
Modelling and Simulation of Ice/Snow Melting

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Group 4

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Abstract

A moving boundary problem, the so-called *Stefan Problem*, for the melting of ice is set up, then solved numerically using MATLAB[®]. Thereby curves for the position of the boundary between ice and water are produced. From these curves the melting time for a given layer thickness of ice/snow can be found. Furthermore, such curves are also presented when salt is added to the ice. It is seen that the melting time decreases substantially when salt is added.

Preface

The present paper is the result of a project in connection with the 22nd ECMI modelling week in Eindhoven, The Netherlands, 17–24 August 2008. The task as presented by the instructor Trond Kvamsdal from NTNU in Norway was to

- (i) model the melting of snow/ice in general and
- (ii) model the effect of adding salt to the ice/snow.

Regarding step (i) the simplest such model is a so-called *one-phase Stefan problem* – a moving boundary problem which is explained in Chapter 2; step (ii) is twofold: salt can either speed up the melting process – this is where the concept of freezing point depression enters – or it can be used to harden the ice surface. However, we have looked at the first aspect only, since the second aspect requires more thermodynamical knowledge than any of us (i.e. the group members) had beforehand – and would be able to achieve in the four days we had for effective work. The concept of freezing point depression that was mentioned above is explained in Chapter 3.

After the one-phase Stefan problem and the concept of the freezing point depression have been established, numerical simulations are carried out in Chapter 4, both for melting in general and in particular for melting with salt present.

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1 Introduction

About 70 % of the earth's surface are covered with water. This water is found in three states, or phases: liquid, which is what we see in lakes, rivers and oceans; solid, which is ice/snow; gas, which is water vapour.

If we have liquid water at a temperature of 0°C , it gradually becomes solid, i.e. it *freezes* to ice; on the contrary, if we have ice, it gradually becomes liquid at the afore-mentioned temperature, i.e. it *melts* to liquid. We say that the melting temperature for ice, respectively the freezing temperature for water, is 0°C .

In this paper we examine the melting of ice through a mathematical model called *the Stefan problem*, which is a so-called *boundary moving problem*. This problem is established in Chapter 2 and solved numerically in Chapter 4. In Chapter 3 the effect on the freezing/melting process of adding salt to water is explained.

2 The Mathematical Model of Phase Change Processes

Before we derive a mathematical model for the melting process, we have to discuss the underlying important physical properties and assumptions. Those will be examined in §2.1. Afterwards we review in §2.2 the heat equation as crucial basis for our mathematical model. In §2.3 we derive the two- and one-phase Stefan problem, which is the mathematical foundation of this paper. More discussions and derivations on this matter can be found in [1, 6].

2.1 Physical properties and assumptions

In order to set up a mathematical model we need to have a clear picture of the underlying assumptions. Since this study concerns phase change processes, our model will involve physical properties for each phase. We restrict ourselves to melting processes and hence consider a material in a liquid and a solid phase separated by an interface. For simplification we assume the density ρ to be constant, which is a necessary but slightly unreasonable assumption. For more realistic cases with $\rho_L \neq \rho_S$ (with the subscripts denoting *liquid* and *solid*, respectively) we refer to [1, Section 2.3]. Our phase change material also has a constant melting temperature T_M and latent heat L . The important case of a melting temperature that varies will also be explained later when we discuss the effect of the melting point depression. Each phase has thermal conductivities k_L, k_S and specific heats c_L, c_S , which are phase-wise constant but with $k_L \neq k_S$ and $c_L \neq c_S$. Furthermore we assume that heat is transferred isotropically (i.e. equal in all directions) by conduction only and omit a possible heat transfer by convection or radiation. Also we consider neither supercooling effects, gravitational, elastic nor electromagnetic effects, but we will discuss the chemical effect when foreign particles (as salt) are added to the liquid phase. For the surface separating each phase we assume it to be sharp, planar, without surface tension and of zero thickness.

2.2 The heat equation

A basic quantity involved in heat conduction is the temperature which represents the molecular movement. It is measured in degrees Kelvin or Celsius. A material under constant pressure can absorb heat whose quantity is called enthalpy or thermal energy. The thermal energy per unit mass is denoted by e and per unit volume by E , measured in kJ/kg and kJ/m³, respectively. We consider a pure material under constant pressure without volume changes, then the absorbed heat is related to the change in the temperature by

$$de = c dT, \quad (2.1)$$

where c is the specific heat capacity. The heat flux \mathbf{q} is the amount of heat crossing a unit area per time and given by *Fourier's Law*,

$$\mathbf{q} = -k \nabla T, \quad (2.2)$$

where k is the thermal conductivity. Since we assume isotropic conduction, $k > 0$ is a scalar, otherwise k can be a tensor. The heat flux points in direction of the heat flow and is measured in kJ/(m·K). The *First Law of Thermodynamics* in differential form gives us the *Energy Conservation Law*,

$$\frac{\partial}{\partial t}(\rho e) + \nabla \cdot \mathbf{q} = f, \quad (2.3)$$

where the function f represents either a heat sink or a heat source. Inserting (2.1) and (2.2) in (2.3) leads to the *Heat Conduction Equation*

$$\rho c \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + f. \quad (2.4)$$

This is a partial differential equation (PDE) which is satisfied by a temperature distribution $T(\mathbf{x}, t)$. In order to have a well-posed problem in a domain Ω for $t > 0$ we have to combine the PDE (2.4), which holds in the interior of Ω , with

$$(i) \text{ an initial condition } T(\mathbf{x}, 0) = T_{\text{init}}(\mathbf{x}), \quad \forall \mathbf{x} \in \Omega, \text{ and} \quad (2.5)$$

$$(ii) \text{ boundary conditions for } T(\mathbf{x}, t), \quad \forall \mathbf{x} \in \partial\Omega, \quad t > 0. \quad (2.6)$$

