Optimal Control of a Moving Boundary by Laser Heating in a 2-Phase Stefan Problem

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Abstract

The 2-phase heat control problem by a single laser point input is studied and a method of overcoming the moving boundary problem is introduced. This is achieved by applying a sequence of linear time varying control problems which converge to the single nonlinear problem which can be obtained from the joint moving boundary problems.

Key words: Moving boundary problems, Linear time varying systems, Optimal control

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Laser interactions with materials play a pivotal role in very many applications ranging from industrial scale cutting and welding, through to delicate surgery and machining of nanoscale features for microstructure manufacture. These applications have highly varied goals; for example, certain processes may require large amounts of material to be ablated per pulse, whilst others necessitate that laser-induced modification of the target is restricted to regions that may be sub-micron in size. The timescale on which the target reacts to the laser, for example phase front propagation velocities, can also be very important in determining the quality of the final result. For all of these processes, the common factor is that knowledge of how the target material reacts after irradiation with the laser is vital for accurate control of the result.

Since the invention of the laser, such interactions have been studied extensively. These studies have been almost exclusively based around the resultant thermal processes in the target material given specified laser parameters. However, as most of the applications involving laser processing have relatively well-defined goals, it is apparent that a method

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where the desired modifications to the target are specified initially, and then a suitable laser input is calculated, would be a highly desirable tool.

Recently we demonstrated a technique for determining an optimum control by classical methods for 2-phase heat diffusion (Stefan) problems (Banks, 2007). In this work we apply our technique to the situation of laser heating. A desired temperature profile within the target is specified and then the corresponding time-varying laser input required to obtain such a profile is calculated.

1. Background

1.1. *Laser Temporal Control*

Temporal control of a processing laser beam is well-known to have significant effects on the subsequent thermal processes in the target. With the correct selection of the temporal profile, significant benefits can be achieved in many applications including micromachining (Dachraoui, 2006; Stoian, 2002), and cutting and welding (Simon, 1993). However, the determination of the optimal temporal form of the laser is a major challenge both experimentally and theoretically.

The most common form of temporal control is to simply pulse the incident laser at a constant frequency, either by direct modulation of the laser source into a train of identical pulses (Simon, 1993) or by splitting a single incident pulse into multiple pulses, very closely spaced in time (Stoian, 2002). However, many techniques have been successfully demonstrated for modifying the temporal intensity distributions of lasers. Such techniques are readily available and are versatile enough to allow essentially arbitrary temporal waveforms to be generated. The effects of temporal pulse shaping of single pulses (Dachraoui, 2006) and pulse trains (Low, 2000) on the target material have received significant study. It is apparent from many of these studies that control of the temporal profile of the laser beyond simple pulsing is necessary to optimise the interaction with the target material.

The difficulty with optimising a laser-matter interaction through temporal pulse shaping is that typically no prior knowledge of a suitable profile is available. To get around this difficulty, evolutionary algorithms are commonly employed to optimise the pulse shaping (Dachraoui, 2006). However this method can be relatively time-consuming, especially when no good "first guess" of the optimal profile is available. A further problem that can arise is that a quantifiable measure of the success of a particular pulse form may be hard to obtain *in situ* experimentally.

1.2. *The Stefan Problem*

In this paper we consider the general 2-phase Stefan problem in a region $\Omega \subseteq \Re^n$. Thus we assume that Ω is divided into two (initially unknown) regions Ω_1, Ω_2 in which the material is respectively liquid (in Ω_1) and solid (in Ω_2). The phase change takes place on the boundary $\partial\Omega_1 = \partial\Omega_2$ and in the open regions Ω_1, Ω_2 we have the standard heat conduction equations

$$
\begin{aligned}
\frac{\partial T}{\partial t} &= \alpha_L \nabla^2 T, \quad (x,t) \in \Gamma_1 = \Omega_1 \times (0,\tau) \\
\frac{\partial T}{\partial t} &= \alpha_S \nabla^2 T, \quad (x,t) \in \Gamma_2 = \Omega_2 \times (0,\tau)
\end{aligned} \tag{1}
$$

for some time $\tau > 0$, assuming constant thermal conductivity in each phase.

