FLATNESS BASED OPEN LOOP CONTROL FOR A PARABOLIC PARTIAL DIFFERENTIAL EQUATION WITH A MOVING BOUNDARY

Christian Fleck†, Thomas Paulus*, Dirk Abel*

* Institute of Automatic Control
Aachen University, Steinbachstrasse 54, 52056 Aachen, Germany
Phone: ++49-241-8027482, Fax: ++49-241-8022296
*Email: Th.Paulus@irt.rwth-aachen.de
†Email: Ch.Fleck@irt.rwth-aachen.de

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Abstract

The present paper deals with the flatness based open loop boundary control of a solidification process. A model to describe solidification is well-known as the Stefan problem. Depending on the mathematical model of the phase between solidus and liquidus one can differentiate between the one phase and the two phases Stefan problem. The paper presents a method for both cases to show that this moving boundary value problem described by a parabolic partial differential equation is flat and the boundary control can be easily calculated from the flat output. The results achieved using a Taylor series expansion will be compared with numerical solutions. The solution is facilitated by coordinate transformations.

1 Introduction

The Stefan problem [7] is probably the simplest mathematical model of conduction of heat accompanied by a phenomenon of change of phase. Therefore it can be used to determine various crystal growth manufacturing processes, e.g. Bridgman [1] or Czochralski crystal growth process, but also processes mathematical similar to it. The growth of the crystal is mainly influenced by the velocity of the phase interface and the temperature gradient at this point. On this account it is obvious to control these variables in applications, i.e. to determine trajectories for the input variables in the one phase and two phases case to fulfil the requirements for the temperature gradient and the velocity of the phase interface.

When a change of phase takes place, a latent heat is either absorbed or released, while the temperature of the material changing its phase remains constant. In the following (cp. Fig. 1) we denote by $u_i(t)$ the input variables at the boundary i, $T_i(x,t)$ the temperature of the liquid or solid material and $\xi(t)$ the movement of the phase interface. For the sake of simplicity any volume change in the material undergoing the change of phase is neglected and the critical temperature T_s of change of phase is assumed to be constant.

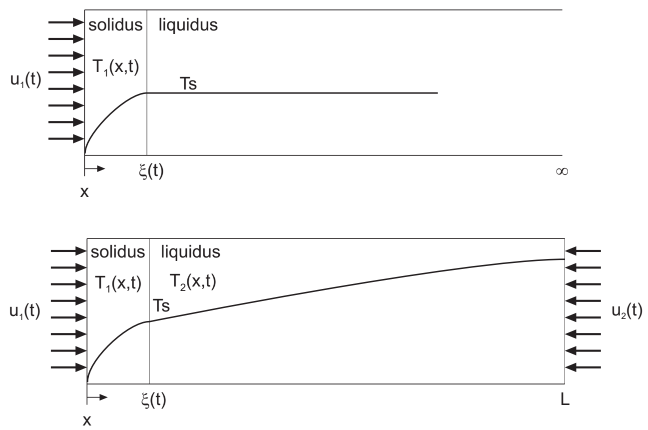

Figure 1: Schematic diagram of the one phase (top) and two phases (bottom) Stefan problem

Taking these assumptions into account the calculation of the thermal balance at the interface yields for the two phases problem, as shown by Stefan, the condition [6]:

$$\frac{\partial \xi}{\partial t}(t) = \left(k_1 \cdot \frac{\partial T_1}{\partial x}(x,t) - k_2 \cdot \frac{\partial T_2}{\partial x}(x,t) \right) \Bigg|_{x=\xi(t)} \tag{1}$$

$$k_1 = \frac{\lambda_1}{\rho \Delta H} \tag{2}$$

$$k_2 = \frac{\lambda_2}{\rho \Delta H} \tag{3}$$

and if the liquid phase is at constant temperature equation (1) reduces to the one phase problem:

$$\frac{\partial \xi}{\partial t}(t) = k_1 \cdot \frac{\partial T_1}{\partial x}(x,t) \Bigg|_{x=\xi(t)} \tag{4}$$

In both cases ΔH is the latent heat; ρ is the density of the material in its origin phase state and λ_1, λ_2 are the conductivity coefficients corresponding to the liquid and the solid phase.