Some common boundary conditions for (2.6) will be considered later. In §2.1 we imposed a constant thermal conductivity k and therefore introduce the thermal diffusivity,

$$\alpha = \frac{k}{\rho c}, \quad (2.7)$$

which is measured in m²/s. Hence, Eq. (2.4) can be written as the *Heat Equation*,

$$\frac{\partial T}{\partial t} = \alpha \nabla^2 T + f, \quad (2.8)$$

which is a linear parabolic PDE. We may restrict ourselves to the one-dimensional case, i.e. $\Omega = [0, \infty)$, without any heat sink or source, i.e. $f = 0$. Then Eq. (2.8) transforms to

$$T_t = \alpha T_{xx}, \quad (2.9)$$

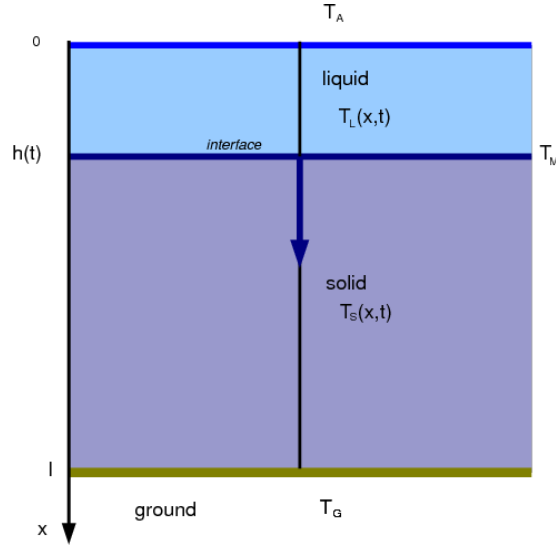


FIG. 2.1: Liquid and solid phases with interface $h(t)$ and imposed boundary temperatures.

where T_t and T_{xx} denote the second temporal derivative and the second spatial derivative, respectively. Common boundary conditions (2.6) for the case $\Omega = [0, \infty)$ are for instance an *imposed temperature*,

$$T(0, t) = T_0(t) \text{ and } \lim_{x \rightarrow \infty} T(x, t) = T_\infty(t), \quad (2.10)$$

or an *imposed flux*

$$-kT_x(0, t) = q_0(t) \text{ and } -k \lim_{x \rightarrow \infty} T_x(x, t) = q_\infty(t). \quad (2.11)$$

Other possibilities are a convective or radiative flux (see [1, Chapter 1.2.D]).

2.3 The classical Stefan problem

For our melting process we divide the domain Ω into a liquid and a solid phase separated by an interface $h(t)$, see FIG. 2.1, which illustrates the model we use in the following. As simplification we consider the phase change process in a one-dimensional region $\Omega = (0, l)$ of a cross-sectional area A , i.e. a slab of ice with length l . On the upper boundary we impose a temperature $T_A > T_M$ and on the lower boundary a temperature T_G (the subscripts A and G denote *air* and *ground*, respectively). The liquid phase in the subregion $0 < x < h(t)$ is separated by the sharp interface $h(t)$ from the solid phase in the subregion $h(t) < x < l$. Both phases have their own temperature distributions $T_L(x, t)$ and $T_S(x, t)$. Hence we have a heat equation (2.9) for both phases:

$$\begin{aligned} T_t &= \alpha_L T_{xx} \text{ for } 0 < x < h(t) \text{ (liquid phase),} \\ T_t &= \alpha_S T_{xx} \text{ for } h(t) < x < l \text{ (solid phase),} \end{aligned}$$

where we used as simplification the same symbolic $T(x, t)$ for both phases and $\alpha_L = k_L/\rho c_L$, $\alpha_S = k_S/\rho c_S$. To derive a condition for the interface we consider

the total enthalpy, referred to the melt temperature T_M ,

$$E(t) = A \left[\int_0^{h(t)} \{ \rho c_L (T(x, t) - T_M) + \rho L \} dx + \int_{h(t)}^l \rho c_S (T(x, t) - T_M) dx \right], \quad (2.12)$$

with L as the latent heat of the material. Applying Leibniz's integral rule to (2.12) leads to

$$\begin{aligned} \frac{1}{A} \frac{dE}{dt} &= \rho c_L (T(h(t), t) - T_M) \cdot h'(t) + \int_0^{h(t)} \rho c_L T_t(x, t) dx \\ &\quad + \rho L h'(t) - \rho c_S (T(h(t), t) - T_M) \cdot h'(t) + \int_{h(t)}^l \rho c_S T_t(x, t) dx. \end{aligned} \quad (2.13)$$

Since we impose $T(h(t), t) = T_M$, Eq. (2.13) becomes

$$\frac{1}{A} \frac{dE}{dt} = \int_0^{h(t)} \rho c_L T_t(x, t) dx + \rho L h'(t) + \int_{h(t)}^l \rho c_S T_t(x, t) dx \quad (2.14)$$

and by substituting the heat equation (2.9) for each phase we get

$$\frac{1}{A} \frac{dE}{dt} = k_L T_x(h(t), t) - k_L T_x(0, t) + \rho L h'(t) + k_S T_x(l, t) - k_S T_x(h(t), t).$$

The terms $-k_L T_x(0, t)$ and $k_S T_x(l, t)$ can be considered as the heat fluxes $q(0, t)$ and $-q(l, t)$ through the boundary of Ω . Furthermore, we can use the global heat balance, which states that the heat change is the difference between incoming and outgoing heat, to retrieve

$$\frac{dE}{dt} = A [q(0, t) - q(l, t)].$$

Altogether, (2.14) simplifies to the one-dimensional *Stefan Condition*,

$$\rho L h'(t) = k_S T_x(h(t), t) - k_L T_x(h(t), t), \quad (2.15)$$

which expresses that the velocity $h'(t)$ of the interface $h(t)$ is proportional to the jump of the heat flux across the interface. This enables us to describe a mathematical model for a phase change process with the assumptions of section §2.1.

