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CONTROL OF INTERFACE ACCELERATION DURING SOLIDIFICATION PROCESSES USING INVERSE HEAT TRANSFER METHODS

A. Abbasnejad[a], M.J. Maghrebi[a] & H. Basirat Tabrizi[b]
[a]*Faculty of Mechanical Engineering, Shahrood University of Technology, Shahrood, Iran*
[b]*Faculty of Mechanical Engineering, Amirkabir University of Technology, Tehran, Iran*

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Abstract: *In this study, a computational method is established for controlling acceleration of phase interface motion during solidification in pure materials. Inverse heat transfer method is applied to estimate the required time-dependent boundary conditions. Enthalpy formulation is employed to avoid the solution problem for solid and liquid phases separately. Conjugate gradient along with adjoint method is used to minimize the objective function. Constant velocity and constant interface acceleration are also investigated. Simulation result is validated with analytical solution existing just for zero acceleration. Furthermore, the estimated boundary heat flux is taken as an input for direct solution and it is observed that desired acceleration can be achieved.*

1. INTRODUCTION

Solidification processes play an important role in many branches of technology such as casting and welding. A desired solidification microstructure in the final products dictates a certain type of solid-liquid interface motion[1]. Thus finding a boundary condition e.g. Heat Flux, which leads to desired interface motion, is of paramount importance to the microstructure formation of solidified material. The main aim of this paper is to present an inverse numerical technique to find time-dependent boundary conditions which cause the desired interface acceleration. These kinds of problems are classified as inverse problems. In inverse solidification problems, the velocity or acceleration is prescribed at the interface thus the boundary conditions (temperature or heat flux) remain to be computed using a proper inverse heat transfer method. Due to the presence of the solid-liquid moving interface, these problems may become strongly nonlinear.

A wide variety of numerical methods have been used for direct and inverse modeling of solidification problems. Voller [2] presented an enthalpy method with future time stepping to solve inverse Stefan problem. The problem was investigated by references [3-10] with and without fluid flow consideration using Beck's method [11], the steepest descent method and conjugate gradient method. They used front fixing and front tracking finite element method. In their approach the problem should be treated as two distinct inverse problems for both liquid and solid phases.

Frankel, Keyhani [12] and Hale et. al. [13] applied the global time method (GTM) to control interfacial temperature gradient and velocity. Xu and Naterer [14-16] estimated boundary temperature history to control the velocity and acceleration of the interface using combined experimental and numerical techniques. The numerical method was developed for enthalpy with control volume based finite element method and Beck's inverse method. Recently, Okamoto and Li [17] used Tikhonov regularization method to control the velocity and the shape of the solid-liquid interface. Hinze and Ziegenbaly [18] solved inverse Stefan problem for one and two region problems via steepest descent method.

Most of the studies employed the deforming grid and solved the two distinct problems for each phase, separately. In this study, we present a numerical method to control the acceleration of the solid-liquid interface for controlling the quality of solidified material. This is based on fixed grid (enthalpy) method and highly accurate time advancement scheme.

The inverse acceleration control problem minimizes the objective function defined based on the temperature difference between the desired temperature (melting point) and the computed temperature at a desired interface location. Adjoint method, which yields the sensitivity, and adjoint equations are developed in conjunction with the conjugate gradient method (CGM).

Different cases with constant velocity and constant acceleration are tested. The obtained boundary heat flux from inverse solution is applied as an input boundary condition of direct problem to evaluate the accuracy of the inverse numerical solution.