The complete mathematical model of two phases problem, including boundary and initial conditions is described by the following equations:

$$\begin{aligned}
\frac{\partial T_1}{\partial t}(x,t) &= \frac{c_{p_1}\rho}{\lambda_1}\cdot\frac{\partial^2 T_1}{\partial x^2}(x,t) \quad 0\le x\le \xi(t) && (5)\\
\frac{\partial T_2}{\partial t}(x,t) &= \frac{c_{p_2}\rho}{\lambda_2}\cdot\frac{\partial^2 T_2}{\partial x^2}(x,t) \quad \xi(t)\le x\le L && (6)\\
T_1(x,0) &= T_s && (7)\\
\xi(0) &= 0 && (8)\\
T_1(\xi(t),t) &= T_s && (9)\\
T_2(\xi(t),t) &= T_s && (10)\\
T_1(0,t) &= u_1(t) && (11)\\
T_2(L,t) &= u_2(t) && (12)
\end{aligned}$$

and for the one phase problem the mathematical model reduce to:

$$\begin{aligned}
\frac{\partial T_1}{\partial t}(x,t) &= \frac{c_{p_1}\rho}{\lambda_1}\cdot\frac{\partial^2 T_1}{\partial x^2}(x,t) \quad 0\le x\le \infty && (13)\\
\xi(0) &= 0 && (14)\\
T_1(x,0) &= T_s && (15)\\
T_1(\xi(t),t) &= T_s && (16)\\
T_1(0,t) &= u_1(t) && (17)
\end{aligned}$$

2 Solution of the boundary control problem

The solution of the open loop boundary control problem corresponds to the solution of the inverse dynamic system. A suitable way to deal with this problem is differential flatness. Flatness was first introduced by Fliess et. al. [2] for finite dimensional systems and was extended by Martin et. al. [4] for infinite dimensional systems. If a system is flat, it can be parametrized by the flat output. Is the flat output equal to the output variable of the system, it is simple to determine the input trajectory of the system for a given output trajectory without integrating. Thus the open loop control problem is solved. The following considerations refer to the method of determination the flat output for the Stefan problem and the solution of the control task.

To facilitate the problems for calculation and analysis, especially for the numerical simulations, it appears advantageous to work in domain with unchanging size in which the phase interface $\xi(t)$ is fixed for all time. This can be done by defining new space coordinates for the solid and the liquid phase [5, 3]:

$$\begin{aligned}
x_1 &= \frac{x}{\xi(t)} \qquad 0\le x_1\le 1 && (18)\\
x_2 &= \frac{x-\xi(t)}{L-\xi(t)} \qquad 0\le x_2\le 1 && (19)
\end{aligned}$$

Using this simplification the equations (1), (4), (5)-(12), (13)-(17) have to be transformed.

2.1 One phase Stefan problem

In the case of the one phase Stefan problem the moving boundary $y_{f_1}(t)=\xi(t)$ is the flat output. The following considerations will proof this assumption.

From condition (16) follows after transformation:

$$T_1(1,t) = T_s \tag{20}$$

and

$$\left.\frac{\partial T_1}{\partial t}(x_1,t)\right|_{x_1=1} = 0 \tag{21}$$

The transformation of the moving boundary condition (4) results in

$$\left.\frac{\partial T_1}{\partial x_1}(x_1,t)\right|_{x_1=1} = k_1\cdot\dot{\xi}(t)\cdot\xi(t) \tag{22}$$

The derivatives $\frac{\partial T_1}{\partial x_1}$ and $\frac{\partial T_1}{\partial t}$ in $x_1=1$ are only depending on $\xi(t)$ or are equal to zero. Taking the partial differential equation (13) into account, the second derivative $\frac{\partial^2 T_1}{\partial {x_1}^2}$ in $x_1=1$ is also determined and only parametrized by $\xi(t)$. Therefore $\xi(t)$ is obviously the flat output.