We consider a slab $0 < x < l$ of a material which is initially solid at an initial temperature $T_{\text{init}} < T_M$. Since we impose a higher temperature $T_A > T_M$ at $x = 0$ melting occurs. At $x = l$ we assume a temperature T_G . For each $t > 0$ the liquid occupies $[0, h(t))$ and the solid $(h(t), l]$, respectively. The interface location is denoted by $h(t)$. This leads to the *two-phase Stefan problem*, where we have to find a temperature distribution $T(x, t)$ in $[0, l] \times (0, \infty)$ and a interface location $h(t)$ for $t > 0$ that satisfy

(i) Heat equations:

$$\begin{aligned} T_t &= \alpha_L T_{xx} \text{ for } 0 < x < h(t), \quad t > 0, \\ T_t &= \alpha_S T_{xx} \text{ for } h(t) < x < l, \quad t > 0. \end{aligned} \quad (2.16)$$

(ii) Interface conditions:

$$\begin{aligned} T(h(t), t) &= T_M \text{ for } t > 0, \\ \rho L h'(t) &= k_S T_x(h(t), t) - k_L T_x(h(t), t) \text{ for } t > 0. \end{aligned} \quad (2.17)$$

(iii) Initial conditions:

$$\begin{aligned} h(0) &= 0 \text{ (material initially solid),} \\ T(x, 0) &= T_{\text{init}} < T_M \text{ for } 0 \leq x \leq l. \end{aligned} \quad (2.18)$$

(iv) Boundary conditions:

$$\begin{aligned} T(0, t) &= T_A > T_M \text{ for } t > 0, \\ T(l, t) &= T_G < T_M \text{ for } t > 0. \end{aligned} \quad (2.19)$$

Note that the second equation in (2.18) can be substituted by $-k_S T_x(l, t) = 0$ for $t > 0$ to include a insulated boundary at $x = l$.

This one-dimensional *classical Stefan problem* is a famous example of a *moving boundary problem*. Such problems arise also in the mathematical modelling of solidification processes, combustion, flows through porous media and molecular diffusions to name at least a few. Generalisations to multidimensional cases can be found in [6]. If we neglect the assumption $\rho_L = \rho_S$ and consider the case $\rho_L > \rho_S$ for water and ice, the former occupies less volume than the latter. Therefore a void between the boundary $x = 0$ and a second interface $s(t)$ is formed through the melting process. More details on this matter can be found in [1, Section 2.3.D]. A common simplification to the two-phase Stefan problem is to assume that the slab is initially solid at the melt temperature $T_{\text{init}} = T_M$, which implies that only one phase is considered as active. Since the boundary at $x = l$ is not important anymore, we can consider the slab as semi-infinite and hence the domain Ω is $[0, \infty)$. This leads to the *one-phase Stefan problem* which is solved by a temperature distribution $T(x, t)$ and an interface location $h(t)$ that fulfil the following:

$$\begin{aligned} T_t &= \alpha_L T_{xx} \text{ for } 0 < x < h(t), \ t > 0, \\ T(h(t), t) &= T_M \text{ for } t > 0, \\ \rho L h'(t) &= -k_L T_x(h(t), t) \text{ for } t > 0, \\ h(0) &= 0, \\ T(0, t) &= T_A(t) > T_M \text{ for } t > 0. \end{aligned} \quad (2.20)$$

This is the type of problem we will use from now on throughout this paper, but we will include a changing melt temperature T_M by the effect of the melting point depression, which will be explained in the following.

3 Why Salt Melts Ice

Combining ice and salt produces a remarkable reaction that is important both for hardening of snow surfaces and for melting of ice on roads by adding salt. To understand this phenomenon we first need to take a closer look at a plain



FIG. 3.1: *Left:* Melting of ice on roads. *Right:* Hardening of snow surfaces. *Source:* 22nd ECMI Modelling Week, presentation by Trond Kvamsdal.

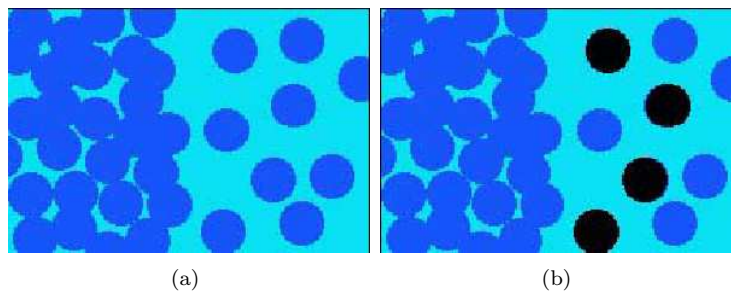


FIG. 3.2: *Left:* Ice-water mixture. *Right:* Ice-water mixture with salt. *Source:* <http://www.waynesthisandthat.com/saltice.html>.

ice-water mixture.

In FIG. 3.2(a) the densely packed blue spheres on the left represent water molecules solidified into ice; the looser spheres on the right are water molecules. Ice consists of water molecules locked in a crystalline structure. Liquid water consists of free water molecules randomly moving around in all directions.