The problem consists of two linear equations in unknown regions. In order to solve the problem, we show how to convert it into a single nonlinear diffusion equation with a temperature-dependant heat coefficient $\alpha(T)$. To do this note that the classical Stefan boundary condition is given by

$$
\rho L V_n = \Big[-\kappa \frac{\partial T}{\partial n} \Big]_-^+ \quad \text{on } \partial\Gamma_1,
$$

where V_n is the velocity of the moving boundary, ρ is the density, L is the latent heat, κ is the thermal conductivity, and n is the normal to the phase boundary. The energy content in the liquid region is given by

$$
e^L(T) = L + \int_{T_m}^{T} C_L(\overline{T}) d\overline{T}, \quad T > T_m
$$

and by

$$
e^S(T) = \int_{T}^{T_m} C_S(\overline{T}) d\overline{T}, \quad T < T_m
$$

where C_L and C_S are the respective specific heats. The corresponding conductivity coefficients (assuming the densities of each phase are equal and constant) are given by

$$
\alpha_L(T) = \frac{\kappa_L}{\rho C_L(T)}, \quad \alpha_S(T) = \frac{\kappa_S}{\rho C_S(T)},
$$

and the energy expressions can be unified by defining the specific heat

$$
C(T) = \begin{cases} L\delta(T - T_m) + C_L(T), & T \geq T_m \\ C_S(T), & T < T_m, \end{cases}
$$

and so the conductivity coefficient becomes

$$
\alpha(T) = \begin{cases} \alpha_L(T) = \kappa_L / \rho C_L(T), & T \geq T_m \\ \alpha_S(T) = \kappa_S / \rho C_S(T), & T < T_m. \end{cases}
$$

For simplicity we shall assume the conductivity coefficient is constant in each phase, i.e.

$$
\alpha(T) = \begin{cases} \alpha_L(T), & T \geq T_m \\ \alpha_S(T), & T < T_m. \end{cases} \tag{2}
$$

This gives a reasonable approximation in most cases. Thus, the equations (1) can be unified into the equation

$$
\frac{\partial T}{\partial t} = \alpha(T) \nabla^2 T, \quad (x,t) \in \Omega \times (0,\tau), \tag{3}
$$

where $\alpha(T)$ is given by (2).

2. Solution of the Unforced System

To solve the uncontrolled system (3), we introduce a sequence of linear, time-varying problems:

$$\frac{\partial T^{[i]}}{\partial t}(x,t) = \alpha\big(T^{[i-1]}(x,t)\big)\nabla^2 T^{[i]}(x,t), \tag{4}$$

with some given initial conditions

$$\begin{aligned} T^{[i]}(x,0) &= f(x), \quad x \in \Omega \\ T^{[0]}(x,t) &= f(x), \quad t \in (0,\tau) \end{aligned}$$

and a Dirichlet boundary condition

$$T^{[i]}(\partial\Omega, t) = 0, \quad \text{say.}$$

For the first approximation $T^{[1]}$ we can take the solution of the system

$$\frac{\partial T^{[1]}}{\partial t}(x,t) = \alpha\big(T^{[0]}(x,t)\big)\nabla^2 T^{[1]}(x,t). \tag{5}$$