The solution of the one phase Stefan problem can now be calculated with the aid of Taylor series expansion in $x_1=1$:

$$\begin{aligned}
T_1(x_1,t) &= T_1(1,t)+\sum_{i=1}^{\infty}\frac{\partial^i T_1}{\partial x_1^i}(1,t)\cdot\frac{(x_1-1)^i}{i!} && (23)\\
&= f_{1,0}(t)+\sum_{i=1}^{\infty} f_{1,i}(t)\cdot\frac{(x_1-1)^i}{i!} && (24)\\
&\quad 0\le x_1\le 1
\end{aligned}$$

Regarding the partial differential equation (13) and defining:

$$\begin{aligned}
b_1(t) &= \xi^2(t)\frac{\lambda_1}{c_{p_1}\rho}\\
c_1(t) &= \frac{\dot{\xi}(t)}{\xi(t)}
\end{aligned}$$

the coefficients of the Taylor series $f_{1,i}(t)$ can be obtained after simple calculations:

$$\begin{aligned}
f_{1,0}(t) &= T_1(1,t)=T_s && (25)\\
f_{1,1}(t) &= \left.\frac{\partial T_1}{\partial x_1}(x_1,t)\right|_{x_1=1}\\
&= \dot{\xi}(t)\cdot\xi(t)\cdot k_1 && (26)\\
f_{1,2}(t) &= \left.\frac{\partial^2 T_1}{\partial x_1^2}(x_1,t)\right|_{x_1=1}\\
&= -b_1(t)\cdot c_1(t)\cdot f_{1,1}(t) && (27)
\end{aligned}$$

It is possible to determine a recursion formula for the coefficients:

$$\begin{aligned}
f_{1,n}(t) = b_1(t)\cdot\Bigg(&\frac{\partial f_{1,n-2}}{\partial t}(t)-\\
&-c_1(t)\cdot\big((n-2)f_{1,n-2}(t)+f_{1,n-1}(t)\big)\Bigg) && (28)\\
&n\ge 2
\end{aligned}$$

The transformation of equation (24) into the origin domain yields the solution:

$$
\begin{aligned}
T_1(x,t) &= T_s + \sum_{i=1}^{\infty} \frac{f_{1,i}(t)}{i!} \cdot \frac{(x-y_{f_1})^i}{y_{f_1}^i} \qquad (29)\\
f_{1,i}(t) &= \varphi(y_{f_1}, \dot{y}_{f1}, \ldots, y_{f_1}^{(q)})
\end{aligned}
$$

From equation (17) the input $u_1(t)$ is determined:

$$
\begin{aligned}
u_1(t) &= T_s + \sum_{i=1}^{\infty} \frac{(-1)^i}{i!} \cdot f_{1,i}(t) \qquad (30)\\
f_{1,i}(t) &= \varphi(y_{f_1}, \dot{y}_{f_1}, \ldots, y_{f_1}^{(q)})
\end{aligned}
$$

For crystal growth, as mentioned above, it is desirable to control the velocity of the phase interface $\dot{\xi}(t)$. From equations (30) and (29) the input $u_1(t)$ and the temperature profile $T_1(x,t)$ are parametrized by the flat output $y_{f_1}(t) = \xi(t)$. For this reason the system is flat and the control trajectory can be calculated for a given velocity.

2.2 Two phases Stefan problem

In the case of the two phases Stefan problem the flat output is determined by

$$
\begin{aligned}
y_{f_2}(t) &= \big(y_{f_{2,1}}(t), y_{f_{2,2}}(t)\big)\\
&= \left(\xi(t), \left.\frac{\partial T_1}{x_1}(x_1,t)\right|_{x_1=\xi(t)}\right) \qquad (31)
\end{aligned}
$$