Assuming there are no outside sources of heat or cold, the ice and water will be in equilibrium (0°C). However, this does not mean that everything is static. Every once in a while a free-swimming water molecule will collide with an ice molecule and thus gives the ice molecule sufficient energy to break away from the ice block. This free water molecule has a certain amount of energy stored in the form of kinetic energy. After the collision, the original free-swimming molecule will move slower and therefore has less energy. The difference between the amount of energy it had before and after the collision is same as the amount of energy it took to break the frozen ice molecule free. The temperature of water is a measure of how fast the average water molecule is moving. The hotter the water, the faster the molecules are moving. When the water molecule collided with the ice and hence slowed down, it can now

be thought of as being cooler. If this happens to enough water molecules the water as a whole will get cooler.

On the other side, free-swimming water molecules can collide with the ice in a way that causes them to stick to it, or freeze. In doing so, they release energy to the water/ice mixture from their loss of kinetic energy and the energy released as they create a molecular bond with the ice. This energy goes into the remaining water, making the molecules travel faster and hence heating the water up.

In a stable mixture of water and ice the rate of ice molecules being broken free (and taking energy from the mixture) and water molecules freezing to ice (and giving up energy to the mixture) is the same, so that over time both the amount of water and ice and the temperature (a measure of the kinetic energy in the system) is constant.

Now let us assume that we want to melt ice on a driveway. One can sprinkle a little salt on it and the ice starts to melt. What happens? In FIG. 3.2(b) we have the same water-ice mixture as we had in the first picture, except this time salt (black spheres) has dissolved into the water and displaced some of the water molecules. Because the salt molecules have replaced some of the water molecules, there are less water molecules left to collide with the ice. The result is, that there are more ice molecules melting than there are water molecules freezing. Because the salt is not used up in this process the melting continues. This is why only a little salt is needed to melt a lot of ice.

One curiosity about this process is that the melting ice is actually colder than it was before the salt was added. We take advantage of this phenomenon to harden snow surfaces or to make ice cream at home.

3.1 Calculation of the melting point depression

The *melting point* of a solid is the temperature range at which it changes state from solid to liquid. For most substances (e.g. water) melting and freezing points are essentially equal. The melting point is relatively insensitive to pressure because the solid-liquid transition represents only a small change in volume. The melting point of a pure substance is always higher than the melting point of an impure substance. The more impurity is present, the lower the melting point.

Melting point depression describes this phenomenon that the melting point of a liquid (the solvent) is depressed when another compound (the solute) is added, meaning that a solution has a lower melting point than a pure solvent. The melting point depression $\Delta T_f (= T_{f(\text{pure solvent})} - T_{f(\text{solution})})$ for the solvent is proportional to the molality m_B of the solute:

$$\Delta T_f = K_f \cdot m_B.$$

The value K_f is called the *cryoscopic constant*, depending only on the solution and not on the solute. For water $K_f = 1.86 \text{ (K}\cdot\text{kg)/mol}$, which means that the melting point is decreased by 1.86°C if one adds one mole of a solute to one kilogram of water. It can be calculated as

$$K_f = R \frac{T_M^2}{\Delta H_f},$$

where

- R is the gas constant (8.314 472 J/(mol·K)),
- T_M is the melting point of the pure solvent in K and
- ΔH_f is the heat of fusion of the solution in J/kg.

m_B is the molality of the solution, calculated by taking dissociation into account since the melting point depression is a colligative property, dependent on the number of particles in solution. This is most easily done by using the *van't Hoff factor*, i , as

$$m_B = i \cdot m_{\text{solute}}.$$

The factor i accounts for the number of individual particles (typically ions) formed by a compound in solution. Examples of values of i are:

- $i = 1$ for sugar in water;
- $i = 2$ for sodium chloride (cooking salt) in water, due to dissociation of NaCl into Na^+ and Cl^- ;
- $i = 3$ for calcium chloride in water, due to dissociation of CaCl_2 into Ca^{2+} and 2Cl^- ;
- $i = 2$ for hydrogen chloride in water, due to complete dissociation of HCl into H^+ and Cl^- .

Finally, $m_{\text{solute}} = \frac{m}{M}$, where m is the solute in gram per 1.0 kg solvent and M the molar mass of the solvent.

3.1.1 Example

We want to solubilize 58.44 g of cooking salt (NaCl) in 0.5 kg of water. m calculates to:

$$m = \frac{58.44 \text{ g}}{0.5 \text{ kg}} = 116.88 \text{ g/kg}.$$

This means we have 116.88 g of salt per 1 kg of water. The molar mass of salt is 58.44 g/mol, so we get

$$m_{\text{solute}} = \frac{116.88 \text{ g/kg}}{58.44 \text{ g/mol}} = 2 \text{ mol/kg}.$$

m_B is then $2 \cdot m_{\text{solute}} = 4 \text{ mol/kg}$ (since $i = 2$ for NaCl), so in summary we get:

$$\Delta T = K_f \cdot m_B = 1.86 \text{ (kg·K)/mol} \cdot 4 \text{ mol/kg} = 7.44 \text{ K}.$$

4 Solution of The Stefan Problem

After we have derived the moving boundary problem (2.20) we now set out to solve the problem. In the present chapter we first show that a given analytical expression solves the problem, then we set up a numerical model which is solved with the use of MATLAB[®].