It is well-known that each of the equations (4) has a unique solution. To prove the convergence of the sequence of solutions, we approximate each system (4) by a finite-dimensional approximation. For simplicity, we consider the one spatial dimensional case- the general case follows similarly. Thus consider the one-dimensional bar with temperature $T(x,t)$, $0 \le x \le l$. Write

$$T_j^{[i]}(t) = T^{[i]}(t, jl/N), \quad j = 1, 2, \ldots, N.$$

Then we have the system

$$\frac{d}{dt}\begin{pmatrix} T_1^{[i]} \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ T_N^{[i]} \end{pmatrix} = \frac{1}{(\Delta x)^2}\times$$

$$\begin{pmatrix} -2\alpha(T_1^{[i-1]}) & \alpha(T_1^{[i-1]}) & 0 & \cdots & \cdots & \cdots & 0 \\ \alpha(T_2^{[i-1]}) & -2\alpha(T_2^{[i-1]}) & \alpha(T_2^{[i-1]}) & 0 & \cdots & \cdots & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ \cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & \cdots & \cdots & \cdots & 0 & \alpha(T_N^{[i-1]}) & -2\alpha(T_N^{[i-1]}) \end{pmatrix}\begin{pmatrix} T_1^{[i]} \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ T_N^{[i]} \end{pmatrix}$$

where

$$T^{[i]}(0) = T_0, \quad T^{[i]} = (T_1^{[i]}, \cdots, T_N^{[i]})^T,$$

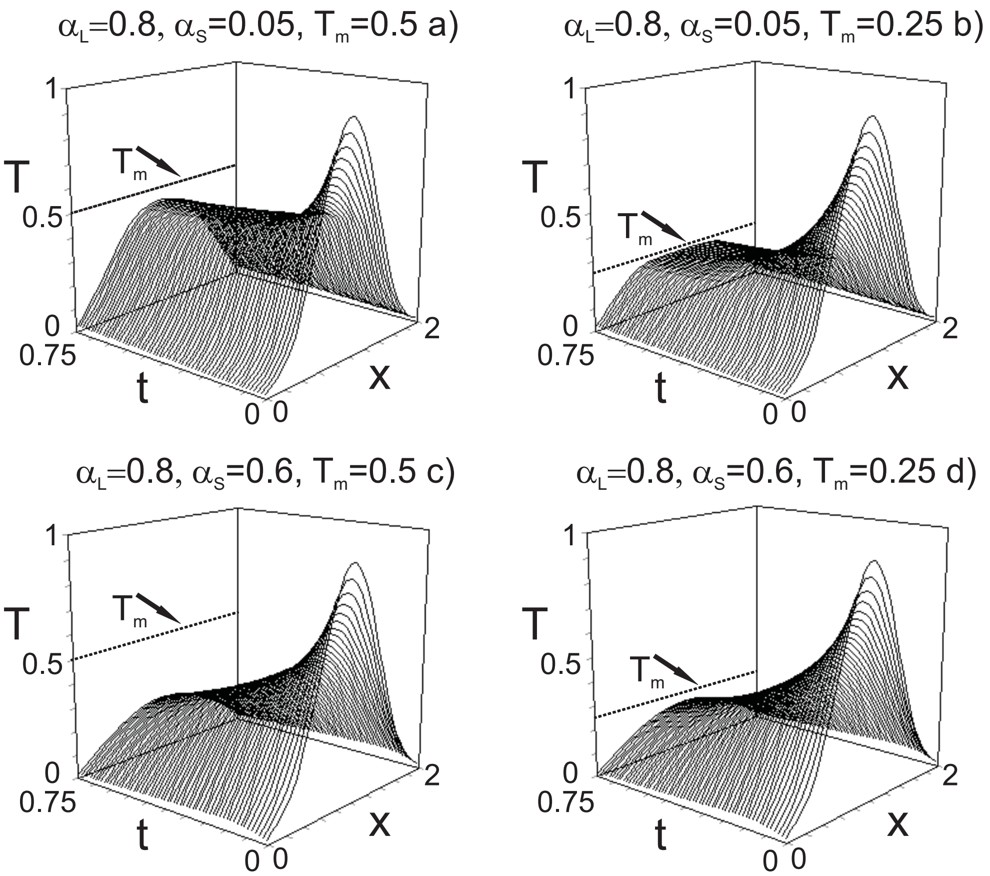

Fig. 1. Plots of the solution of the unforced system with $f(x) = e^{(4(x-1)^2)}$ and various values of α_L, α_S, and T_m.

and

$$T_0 = \Big(f(l/N), f(2l/N), \cdots, f\big((N-1)l/N\big), f(l))\Big).$$

(f is the initial condition, as above).