2. GOVERNING EQUATIONS

The unidirectional conduction-dominated solidification of a pure material with boundary conditions is shown in Fig.1. Thus, the non-dimensional model equations describing the temperature distribution in the solidifying region based on enthalpy form can be written as [19]:

$$\frac{\partial H}{\partial t} = \frac{\partial^2 T}{\partial x^2} \qquad 0 < x < 1 \qquad 0 < t \le t_f \tag{1a}$$

$$\left.\frac{\partial T}{\partial x}\right|_{x=0} = q(t) \qquad x = 0 \qquad 0 < t \le t_f \tag{1b}$$

$$\left.\frac{\partial T}{\partial x}\right|_{x=1} = 0 \qquad x = 1 \qquad 0 < t \le t_f \tag{1c}$$

$$T = T_i \ or \ H = H_i \qquad 0 \le x \le 1 \qquad t = 0 \tag{1d}$$

And enthalpy-temperature relations are:

$$H(x,t) = \begin{cases} T & T < 0 \quad \text{Solid region} \\ [0, Ste] & T = 0 \\ T + Ste & T > 0 \quad \text{Liquid region} \end{cases} \tag{2a}$$

$$T(x,t)=\begin{cases} H & H<0 & \text{Solid region} \\ 0 & 0\le H\le Ste & \text{Interface} \\ H-Ste & H>Ste & \text{Liquid region} \end{cases} \tag{2b}$$

Where, Ste is the non-dimensional form of latent heat known as Stefan's number.

The direct problem given by the sets of equations (1) and (2) is for the determination of the temperature field $T(x, t)$ and interface velocity when the boundary heat flux $q(t)$ at $x = 0$ is known.

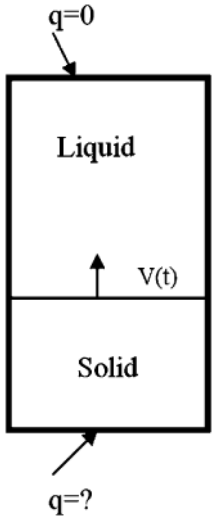

Figure. 1: Schematic Diagram of Problem

On the other hand for the inverse problem, the heat flux $q(t)$ at $x = 0$ is unknown while the velocity, acceleration or location of interface is known.However it can be estimated by using measured temperatures or desired temperatures (pseudo measured temperatures).

So the inverse problem is established which minimizes the objective function defined base on the L_2 norm of the error between the calculated temperature at the desired interface (x_{sd}: measurement point) and a given melting (fusion) temperature (T_f). In other words:

$$s[q(t)] \;=\; \| T_t - T(x_{sd},t;q(t)) \|^2 = \int_0^{t_f} [T_f - T(x_{sd},t;q(t))]^2\, dt \tag{3}$$

The conjugate gradient method with adjoint problem is applied to minimize the cost function of (3).

3. THE SENSITIVITY PROBLEM

It is assumed that the temperature $T(x, t)$ and the enthalpy $H(x, t)$ change with an amount $\Delta T(x, t)$ and $\Delta H(x, t)$, respectively when $q(t)$ undergoes a perturbation $\Delta q(t)$. By substituting $[T + \Delta T]$ for $T(x, t)$, $[H, \Delta H]$ for $H(x, t)$ and $[q + \Delta q]$ for $q(t)$ in the direct problem (equations (1a)-(1d)) and subtracting the original direct problem the following expressions are obtained as introduced in [20]:

$$\frac{\partial \Delta H}{\partial t}=\frac{\partial^2 \Delta T}{\partial x^2} \qquad 0<x<1 \qquad 0<t\le t_f \tag{4a}$$

$$\frac{\partial \Delta T}{\partial x} = \Delta q \qquad x = 0 \qquad 0 < t \le t_f \tag{4b}$$

$$\frac{\partial \Delta T}{\partial x} = 0 \qquad x = 1 \qquad 0 < t \le t_f \tag{4c}$$

$$\Delta T = 0 \qquad 0 \le x \le 1 \qquad t = 0 \tag{4d}$$

And $\Delta H = \Delta T$.

Clearly $\Delta T(x, t)$ represents changes in $T(x, t)$ with respect to changes in the unknown $q(t)$; hence it is a sensitivity function. The equations (4a-d) can be solved to obtain an optimal search step size.