The verification of the flat output and the solution of the two phases Stefan problem is analogous to the one phase problem. In contrary to equation (26) the coefficient $f_{1,1}$ is part of the flat output. After the coordinate transformation (19) equation (10) becomes:

$$T_2(0,t) = T_s \qquad (32)$$

and

$$\left.\frac{\partial T_2}{\partial t}(x_2,t)\right|_{x_2=0} = 0 \qquad (33)$$

The relationship between the solid and liquid phase for the two phases problem is given by equation (1). The coordinate transformation in the unchanging size domain changes the condition to:

$$
\begin{aligned}
&\left.\frac{\partial T_2}{\partial x_2}(x_2,t)\right|_{x_2=0} =\\
&= -\frac{L-\xi(t)}{k2} \cdot \left(\frac{\partial \xi}{\partial t}(t) - \frac{k_1}{\xi(t)} \cdot \left.\frac{\partial T_1}{\partial x_1}\right|_{x_1=1}\right) \qquad (34)
\end{aligned}
$$

The derivatives in $x_2 = 0$ are only depending on $\xi(t)$ and $\frac{\partial T_1}{x_1}$. Using equation (6) the second derivative $\frac{\partial^2 T_2}{\partial x_2{}^2}$ in $x_2 = 0$ is determined. Therefore the two phases Stefan problem is flat and the solution can be found using a Taylor series expansion in $x_2 = 0$:

$$
\begin{aligned}
T_2(x_2,t) &= T_2(0,t) + \sum_{i=1}^{\infty} \frac{\partial^i T_2}{\partial x_2^i}(0,t) \cdot \frac{x_2^i}{i!} \qquad (35)\\
&= f_{2,0}(t) + \sum_{i=1}^{\infty} f_{2,i}(t) \cdot \frac{x_2^i}{i!} \qquad (36)\\
&\quad 0 \le x_2 \le 1
\end{aligned}
$$

Regarding the partial differential equation (6) and defining:

$$
\begin{aligned}
b_2(t) &= (L-\xi(t))^2 \cdot \frac{\lambda_2}{c_{p_2}\rho}\\
c_2(t) &= \frac{\dot{\xi}(t)}{L-\xi(t)}
\end{aligned}
$$

we obtain the coefficients with the same method used in the one phase case:

$$
\begin{aligned}
f_{2,0}(t) &= T_2(0,t) = T_s \qquad (37)\\
f_{2,1}(t) &= \left.\frac{\partial T_2}{\partial x_2}(x_2,t)\right|_{x_2=0}\\
&= -\frac{L-\xi(t)}{k2}\left(\frac{\partial \xi}{\partial t}(t) - \frac{k_1}{\xi(t)} \cdot \left.\frac{\partial T_1}{\partial x_1}\right|_{x_1=1}\right) \qquad (38)\\
f_{2,2}(t) &= \left.\frac{\partial^2 T_2}{\partial x_2^2}(x_2,t)\right|_{x_2=0}\\
&= -b_2(t) \cdot c_2(t) \cdot f_{2,1}(t) \qquad (39)
\end{aligned}
$$

For the two phases problem a recursion formula can be developed as well:

$$
\begin{aligned}
f_{2,n}(t) = b_2(t) \cdot \Bigg(&\frac{\partial f_{2,n-2}}{\partial t}(t) +\\
&+ c_2(t) \cdot \big((n-2)f_{2,n-2}(t) - f_{2,n-1}(t)\big)\Bigg) \qquad (40)\\
n \ge 2&
\end{aligned}
$$

After the transformation of (36) in the origin domain the temperature profile can be specified:

$$
\begin{aligned}
T_2(x,t) &= T_s + \sum_{i=1}^{\infty} \frac{f_{2,i}(t)}{i!} \cdot \left(\frac{x-y_{f_{2,1}}}{L-y_{f_{2,1}}}\right)^i \qquad (41)\\
f_{2,i}(t) &= \varphi(y_{f_2}, \dot{y}_{f_2}, \ldots, y_{f_2}^{(q)})
\end{aligned}
$$

Using equation (12) it is possible to calculate the input $u_2(t)$:

$$
\begin{aligned}
u_2(t) &= T_s + \sum_{i=1}^{\infty} \frac{f_{2,i}(t)}{i!} \qquad (42)\\
f_{2,i}(t) &= \varphi(y_f, \dot{y}_f, \ldots, y_f^{(q)})
\end{aligned}
$$

The temperature profile and the input variable of the solid phase are equal to (29) and (30). In the case of the two phases Stefan problem the input variables and the temperature profiles are parametrized by the flat output $y_f(t)$. Therefore the system is flat and the boundary control for a given temperature gradient at the phase interface and given velocity of the interface can be calculated.