Hence we can write the systems in the form

$$\frac{dT^{[i]}}{dt}(t) = A(T^{[i-1]})T^{[i]}, \quad T(0) = T_0. \tag{6}$$

Since A is locally Lipschitz, we have the following theorem (Tomas-Rodriguez, 2003):

Theorem 1 *The sequence of temperatures $T^{[i]}(t)$ defined by (6) is uniformly convergent on any compact time interval.* □

Combining this with the well-known theory of convergence for finite-dimensional approximations of diffusion systems, we have

Theorem 2 *The sequence $T^{[i]}(t)$ converges uniformly almost everywhere on compact time intervals, as $i \to \infty$ and $N \to \infty$, to the solution of (4).* □

To demonstrate the ability of the technique to model heat flow in a 2-phase system, some simple unforced diffusion problems have been solved with $f(x) = e^{(4(x-1)^2)}$ (i.e. some

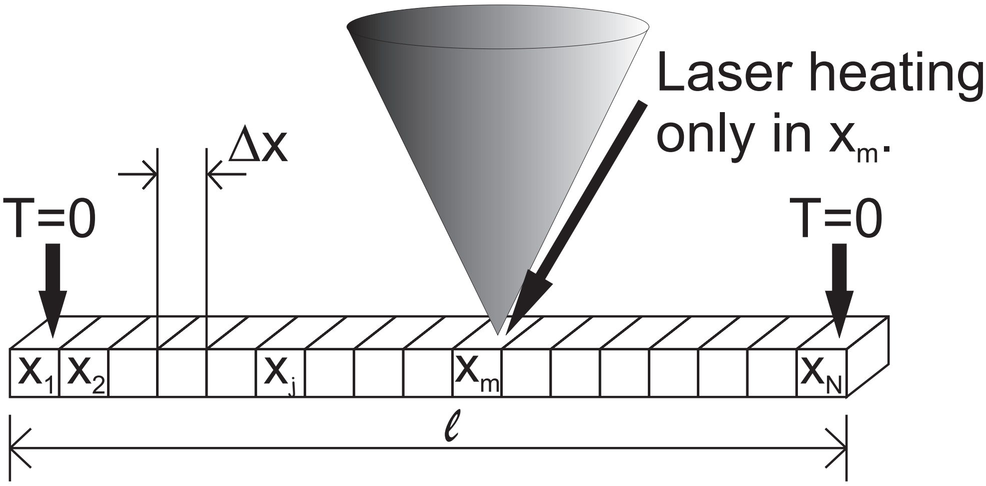

Fig. 2. Plots of the solution of the unforced system with $f(x) = e^{(4(x-1)^2)}$ and various values of α_L, α_S, and T_m.

regions liquid and some solid at $t = 0$)), $l = 2$, $N = 30$, and $\tau = 0.75$; 300 time steps were used. Figures 1(a) & (b) show results using $\alpha_L = 0.8$ and $\alpha_S = 0.05$ (i.e. relatively large conductivity ratio α_L/α_S). Figures 1(c) & (d) show results using $\alpha_L = 0.8$ and $\alpha_S = 0.6$ (i.e. relatively small conductivity ratio). The melt temperature was taken to be $T_m = 0.5$ (fig. 1(a&c)) and $T_m = 0.25$ (fig. 1(b&d)). As can be seen, the heat diffused out of the higher-conductivity liquid region rapidly, but diffused more slowly in the lower-conductivity solid regions, as would be expected. The model required $\approx 4 - 5$ iterations to converge.