To set the record straight, let us first state the problem (2.20) once more. We have the heat equation,

$$T_t = \alpha T_{xx}, \quad 0 \leq x \leq h(t), \quad t > 0, \quad (4.1)$$

subject to boundary conditions

$$T(0, t) = T_A, \quad T(h(t), t) = T_M, \quad \forall t > 0. \quad (4.2)$$

Furthermore, we have the Stefan condition, which governs the position of the moving boundary:

$$h'(t) = -\beta T_x(h(t), t), \quad (4.3)$$

where $\beta = k_L/(\rho_L L)$.

Now we have stated the problem the next step is show that a given analytical expression solves the problem. This is done in the next section, §4.1. In §4.2 a numerical model is set up and solved/analyzed in §4.3.

4.1 Analytical solution of the Stefan problem

If the initial boundary position is

$$h(0) = h_0 \quad (4.4)$$

and the initial temperature distribution is

$$T(x, 0) = \begin{cases} T_A - \Delta T_L \frac{\operatorname{erf}\left(\frac{x}{2\sqrt{\alpha t_0}}\right)}{\operatorname{erf}(\lambda)}, & 0 \leq x \leq h_0, \\ T_M, & x > h_0, \end{cases} \quad (4.5)$$

where $\operatorname{erf}(x) = \frac{2}{\sqrt{\pi}} \int_0^x \exp(-s^2) ds$, λ is the solution of the equation

$$\lambda \exp(\lambda^2) \operatorname{erf}(\lambda) = \frac{c_L \Delta T_L}{L\sqrt{\pi}} \quad (4.6)$$

and $t_0 = h_0^2/(4\lambda^2\alpha)$, then the solution of the Stefan problem is:

$$h(t) = 2\lambda\sqrt{\alpha(t+t_0)} \quad (4.7)$$

$$T(x, t) = \begin{cases} T_A - \Delta T_L \frac{\operatorname{erf}\left(\frac{x}{2\sqrt{\alpha(t+t_0)}}\right)}{\operatorname{erf}(\lambda)}, & 0 \leq x \leq h(t), \\ T_M, & x > h(t). \end{cases} \quad (4.8)$$

In the following the solution (4.7)–(4.8) to the problem (4.1)–(4.3) is verified.

We can see by substituting $t = 0$ that the given functions (4.8) and (4.7) satisfy the initial conditions (4.5) and (4.4). Also, since $\operatorname{erf}(0) = 0$, (4.8) satisfies the boundary conditions (4.2). We have yet to show that (4.7) and (4.8) satisfy the differential equations (4.1) and (4.3).

Differentiating (4.8) wrt. time yields:

$$\frac{\partial T}{\partial t}(x, t) = -\frac{\Delta T_L}{\operatorname{erf}(\lambda)} \frac{2}{\sqrt{\pi}} \frac{\partial}{\partial t} \int_0^{\frac{x}{2\sqrt{\alpha(t+t_0)}}} \exp(-s^2) ds$$

With a change of variable $w = \frac{x^2}{4\alpha s^2} - t_0$ we have:

$$\int_0^{\frac{x}{2\sqrt{\alpha(t+t_0)}}} \exp(-s^2) ds = -\frac{1}{2} \int_{\infty}^t \frac{x}{\sqrt{4\alpha}} (w+t_0)^{-3/2} \exp\left(-\frac{x^2}{4\alpha(w+t_0)}\right) dw$$

and since for any C :

$$\frac{\partial}{\partial t} \int_C f(w) dw = f(t), \quad (4.9)$$

we have:

$$\frac{\partial T}{\partial t}(x, t) = \frac{\Delta T_L}{\operatorname{erf}(\lambda)} \frac{1}{2\sqrt{\pi}} \frac{x}{\sqrt{\alpha}} (t+t_0)^{-3/2} \exp\left(-\frac{x^2}{4\alpha(t+t_0)}\right).$$

Differentiating (4.8) wrt. x yields:

$$\frac{\partial T}{\partial x}(x, t) = -\frac{\Delta T_L}{\operatorname{erf}(\lambda)} \frac{2}{\sqrt{\pi}} \frac{\partial}{\partial x} \int_0^{\frac{x}{2\sqrt{\alpha(t+t_0)}}} \exp(-s^2) ds.$$

With a change of variable $u = s \cdot 2\sqrt{\alpha(t+t_0)}$ we have

$$\int_0^{\frac{x}{2\sqrt{\alpha(t+t_0)}}} \exp(-s^2) ds = \int_0^x \exp\left(-\frac{u^2}{4\alpha(t+t_0)}\right) \frac{1}{2\sqrt{\alpha(t+t_0)}} du.$$

Using (4.9) we have:

$$\frac{\partial T}{\partial x}(x, t) = -\frac{\Delta T_L}{\operatorname{erf}(\lambda)} \frac{1}{\sqrt{\pi}} \frac{1}{\sqrt{\alpha(t+t_0)}} \exp\left(-\frac{x^2}{4\alpha(t+t_0)}\right). \quad (4.10)$$

Differentiating with respect to x we have:

$$\frac{\partial^2 T}{\partial x^2}(x, t) = \frac{\Delta T_L}{\operatorname{erf}(\lambda)} \frac{1}{2\sqrt{\pi}} \frac{1}{\alpha} \frac{x}{\sqrt{\alpha}} (t+t_0)^{-3/2} \exp\left(-\frac{x^2}{4\alpha(t+t_0)}\right).$$

Now we see that

$$\frac{\partial^2 T}{\partial x^2}(x, t) = \frac{1}{\alpha} \frac{\partial T}{\partial t}(x, t),$$

which upon multiplication by α leads to the heat equation (4.1).