4. THE ADJOINT PROBLEM

To derive the adjoint problem, a new function $\lambda(x, t)$ called Lagrange multiplier is introduced. In adjoint problem the governing equations are multiplied by $\lambda(x, t)$ and then integrated over the spatial and temporal domains. The results are then added to the cost functional equation (3) as achieved in [20]:

$$s[q(t)] = \int_0^{t_f} [T_f - T(x_m, t; q(t))]^2 dt + \int_0^{t_f} \int_0^1 \lambda(x,t)[k\frac{\partial^2 T}{\partial x^2} - \rho\frac{\partial H}{\partial t}]dxdt \tag{5}$$

The following adjoint problem can be obtained by replacing T with $[T + \Delta T]$, q with $[q + \Delta q]$ and $s(q)$ with $[s(q) + \Delta s(q)]$ in equation (5) and then subtracting the obtained result from equation (5) and further using boundary and initial conditions and allowing terms containing $\Delta T(x, t)$ to vanish,:

$$\frac{\partial \lambda(x,t)}{\partial t} + \frac{\partial^2 \lambda(x,t)}{\partial x^2} + 2[T - T_f]\delta(x - x_{sd}) = 0 \qquad 0 < x < 1 \qquad 0 < t \le t_f \tag{6a}$$

$$\frac{\partial \lambda}{\partial x} = 0 \qquad x = 0 \qquad 0 < t \le t_f \tag{6b}$$

$$\frac{\partial \lambda}{\partial x} = 0 \qquad x = 1 \qquad 0 < t \le t_f \tag{6c}$$

$$\lambda = 0 \qquad 0 \le x \le 1 \qquad t = t_f \tag{6d}$$

After eliminating the terms containing $\Delta T(x,t)$, the following integral term is left.

$$\Delta s(q) = \int_0^{t_f} \lambda(0,t)\Delta q dt \tag{7a}$$

Since $q(t) \in L_2(0, t_f)$, one can write:

$$\Delta s(q) = \int_0^{t_f} \Delta q \nabla s[q(t)]dt \tag{7b}$$

Comparing the last two equations, one obtains:

$$\nabla s[q(t)] = -\lambda(0,t) \tag{7c}$$

Equation (7c) is used to calculate the objective function gradient. Note that in the adjoint problem the condition (6d) is the value of $\lambda(x, t)$ at $t = t_f$. However, the final value problem (6a-6d) can be transformed into an initial value problem by defining a new time variable given by $\tau = t_f - t$.

5. THE CONJUGATE GRADIENT ALGORITHM (CGM)

The unknown function $q(t)$ can be determined by a procedure based on minimizing the objective function $s[q(t)]$ with an iterative approach by properly selecting the direction of descent and the search step size. The following iterative scheme is considered as conjugate gradient method (CGM) to estimate the unknown heat flux[20]:

$$q^{k+1}(t) = q^k(t) - \beta^k d^k(t) \tag{8a}$$

Where, k denotes the iteration number. The direction of descent $d^k(t)$ is approximated from the following formula:

$$d^k(t) = -\nabla s[q^k(t)], \text{ for } k = 0$$

$$d^k(t) = -\nabla s[q^k(t)] + \gamma^k d^{k-1}(t), \text{for other } k \tag{8b}$$

The conjugate coefficient is defined by to the following expression:

$$\gamma^0 = 0$$

$$\gamma^k = \frac{\int_0^{t_f} \left\{\nabla s[q^k(t)] - \nabla s[q^{k-1}(t)]\right\} \nabla s[q^k(t)]dt}{\int_0^{t_f} \left\{\nabla s[q^{k-1}(t)]^2\right\} dt} \tag{8c}$$

To implement the iterative procedure, one needs to develop expression for the optimal search step size β^k and solve the sensitivity problem by setting $\Delta q(t) = d^k(t)$. The following formula is used for the calculation of β^k:

$$\beta^k = \frac{\int_0^{t_f} [T(x_{sd}, t; q^k(t)) - T_f]\Delta T(x_{sd}, t; d^k(t))dt}{\int_0^{t_f} [\Delta T(x_{sd}, t; d^k(t))]^2 dt} \tag{8d}$$

The following stopping criterion is chosen to stop the iterative procedure:

$$s[q^{k+1}(t)] < \varepsilon \tag{8e}$$

Where, ε is the specified tolerance and is of order 6. The flow chart of the CGM is illustrated in Fig. 2.