3. The Control Problem

We now consider the problem of controlling the temperature profile in a one-dimensional bar with a pointwise laser heating control. The problem is shown schematically in fig. 2. The equation of the system is given by

$$\frac{\partial T}{\partial t} = \alpha(T)\nabla^2 T + \delta(x - \bar{x})u \tag{7}$$

where u is proportional to the heat input power from the laser. As before we shall apply the above methods to the finite-dimensional approximation

$$\frac{dT^{[i]}}{dt}(t) = A\big(T^{[i-1]}(t)\big)T^{[i]}(t) + Bu, \tag{8}$$

where

$$B = (0, 0, \cdots, 1, 0, \cdots, 0),$$

and the ‘1’ is in the mth place corresponding to the point

$$\bar{x} = ml/N. \tag{9}$$

If $T_d(t)$ is the desired temperature profile, we shall solve the optimal tracking problem of minimising the cost functional

$$\begin{aligned} J =& \frac{1}{2}\big(T^{[i]}(t_f) - T_d(t_f)\big)^T F\big(T^{[i]}(t_f) - T_d(t_f)\big) \\ &+ \frac{1}{2}\int_0^{t_f} \Big\{\big(T^{[i]}(t) - T_d(t)\big)^T Q\big(T^{[i]}(t) - T_d(t)\big) + u^T R u\Big\} dt \end{aligned}$$

where F and Q are positive-semidefinite matrices, and R is positive-definite.

In order to consider the 'trackability' of a given desired temperature profile, we shall consider first the general problem given by the nonlinear (finite-dimensional) control problem

$$\dot{x} = f(x, u).$$

Suppose we desire to track the function $x_d(t)$, then there must exist a control $u_d(t)$ such that

$$\dot{x}_d(t) = f\big(x_d(t), u_d(t)\big) \tag{10}$$

for all $t \geq \bar{t} > 0$, and some finite $\bar{t}$. Let

$$y(t) = x(t) - x_d(t)$$

Then

$$\begin{aligned} \dot{y}(t) &= \dot{x}(t) - \dot{x}_d(t) \\ &= f\big(x(t), u(t)\big) - f\big(x_d(t), u_d(t)\big) \\ &= g\big(y(t), v(t), t\big) \end{aligned}$$

where

$$v(t) = u(t) - u_d(t),$$

and

$$g(0, 0, t) = 0,$$

by Taylor's theorem. We can write this equation in the form

$$\dot{y}(t) = A\big(y(t), v(t), t\big)y(t) + B\big(y(t), v(t), t\big)v(t)$$

for some matrix-valued functions A and B. Hence, we can always rewrite a tracking problem as a regular problem provided the system can track the desired function $x_d(t)$, i.e. there is an (open-loop) control $u_d(t)$ such that (12) holds. If x_d is constant then (12) becomes

$$f(x_d, u_d) = 0 \tag{11}$$

and so for trackability, there must exist a (constant) control u_d such that (11) holds.

Specialising to the heat control problem, if we want to track a given temperature profile T^d, then we must have

$$
\frac{1}{(\Delta x)^2}
\begin{pmatrix}
-2\alpha(T_1^d) & \alpha(T_1^d) & 0 & \cdots & \cdots & \cdots & 0 \\
\alpha(T_2^d) & -2\alpha(T_2^d) & \alpha(T_2^d) & 0 & \cdots & \cdots & 0 \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\cdots & \cdots & \cdots & \cdots & \cdots & \cdots & \cdots \\
\vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\
0 & \cdots & \cdots & \cdots & 0 & \alpha(T_N^d) & -2\alpha(T_N^d)
\end{pmatrix}
\begin{pmatrix} T_1^d \\ T_2^d \\ \vdots \\ \vdots \\ \vdots \\ \vdots \\ T_N^d \end{pmatrix}
= -
\begin{pmatrix} 0 \\ \vdots \\ 0 \\ \vdots \\ 0 \\ \vdots \\ 0 \end{pmatrix} u_d
$$