3 Examples and trajectory planning

In this section the results achieved with the presented method will be compared with numerical results in the unchanging size domain by computing the absolute difference between the temperature profiles of the numerical solution and the solution presented in this paper. The input for the numerical simulations are calculated using the Taylor series expansion for $u_1(t)$ and $u_2(t)$ defined by the equations (30) and (42).
The critical temperature T_s is, without loss of generality, supposed to be zero. The Taylor series expansions are aborted after 10 elements.

3.1 Example for the one phase problem

In the presented example the velocity of the phase interface is assumed to be constant. This is correlated to the requirements in crystal growth applications as mentioned above.

$$y_{f_1}(t) = \xi(t) = c \cdot t \tag{43}$$

The comparison diagrammed in Fig. (4) between the numerical solution and the Taylor series expansion (Fig. 3) shows only a little difference.

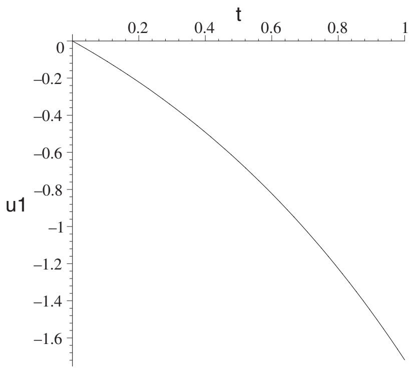

Figure 2: Calculated input trajectory $u_1(t)$

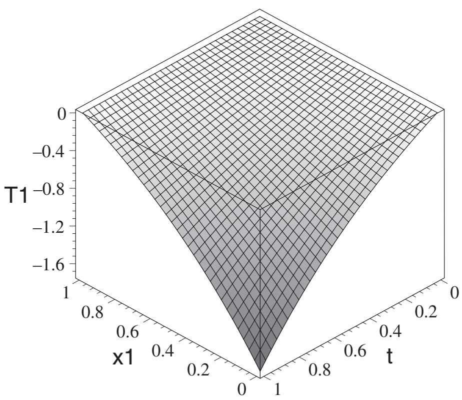

Figure 3: Taylor solution of the one phase Stefan problem $T_1(x_1, t)$

For this reason the presented method is suitable for the one phase Stefan problem and the solution of the open loop control problem.

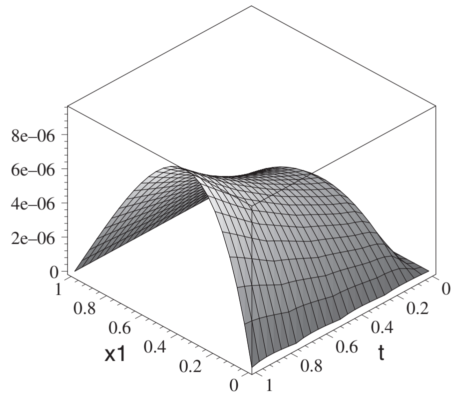

Figure 4: Difference between numerical solution and Taylor solution of the one phase Stefan problem $T_1(x_1, t)$

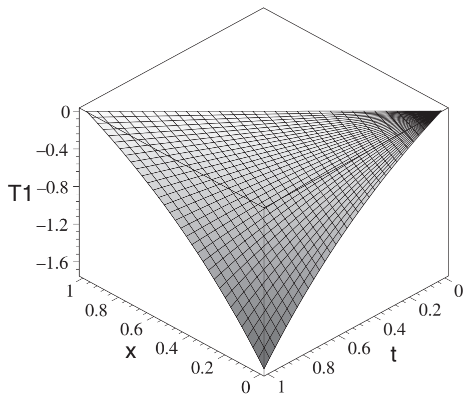

Figure 5: Taylor solution of the one phase Stefan problem in original domain $T_1(x, t)$