Then we check that the boundary moving differential equation (4.3) applies. First let us calculate the derivative of the temperature wrt. x on the boundary. Substitution of $x = h(t) = 2\lambda\sqrt{\alpha(t+t_0)}$ in (4.10) yields:

$$\frac{\partial T}{\partial x}(h(t), t) = -\frac{\Delta T_L}{\operatorname{erf}(\lambda)} \frac{1}{\sqrt{\pi}} \frac{1}{\sqrt{\alpha(t+t_0)}} \exp\left(-\frac{4\lambda^2(\alpha(t+t_0))}{4\alpha(t+t_0)}\right).$$

Since $h'(t) = (\lambda\alpha)/\sqrt{\alpha(t+t_0)}$, we have

$$\frac{\partial T}{\partial x}(h(t), t) = -\frac{\Delta T_L}{\operatorname{erf}(\lambda)} \frac{1}{\sqrt{\pi}} \frac{h'(t)}{\lambda\alpha} \exp(-\lambda^2)$$

By the definition (4.6) of λ we have:

$$\frac{\partial T}{\partial x}(h(t), t) = -\frac{\Delta T_L}{\frac{c_L \Delta T_L}{L\sqrt{\pi}}} \frac{1}{\sqrt{\pi}} \frac{h'(t)}{\alpha} = -\frac{L}{c_L \alpha} h'(t).$$

Substituting the definition of α, β we get:

$$\frac{\partial T}{\partial x}(h(t), t) = -\frac{L\rho_L}{k_L}h'(t) = -\frac{1}{\beta}\frac{\partial h}{\partial t}(t)$$

which upon multiplication by $-\beta$ gives us the boundary movement equation (4.3). Q.E.D.

An important special case of the initial distribution is $h(0) = 0$ and

$$T(x, 0) = \begin{cases} T_A, & x = 0 \\ T_M, & x > 0, \end{cases}$$

for which the results above also hold, see [1]. This corresponds the case with only ice in the beginning.

4.2 Numerical solution of the Stefan problem

We solve the Stefan problem numerically using the following algorithm; the algorithm takes the melting point depression into account. For each time step:

- (i) update the temperature distribution using Eq. (4.1),
- (ii) update the boundary state using Eq. (4.3) and
- (iii) update the melting point.

For steps (i) and (ii) the finite difference method (FDM) is used. For step (i) an implicit scheme is used:

$$\frac{T(x, t + \Delta t) - T(x, t)}{\Delta t} = \alpha \frac{T(x - \Delta x, t + \Delta t) - 2T(x, t + \Delta t) + T(x + \Delta x, t + \Delta t)}{(\Delta x)^2}. \quad (4.11)$$

In step (ii) an explicit method is used,

$$\frac{h(t + \Delta t) - h(t)}{\Delta t} = -\beta \frac{T(h(t), t) - T(h(t) - \Delta x, t)}{\Delta x}, \quad (4.12)$$

while step (iii) is calculated by the explicit formula for freezing point depression when necessary. Now we study these steps more carefully.

4.2.1 Temperature update step

Let our space discretization be $(0, \Delta x, 2\Delta x, \dots, N\Delta x)$ and at time t let $x_0 = n\Delta x$ be the greatest discretization point below $h(t)$, that is

$$x_0 = \max_{n\Delta x < h(t), n \in \mathbb{N}} n\Delta x.$$

Denote vector $\mathbf{T}(t) = [T_1(t) \cdots T_{N+1}(t)]^T$ as the temperature vector in discretization points: $\mathbf{T}(t) = [T(0, t) \cdots T(N\Delta x, t)]^T$. Now by (4.11) we have

$$\mathbf{T}(t + \Delta t) = \begin{bmatrix} T_A \\ T_2(t) + \alpha \frac{T_1(t+\Delta t) - 2T_2(t+\Delta t) + T_3(t+\Delta t)}{(\Delta x)^2} \\ \vdots \\ T_n(t) + \alpha \frac{T_{n-1}(t+\Delta t) - 2T_n(t+\Delta t) + T_{n+1}(t+\Delta t)}{(\Delta x)^2} \\ T_F \\ \vdots \\ T_M \end{bmatrix}.$$

By separating terms with $T(t)$ from terms with $T(t + \Delta t)$ and taking the coefficients in the front of the latter we get

$$\mathbf{T}(t + \Delta t) = \begin{bmatrix} T_A \\ T_2(t) \\ T_3(t) \\ \vdots \\ T_n(t) \\ T_F \\ \vdots \\ T_M \end{bmatrix} + \Delta t/h^2 \underbrace{\begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 \\ 0 & 1 & -2 & 1 \\ & & \ddots & \\ & & & 1 & -2 & 1 & 0 \\ & & & 0 & 0 & 0 & 0 \\ & & & & & \ddots & \\ & & & & & & 0 \end{bmatrix}}_{=\mathbf{A}} \begin{bmatrix} T_1(t + \Delta t) \\ T_2(t + \Delta t) \\ T_3(t + \Delta t) \\ T_4(t + \Delta t) \\ \vdots \\ T_{n-1}(t + \Delta t) \\ T_n(t + \Delta t) \\ T_{n+1}(t + \Delta t) \\ T_{n+2}(t + \Delta t) \\ \vdots \\ T_{N+1}(t + \Delta t) \end{bmatrix}.$$

As we denote the coefficient matrix as \mathbf{A} , we have:

$$(\mathbf{I}_{N+1} - \mathbf{A})\mathbf{T}(t + \Delta t) = [T_A \quad T_2(t) \quad T_3(t) \quad \dots \quad T_n(t) \quad T_M \quad \dots \quad T_M]^T$$

from which we have the update step algorithm:

$$\mathbf{T}(t + \Delta t) = (\mathbf{I}_{N+1} - \mathbf{A})^{-1} [T_A \quad T_2(t) \quad T_3(t) \quad \dots \quad T_n(t) \quad T_M \quad \dots \quad T_M]^T.$$