Hence, if the input is in the mth place, we require

$$
\begin{aligned}
\frac{\alpha(T_1^d)}{(\Delta x)^2}(-2T_1^d + T_2^d) &= 0 \\
\frac{\alpha(T_2^d)}{(\Delta x)^2}(T_1^d - 2T_2^d + T_3^d) &= 0 \\
&\vdots \\
\frac{\alpha(T_{m-1}^d)}{(\Delta x)^2}(T_{m-2}^d - 2T_{m-1}^d + T_m^d) &= 0 \\
\frac{\alpha(T_m^d)}{(\Delta x)^2}(T_{m-1}^d - 2T_m^d + T_{m+1}^d) &= -u_d \\
&\vdots \\
\frac{\alpha(T_{N-1}^d)}{(\Delta x)^2}(T_{N-2} - 2T_{N-1} + T_N) &= 0 \\
\frac{\alpha(T_N^d)}{(\Delta x)^2}(T_{N-1} - 2T_N) &= 0
\end{aligned}
$$

An elementary computation shows that

$$
\begin{aligned}
&T_i = iT_1, \quad T_i = (N-i+1)T_N, \\
&T_N = \frac{iT_1}{N-i+1}
\end{aligned}
$$

and that

$$
u_d = \frac{\alpha(T_i)}{(\Delta x)^2}\frac{N+1}{N-i+1}T_1
$$

Hence, the only constant temperature profiles which are trackable are piecewise linear about the control point.

In the case where we allow time-varying desired temperature profiles, $T_i^d(t)$, we must satisfy the following equations:

$$
\begin{aligned}
T_2^d(t) &= \frac{\dot{T}_1^d(t)}{\beta T_1^d(t)} + 2T_1^d(t) \\
T_3^d(t) &= \frac{\dot{T}_2^d(t)}{\beta T_2^d(t)} + 2T_2^d(t) - T_1^d(t) \\
\dots\dots \\
T_i^d(t) &= \frac{\dot{T}_{i-1}^d(t)}{\beta T_{i-1}^d(t)} + 2T_{i-1}^d(t) - T_{i-2}^d(t)
\end{aligned} \tag{12}
$$

and

$$
\begin{aligned}
T_{N-1}^d(t) &= \frac{\dot{T}_N^d(t)}{\beta T_N^d(t)} + 2T_N^d(t) \\
T_{N-2}^d(t) &= \frac{\dot{T}_{N-1}^d(t)}{\beta T_{N-1}^d(t)} + 2T_{N-1}^d(t) - T_N^d(t) \\
\dots\dots \\
T_i^d(t) &= \frac{\dot{T}_{i+1}^d(t)}{\beta T_{i+1}^d(t)} + 2T_{i+1}^d(t) - T_{i+2}^d(t)
\end{aligned} \tag{13}
$$

where $\beta = \big(1/(\Delta x)^2\big)\alpha(T)$.

To solve (12) we write

$$\Gamma_k = \begin{pmatrix} T_{k-1}^d \\ T_k^d \end{pmatrix}$$

Then the equations become

$$\begin{pmatrix} T_{k-1}^d \\ T_k^d \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ -1 & N \end{pmatrix} \begin{pmatrix} T_{k-2}^d \\ T_{k-1}^d \end{pmatrix}$$

where N is the operator defined by

$$N(T) = \frac{1}{\beta(T)} \frac{dT}{dt}$$

Hence

$$\begin{pmatrix} T_{k-1}^d \\ T_k^d \end{pmatrix} = K \begin{pmatrix} T_{k-2}^d \\ T_{k-1}^d \end{pmatrix}$$

where

$$K = \begin{pmatrix} 0 & 1 \\ -1 & N \end{pmatrix}$$

and so

$$\begin{pmatrix} T_{k-1}^d \\ T_k^d \end{pmatrix} = K^{k-2} \begin{pmatrix} T_1^d \\ T_2^d \end{pmatrix}$$