3.2 Example for the two phases problem

In the example for the two phases Stefan problem the interesting variables are the velocity of the phase interface and the temperature gradient. The calculated inputs $u_1(t)$ and $u_2(t)$ are shown in the figures (7) and (8). The phase interface is given, as in the one phase case, by:

$$y_{f_{2,1}}(t) = \xi(t) = c \cdot t \tag{44}$$

Because of the differentiation in the coefficients of the solution a smooth function for the temperature gradient is needed. Such a function is given by (cp. figure 11):

$$\begin{aligned} y_{f_{2,2}}(t) &= \left.\frac{\partial T_1}{x_1}(x_1, t)\right|_{x_1=\xi(t)} \\ &= \begin{cases} 0 & , t < 0 \\ f_{10}(t) & , 0 \leq t \leq 1 \\ 1 & , t > 1 \end{cases} \end{aligned} \tag{45}$$

with the polynomial $f_{10}(t)$.

For the numerical simulation this function has to be transformed in the unchanging size coordinates.

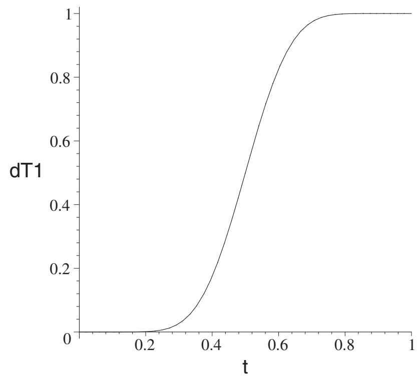

Figure 6: Preset temperature gradient $\frac{\partial T_1}{\partial x}(x,t)\big|_{x=\xi(t)}$

The errors between the numerical and the Taylor solution for the temperature profiles $T_1(x_1,t)$ and $T_2(x_2,t)$ shown in figure (10) and figure (13) are very small. Therefore the presented approach is also suitable for the solution in the two phases case. The solutions for the temperature profiles are shown in the figures (9),(11),(12),(14).

