm, developed above, is applied to the melting and freezing of a Gallium system, based on the melting only set-up originally investigated by Gau and Viskanta[8]. *Figure 2* shows a schematic of the computational domain. The cavity initially contains solid gallium at the phase change temperature (set at $T_m = 0$). Three sides of the cavity are insulated. At time $t = 0$ the temperature along the left hand wall begins to cycle according to

$$T_o = T(0, y, t) = 15 \sin\left(t \frac{\pi}{300}\right) \ [K]; \tag{14}$$

this drives successive melting and freezing of the material in the cavity.

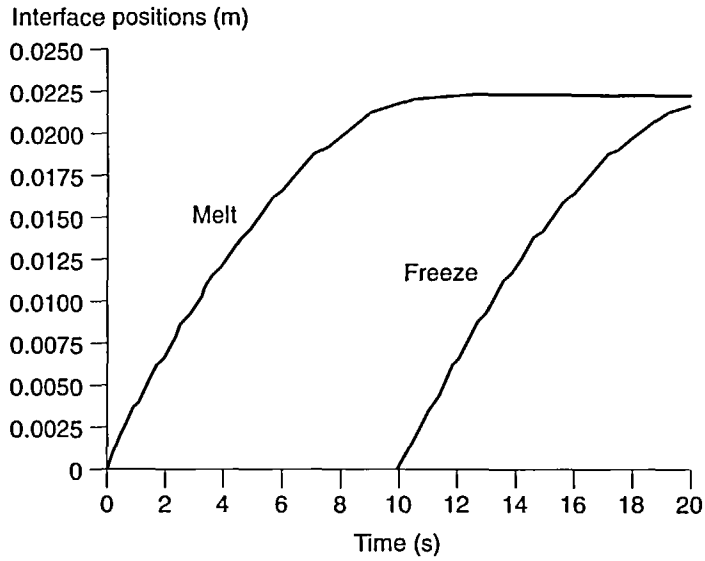

Figure 1 Movement of melting and solidification fronts in one cycle (c.f. Figure 5 in Choi and Hsieh[3])

Following Lacroix and Voller[9] and Brent *et al.*[10] the governing equations are, assuming constant thermal-physical properties and invoking the Boussinesq buoyancy treatment,

Continuity:

$$\frac{\partial u}{\partial x} + \frac{\partial v}{\partial y} = 0 \tag{15}$$

Momentum:

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + v\frac{\partial u}{\partial y} = \nu\left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2}\right) - \frac{\partial P}{\partial x} + S_u \tag{16}$$

$$\frac{\partial v}{\partial t} + u\frac{\partial v}{\partial x} + v\frac{\partial v}{\partial y} = \nu\left(\frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2}\right) - \frac{\partial P}{\partial x} + S_v + g\beta\,(T - T_m) \tag{17}$$

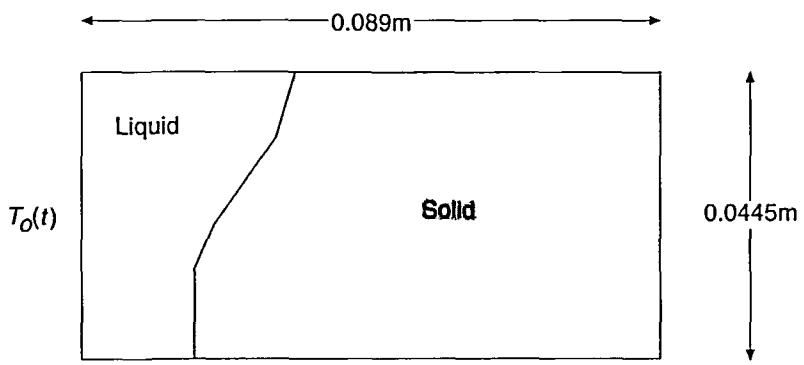

Figure 2 Schematic of cyclic phase change in a Gallium cavity

Energy:

$$\frac{\partial T}{\partial t} + u\frac{\partial T}{\partial x} + v\frac{\partial T}{\partial y} = \alpha\left[\frac{\partial^2 T}{\partial x^2} + \frac{\partial^2 T}{\partial y^2}\right] - \frac{L}{c}\frac{\partial f}{\partial t} \tag{18}$$

where, in the current problem, the kinematic viscosity $v = 2.97\ 10^{-7}$ [m/s], the diffusivity $\alpha = 1.4145\ 10^{-5}$ [m/s], the ratio of latent heat to specific heat $L/c = 195.71$ [K], the acceleration due to gravity $g = 9.81$ [m/s^2], and the thermal coefficient of expansion $\beta = 1.3054\ 10^{-4}$ [1/K].