6. SIMULATION AND RESULTS

A second order central space finite difference and a third order compact Runge-Kutta scheme are considered for computing the spatial derivative and time advancement in direct, sensitivity and adjoint equations, respectively. The time advancement scheme developed by Wray[21] is used for the time marching of the simulation. According to this scheme, the time advancement is performed in three sub-steps. Detailed discussion can be found in [21]. Numerical test case, applied to the following equation, is performed to validate the order of accuracy for the Rung-Kutta time advancement scheme.

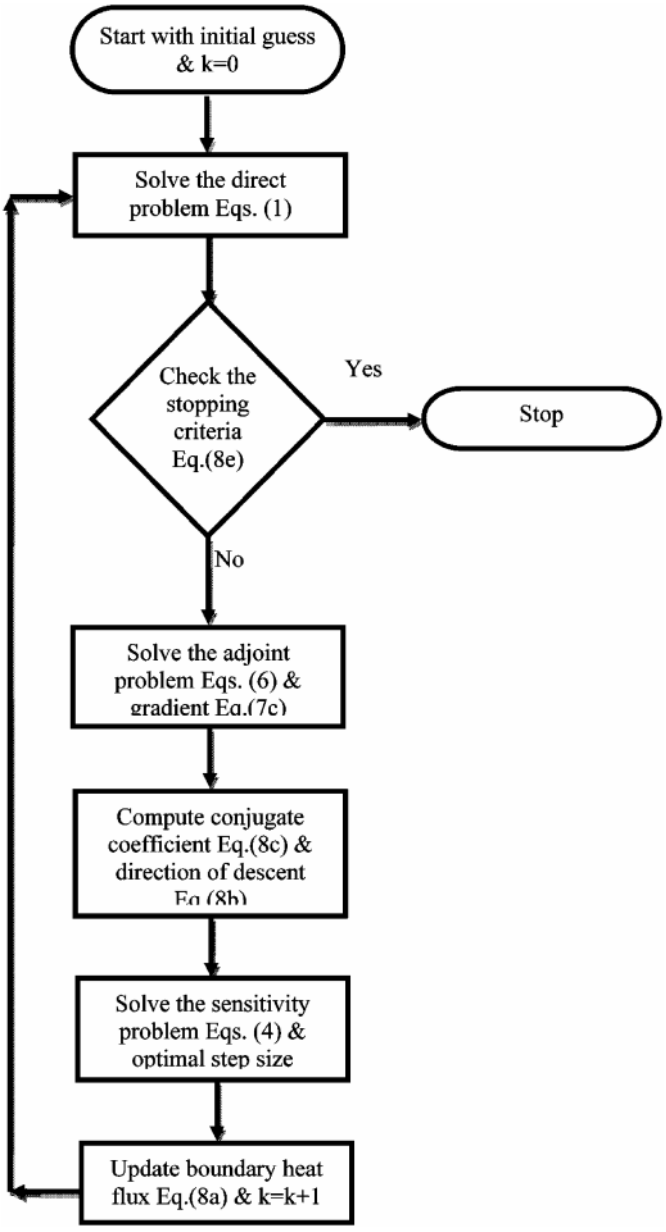

Figure. 2: Flow Chart of Conjugate Gradient Method

$$\frac{du}{dt} = -u(t) \tag{9}$$

Eq. (9) has an exact solution of $u(t) = e^{-t}$ if $u(0) = 1$ is taken as the initial condition. It is solved for $u(t)$ at $t = 1$ using different time increments. A comparison of the order of time advancement scheme for Runge-Kutta and forward in time methods is shown in Fig. 3. This definitely ensures the third order of accuracy for the time advancement of the computation.