4.2.2 Boundary moving step

Let our space discretization be $(0, \Delta x, 2\Delta x, \dots, N\Delta x)$ and at time t let $x_0 = n\Delta x$ be the greatest discretization point below $h(t)$ as in the previous section. We approximate the derivative $T_x(h(t), t)$ as the finite difference between $x_0 - \Delta x$ and x_0 :

$$T_x(h(t), t) \approx \frac{T(x_0, t) - T(x_0 - \Delta x, t)}{\Delta x} = \frac{T_{n+1}(t) - T_n(t)}{\Delta x}.$$

Thus, by (4.12), our update step algorithm is

$$h(t + \Delta t) = h(t) - \beta \frac{T_{n+1}(t) - T_n(t)}{\Delta x} \Delta t.$$

The motivation for using the two last discretization points as finite difference interval points instead of a boundary point and the last discretization point is discussed in §4.3.1.

4.2.3 Melting point update step

The amount of dissolved substance affects the melting point of the solution as presented in Chapter 3. Combining the equations $\Delta T_f = T_{f(\text{pure solvent})} - T_{f(\text{solution})}$, $\Delta T_f = K_f \cdot m_B$, $K_f = RT_M^2/\Delta H_f$ and $m_B = i \cdot m_{\text{solute}}$, we have:

$$T_{\text{solution}} = T_{f(\text{pure solvent})} - K_f \cdot i \cdot m_{\text{solute}},$$

where $K_f = 1.86 \text{ (kg}\cdot\text{K)}/\text{mol}$, i is the number of individual ions in a salt compound and m_{solute} is the molality of solute in the solution, that is the fraction of the amount of substance of solute by the mass of solution. In this simulation we assume that there is a constant amount of substance of solute per unit area (n_A) and that the solute is always uniformly distributed in the current liquid phase. Furthermore we make the approximation that the density of the solution, $\rho = 1000 \text{ kg}/\text{m}^3$, is constant with respect to time and space regardless the amount of substance of solute in water. Since $V_{\text{solution}}(t) = A_{\text{solution}}h(t)$, we have at time t :

$$m_{\text{solute}}(t) = \frac{n_{\text{solute}}}{m_{\text{solution}}(t)} = \frac{n_A A_{\text{solution}}}{\rho V_{\text{solution}}(t)} = \frac{n_A}{\rho h(t)}.$$

Thus we have an explicit formula for the melting point as a function of the boundary position $h(t)$:

$$T_{\text{solution}}(t) = T_{f(\text{pure solvent})} - \frac{K_f \cdot i \cdot n_A}{\rho h(t)},$$

which is recalculated for each time step.

4.3 Simulation

A solution to the Stefan problem with 1.5 cm water layer in the beginning and air temperature $T_A = 273 \text{ K}$ is looked for. The initial temperature distribution is supposed to obey equation (4.5). The considered space is $[0, 10 \text{ cm}]$, which is divided to N parts of same length. Time scale is logarithmic, so that the time step size is small in the beginning and large in the end.

First the effect of the number of space discretization parts N is analyzed. The time step length is set to start from 10^{-5} s and end at 1 s, so that the observed time scale will be from 0 s to about 900 s. The Stefan problem is solved numerically using different space discretization numbers, N , ranging from 15 to 1500. FIG. 4.1 shows the approximate L^2 error between the analytical solution and the numerical solution with different space discretization numbers.

The slope of the logarithmic error by logarithmic space discretization number is $-1.0379 \approx -1$. Thus an empirical convergence rate $\text{Error}_{L^2} \approx C/N$ is derived. It is clear that also the time step size affects to the accuracy of the numerical solution, but that effect is not discussed in this work.

Next the effect of the melting point to the melting time is analyzed. Here a coarser time discretization is used: the time step varies from 10^{-1} s in the beginning to 10^2 s in the end. In FIG. 4.2 curves of boundary position as function of time have been plotted. We see that the smaller the melting point of ice is, the quicker is the melting process.

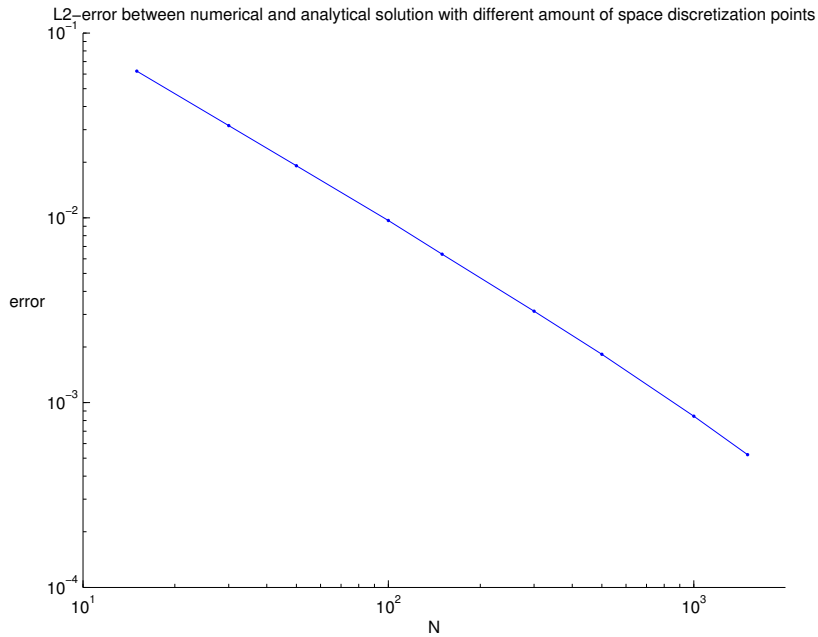


FIG. 4.1: Error of numerical solution as a function of number of space discretization points.