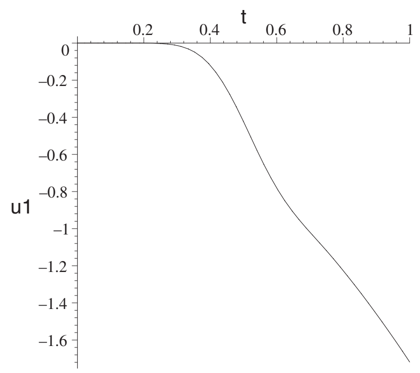

Figure 7: Calculated input variable $u_1(t)$

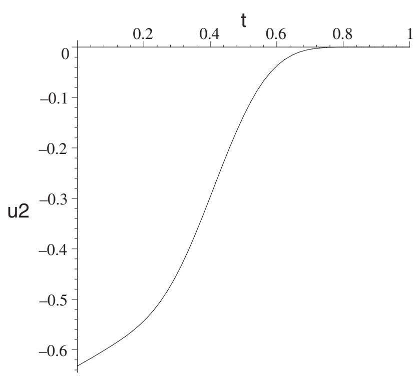

Figure 8: Calculated input variable $u_2(t)$

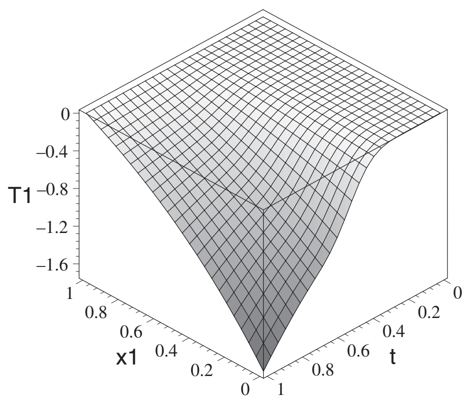

Figure 9: Taylor solution of the two phases Stefan problem $T_1(x_1,t)$

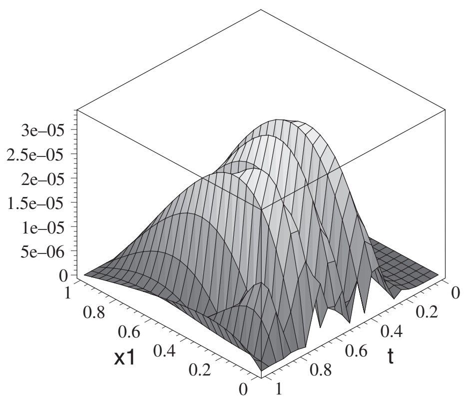

Figure 10: Difference between numerical solution and Taylor solution of the two phases Stefan problem $T_1(x_1,t)$

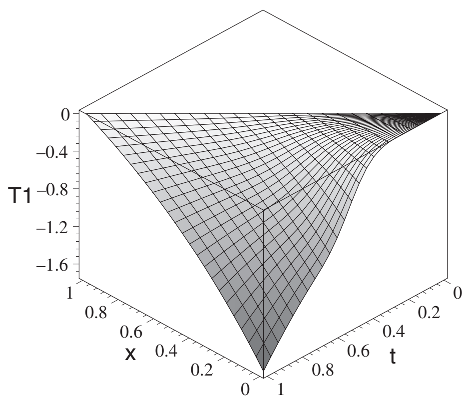

Figure 11: Taylor solution of the two phases Stefan problem in original domain $T_1(x,t)$

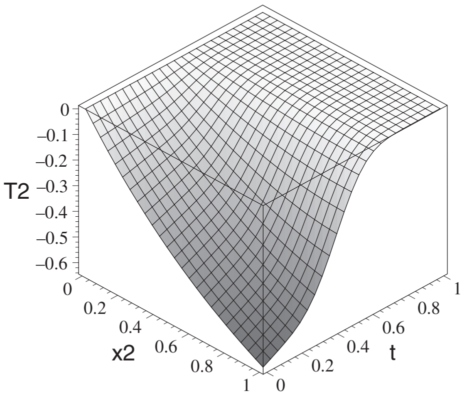

Figure 12: Taylor solution of the two phases Stefan problem $T_2(x_2, t)$

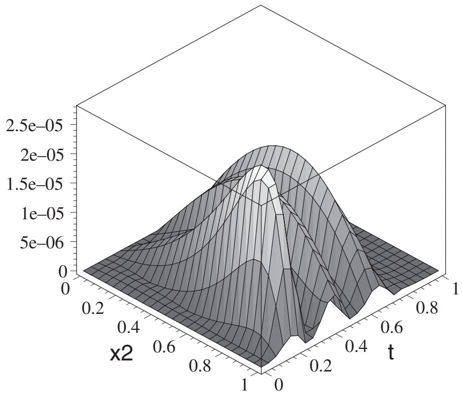

Figure 13: Difference between numerical solution and Taylor solution of the two phases Stefan problem $T_2(x_2, t)$

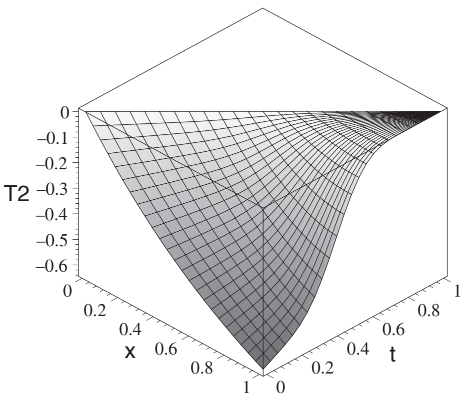

Figure 14: Taylor solution of the two phases Stefan problem in original domain $T_2(x, t)$

4 Concluding Remarks

The results presented in this paper for the Stefan problem, as an example for parabolic partial differential equation with a moving boundary, show that the the one and two phases case are flat and the Taylor series expansion of the temperature profile are equal to the numerical solution. Thus the presented method seems to be a suitable new approach to determine the flat output and for calculating the input variables and the temperature profile. The solution was achieved only in the time domain and no operational calculus was needed.

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