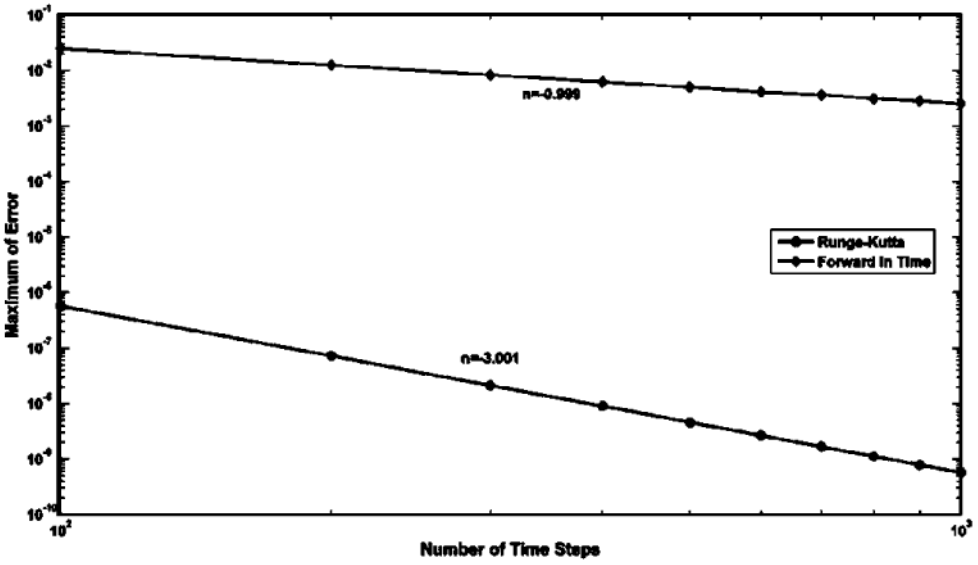

Figure. 3: Order of Time Advancement Scheme for $\frac{du}{dt} = -u(t)$ with $u(0) = 1$

A test case studied for comparison of the results is the zero acceleration (constant velocity) case. The analytical solution is obtained using the following parameters and boundary conditions. $T_i = T_f = 0,\ Ste = 0.5,\ V = 2$. The boundary heat flux is:

$$q(0,t) \quad = \quad e^{4t} \tag{10}$$

A comparison between the present simulation, analytical [22], semi-analytical [10] and a published numerical study in [2] is shown in Figs. 4 and 5. The desired and the computed interface locations can be observed in the figures. According to the figures, the present prediction is good except at the beginning of the simulation.