The governing equations are solved on a fixed computational grid (40 × 20 square control volumes) and a time step of 10s. The iterative solution approach is based on the work of Brent *et al.*[10] with the incorporation of the recent phase change treatment proposed by Swaminathan and Voller[7]. The key steps in this approach are:

(1) A local liquid fraction term, f, that tracks the phase fronts through the fixed computational mesh. The iterative calculation of this variable is identical to the approach used in the conduction problem above.

(2) A porosity source term in the momentum equations, e.g.

$$S_u = -K_0\,(1-f)\,u. \tag{19}$$

This term forces the momentum equations to mimic a Darcy equation in the phase change region. A term that "switches off" the velocity as the local liquid fraction goes to zero. The constant K_o is a morphological constant used to represent the porosity in the phase change region, in the current isothermal phase change case a value of $K_o = 10^5$ is used. (Note in more general phase change cases, which involve a mushy region, it is common to use the Carman-Kozeny equation in place of (19)).

(3) The application of the segregated iterative based SIMPLE algorithm[11] to solve for pressure and velocity.

(4) A line by line TDMA solver[11].

In carrying out the above calculations convergence, within an iteration, is declared when both the maximum mass balance in a computational volume falls below 0.001% of the total mass in the cavity and the heat balance falls below 0.05%. In the current problem, over one cycle of freezing and melting, an average of 28 iterations per time step are required. The position of the phase change fronts can be established, at each time step, on simply interpolating for the position of the 0.5 liquid fraction contours. In the problem investigated, this approach was sufficient to pick up the position of the fronts even when multiple fronts were present in the cavity.

Two comments are made on the solution approach:

(1) No experimental verification for the cyclic case is presented, it is noted, however, that in the case of a constant melting wall temperature the proposed fixed grid approach gives predictions in close agreement with experiments[10] and alternative transformed grid schemes[9].

(2) Although a finite difference control volume method has been employed there is every reason to expect that the proposed cyclic solution approach could be applied on a finite element grid.

Figure 3 shows the predicted position of the solid/liquid interface and the flow field (stream lines) at intervals of 300 seconds up to $t = 48{,}000$ seconds; these "snap shots" reveal the state of the cavity at the end of each melting and freezing cycle. In this figure solid stream lines indicate flow in a clockwise direction and dashed streamlines indicate flow in an anti-clockwise direction (note the stream function values are in $10^{-6} m^2/s$). Solution on an Intel 90MHz Pentium processor (running Fortran 77) requires in the order of 2 CPU hours.

With reference to *Figure 3* the following commentary is made on the evolution of cyclic melting and freezing in the presence of fluid flow:

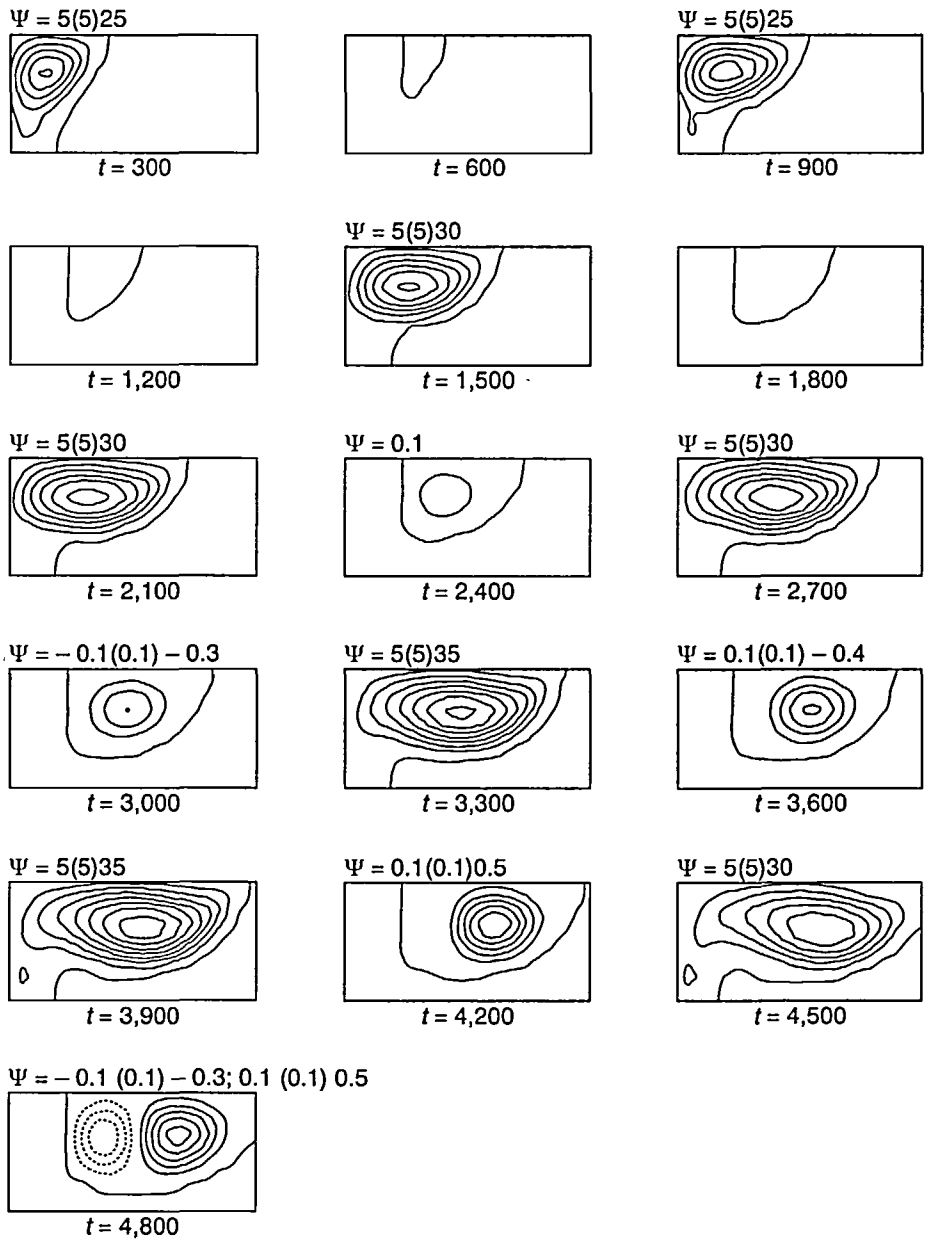

Figure 3 Position of solid/liquid interface and streamlines with time during cyclic phase change in the Gallium cavity. Time, t, is in seconds and the units of the stream function Ψ are $[10^{-6}m^2/s]$

- In the first melting cycle (t = 0s ... 300s) the predictions are similar to predictions obtained in the melting only studies (e.g. Brent *et al.*). In particular the enhancement of melting, in the upper part of the cavity, due to natural convection is evident.
- During the subsequent solidification cycle (t = 300s ... 600s) due to the rapid dissipation of temperature gradients in the melt the movement of the solidification is not modified by the

fluid flow. The reduction in the effectiveness of the heat transfer is noted on observing that a liquid pool still remains at the end of the freezing (t = 600s).

- The above behaviour continues over the next few cycles with an increase in (i) the liquid remaining at the end of solidification and (ii) the stream function intensities. At later stages ($t \geq$ 2100s) the residual flow field in the liquid pool is, although weakened, maintained throughout the freezing cycle. Also note that during the freezing cycle the shape of the liquid pool near the right hand side boundary does not alter in shape. This indicates that the solid in this region remains close to the phase change temperature (T_m = 0).
- The first modification is that the behaviour occurs during the melting cycle from t = 4200s ... 4500s. In this cycle the melting breaks through the solid on the right hand wall. The result is a heating of the right hand wall which leads to a drop of the horizonal temperature gradient in the liquid pool and a decrease in the flow intensity.
- Over the subsequent freezing cycle (t = 4200s ... 4800s), unlike pervious freezing cycles, due to the heated right hand wall the temperature gradients in the liquid pool are not dissipated. The result is a weak but well defined anti-clockwise natural convection flow cell in the left hand part of the liquid pool.

CONCLUSIONS

The central contribution of this paper has been to demonstrate that a basic, but efficient, fixed grid enthalpy scheme[7] can be successfully applied in the solution of problems that involve multiple moving phase change fronts. The only requirement is an appropriate interpretation of the predicted nodal liquid fraction fields. There is no need to explicitly track the movement of the fronts; indeed the movements and positions can be recovered after the fact from the stored liquid fraction field.

Demonstration on a heat conduction controlled cyclic phase change problem produced results, requiring insignificant computing resources, in very close agreement with other researchers[3,6]. Application to problems involving fluid flow in the melt indicated that, under a cyclic boundary condition, the convective enhancement of the heat transfer melting cycles were much more effective than freezing cycles.

The methods and finding from this study will underpin ongoing studies directed at the investigation of "freeze linings" in high temperature processes, e.g., the cryolite ledge in a Hall aluminum reduction Cell.

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