Hence,

$$T_i^d = \left(K^{i-2} \begin{pmatrix} T_1^d \\ \frac{\dot{T}_1^d(t)}{\beta T_1^d(t)} + 2T_1^d(t) \end{pmatrix} \right)_2$$

where $(.)_2$ means the second component. Similarly, starting with (13) we have

$$T_i^d = \left(K^{N-i-1} \begin{pmatrix} T_N^d \\ \frac{\dot{T}_N^d(t)}{\beta T_N^d(t)} + 2T_N^d(t) \end{pmatrix} \right)_1$$

and so we have proved

Theorem 3 *A necessary and sufficient condition for the system (8) to be able to track a desired temperature profile is that (12) and (13) are satisfied and that T_1, and T_N are related by*

$$\left(K^{i-2} \begin{pmatrix} T_1^d \\ \frac{\dot{T}_1^d(t)}{\beta T_1^d(t)} + 2T_1^d(t) \end{pmatrix} \right)_2 = \left(K^{N-i-1} \begin{pmatrix} T_N^d \\ \frac{\dot{T}_N^d(t)}{\beta T_N^d(t)} + 2T_N^d(t) \end{pmatrix} \right)_1$$

moreover, the (open loop) control is given by

$$u_d = \dot{T}_i^d - \beta(T_i^d)(T_{i-1}^d - 2T_i^d + T_{i+1}^d). \quad \square$$

Of course, for the case of laser heating we also have the condition that

$$u_d(t) \geq 0 \quad \text{for all } t \geq 0$$

These conditions are highly nonlinear and can be used as a test for any given desired tracking. In general we will expect perfect tracking only for a very restricted class of functions.

4. Controlled Results

Finally, we apply the model to a real problem. As an example, we consider the case of holding a 1D bar like that in fig. 2 at the melt temperature, *i.e.* $T_d(x,t) = T_m$ for all x and t. The parameters used were $N = 30$, $l = 2$, $\alpha_L = 0.8$, $\alpha_S = 0.02$, $T_m = 0.25$, and $R = 0.5$. The heating point was taken to be in the middle of the bar, *i.e.* $m = 15$, and the time step was $\delta = 0.001$s. The initial condition was $T^[i](x,0) = 0$.

Figure 3 shows results obtained with 5 (fig. 3(a)) and 7 (fig. 3(b)) iterations. As can be seen the model again converged quickly, after around 5 iterations. Initially the control input was on, injecting heat into the bar and raising the temperature. It took just over 2.2 seconds for the heated region of the bar to reach the melting temperature (*i.e.* the desired condition), at which point the heat input was switched off and heat was allowed to diffuse in the bar. Due to the large difference in α_L and α_S heat diffused quickly out of the liquid regions, resulting in rapid solidification and an approximately flat-top temperature profile at around the melting temperature. However, limited diffusion in solid regions resulted in only minimal thermal diffusion following complete solidification and a temperature profile that only matched the desired profile close to the heating point.

Continuing to run the simulation for longer time periods resulted in a oscillating solution where the heat input was turned on until the temperature was raised above the melt