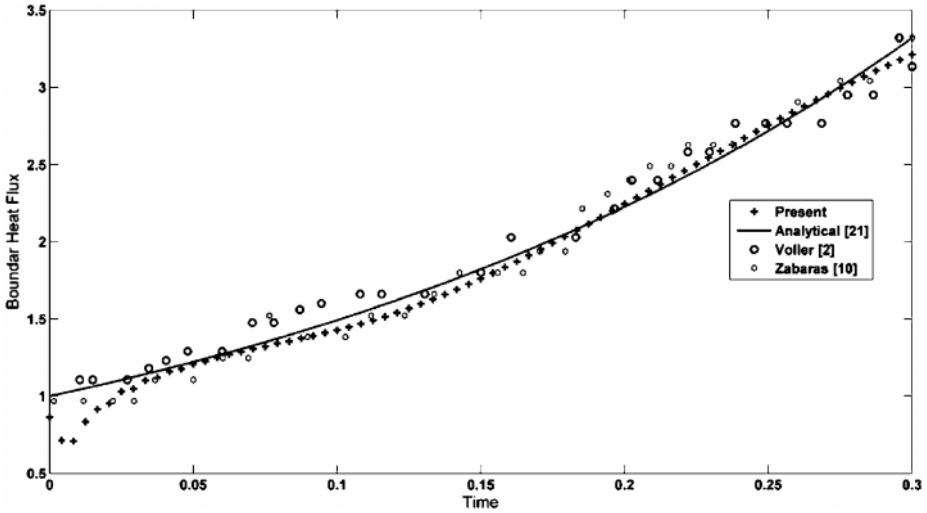

Figure. 4: Required Heat Flux for Constant Velocity

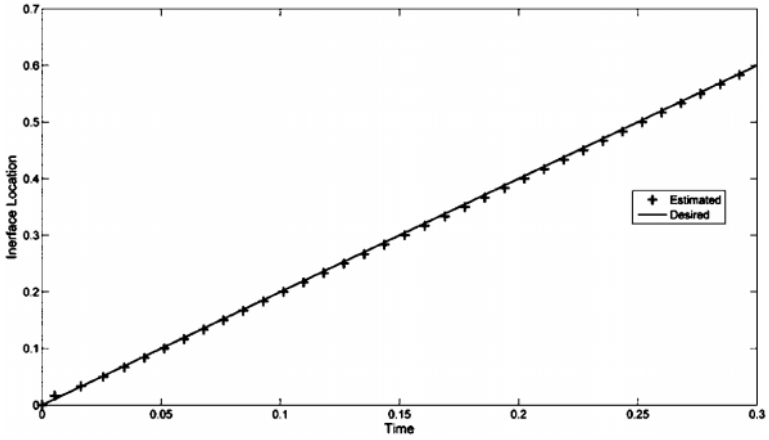

Figure. 5: Desired and Estimated Interface Location for Constant Velocity

In addition for constant acceleration with $Ste = 0.5$, $T_f = 0$ and $T_i = 0.5$, it is assumed that the desired interface location is as follows.

$$X_{sd} = \frac{1}{2} a_d t^2 \tag{11}$$

Where x_{sd} and a_d are the desired interface location and the desired interface acceleration, respectively. To validate the numerical results, the estimated heat flux from inverse solution for different interface accelerations is applied as boundary conditions of direct problem. Then the interface location is computed and compared with the desired location. Estimated heat flux obtained from inverse solution is shown in Fig. 6. Furthermore, the comparison between the desired and the computed interface locations can be seen in Fig.7. The accuracy of the solution can be confirmed by this finding. For quantitative comparison, a relative root mean square error e_{RMS} with the following definition:

$$e_{RMS} = \frac{\sqrt{(1/M)\sum_{m=1}^{M}(x_{sd} - x_{sc})^2}}{\sqrt{(1/M)\sum_{m=1}^{M}(x_{sd})^2}} \times 100 \tag{12}$$

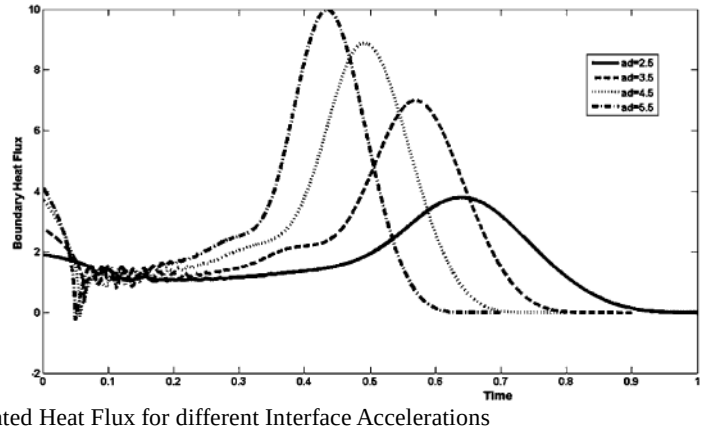

Figure. 6: Estimated Heat Flux for different Interface Accelerations

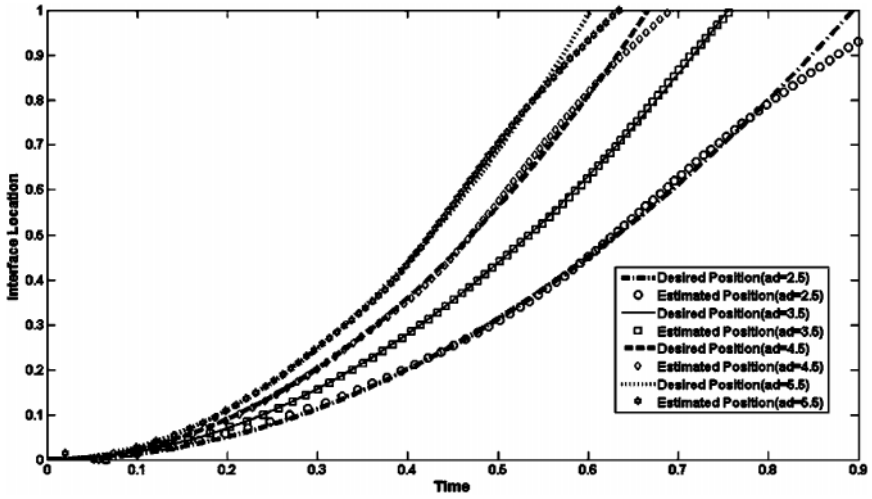

Figure. 7: Desired and Estimated Interface Location for different Accelerations.

Where x_{sc} represents the computed interface location and M is the total number of time steps. For higher accuracy, the required iteration to satisfy the stopping criteria, objective function value at final step and RMS error of the calculations for different interface accelerations are listed in Table 1. To demonstrate the convergence rate of the numerical solution, the rate of reduction of objective function for some cases is presented in Fig. 8.

Table 1
Quantitative Comparison of Results

Case	*Required iterations*	*Objective Function*	e_{RMS}
a_d = 2.5	30	2e-3	6.2
a_d = 3.5	30	1e-3	2.42
a_d = 4.5	30	9e-4	3.37
a_d = 5.5	30	8e-4	4.95

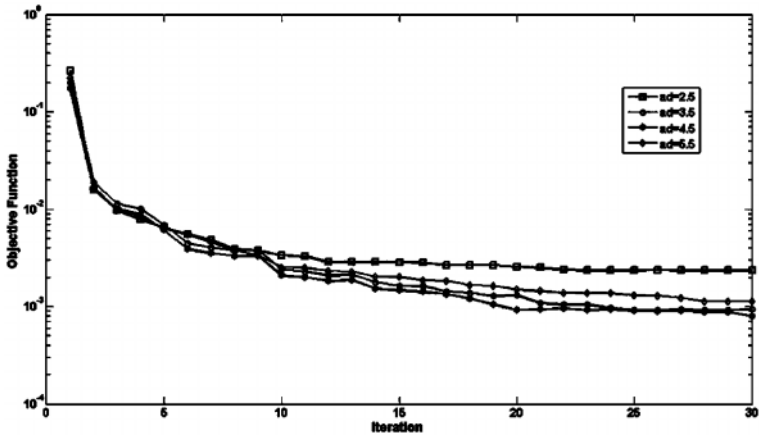

Figure. 8: Rate of Reduction of Objective Function for Different Accelerations

Results reveal a very good convergence and an acceptable output.

7. CONCLUSION

We have formulated and solved a transient inverse heat transfer problem to control the acceleration of solid-liquid interface during solidification processes by applying the conjugate gradient optimization method. In addition, the enthalpy formulation is applied to solve the inverse problem in a fixed domain to avoid the solution for liquid and solid phases separately. Two cases of constant velocity and constant acceleration are investigated. The numerical results at constant the velocity are in good agreement with known analytical and previous numerical studies. For constant acceleration case, the obtained heat flux is applied as an input boundary condition of direct problem and the computed interface location is compared to the desired location. The accuracy and convergence for constant velocity and acceleration cases are shown to be acceptable in the current numerical modeling.

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