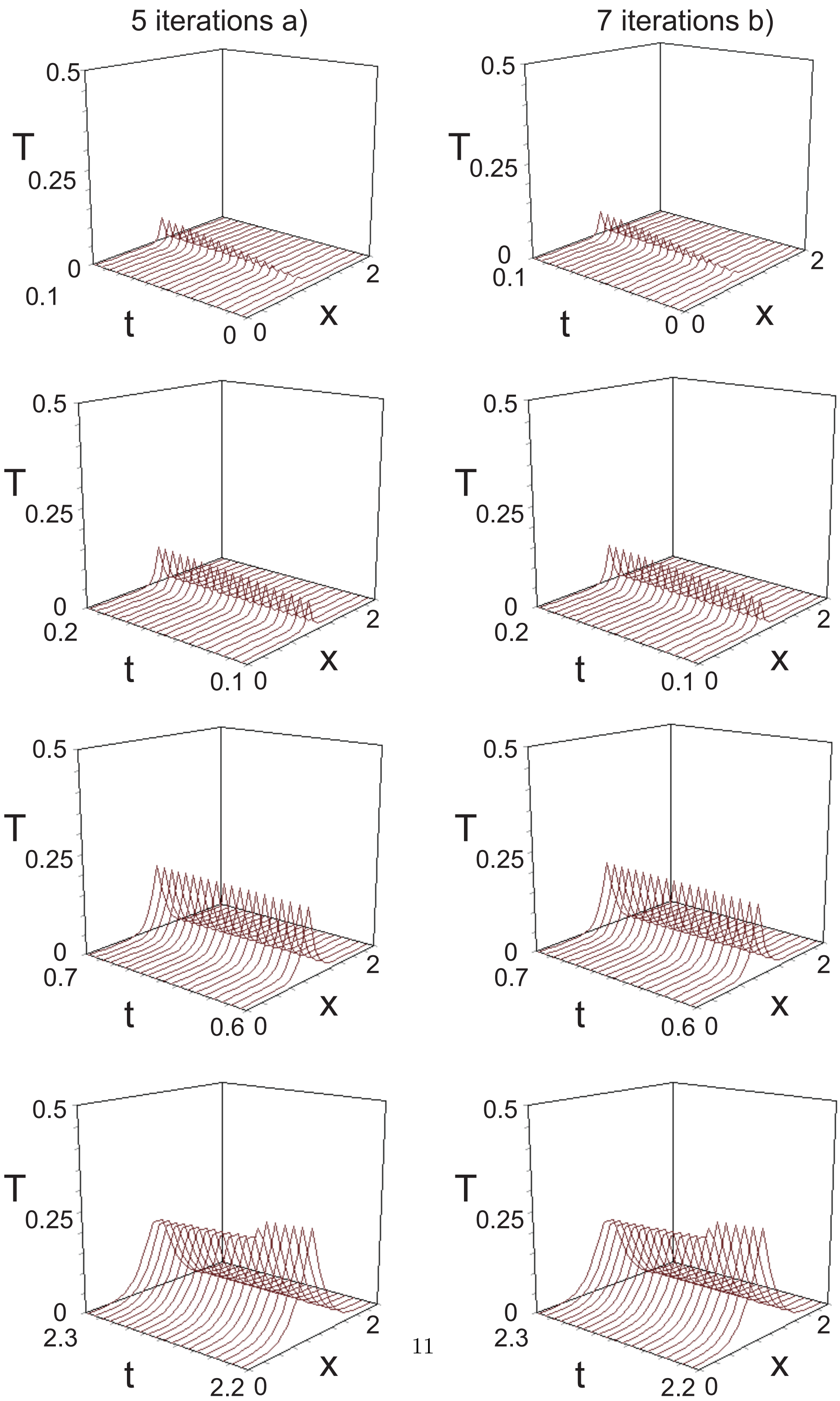

Fig. 3. Plots of the solution of the controlled system using 5 (a) and 7 (b) iterations.

temperature, and then off until sufficient diffusion occurred that the bar cooled below T_m. Heat diffusion in the lateral direction was limited by the small α_S so the temperature profile closely matched the desired condition only close to the heating point. Better tracking of the desired condition was achievable by reducing α_L/α_S.

5. Conclusions

We have shown how to approximate a nonlinear controlled Stefan problem using a linearisation technique. The method allows for the tracking of desired temperature profiles within targets heated by an external heat source, *e.g.* a laser.

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