Next the effect of actually adding salt to the water in the beginning of the melting process is studied. Suppose we have sodium chloride or calcium chloride as a salt, say 10 mol per square metre of water. It is supposed that all added salt is soluted to the current water layer, so the molality of solute varies over time, depending on the height of the water layer. FIG. 4.3 shows the curves of boundary positions. We can see that the melting speed is first much higher when using salt, but by time the effect of salt gets smaller. In this simulation a 0.5 cm starting layer of water has been used with the 10 cm space discretized to 500 parts. The same time discretization and air temperature as in the simulation before has been used.

4.3.1 Analysis of the choice of finite difference points

In our numerical solution we have found some severe stability issues that have to be taken care of. One of them is the choice of discretization points used in the calculation of the finite difference in the boundary moving step. The most natural choice for the space discretization points would be the boundary value and the one before the boundary, but as one can see in FIG. 4.4, this choice leads to unstable values of the derivative of T with respect to x . Therefore the two last discretization points before the boundary have been used in simulations to approximate the derivative.

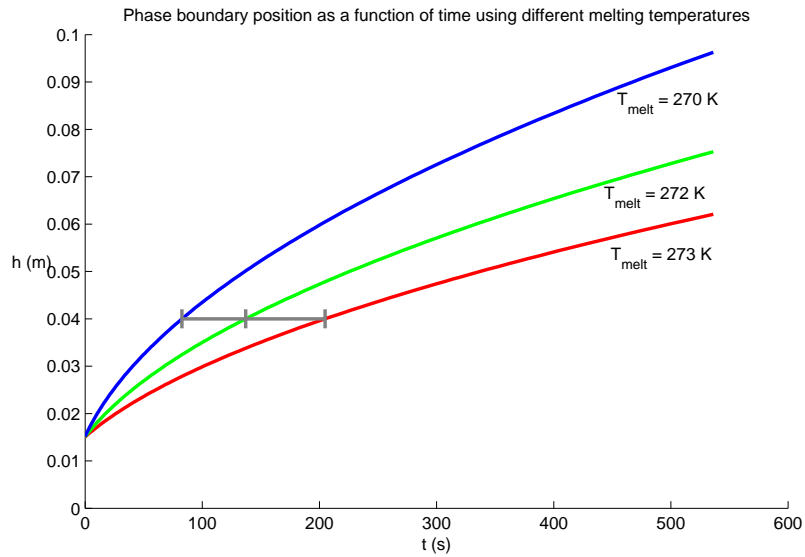


FIG. 4.2: Melting curves for different melting points

5 Conclusion

The classical Stefan problem for the modelling of melting of ice has been derived. Before it was solved, however, it was simplified to a one-phase problem such that only one phase of water and ice is considered as active in the melting process. A numerical model for this simplified problem is then set up, with the concept of melting point depression incorporated. The problem is then solved using MATLAB[®]. The main results are seen in FIG. 4.2 and FIG. 4.3.

As indicated in FIG. 4.2, if we take a layer of ice of thickness 4 cm, then it takes about 80 s to melt the ice with a melting temperature of 270 K; with a melting temperature of 272 K and 273 K, respectively, it takes about 140 s and about 200 s resp.

The melting curves, i.e. the position of the boundary between ice and water, both with and without salt added are seen in FIG. 4.3. If we again take a 4 cm thick layer of ice, then we see that with no salt it takes about 225 s to melt the ice; with NaCl resp. CaCl₂ added it takes about 125 s and about 100 s, resp.

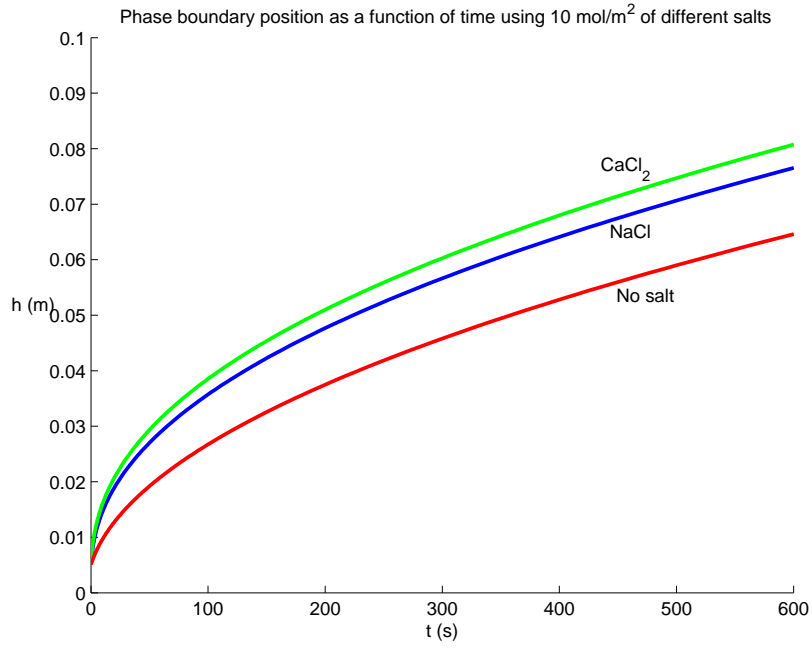


FIG. 4.3: Melting curves for systems with solutes of different salts

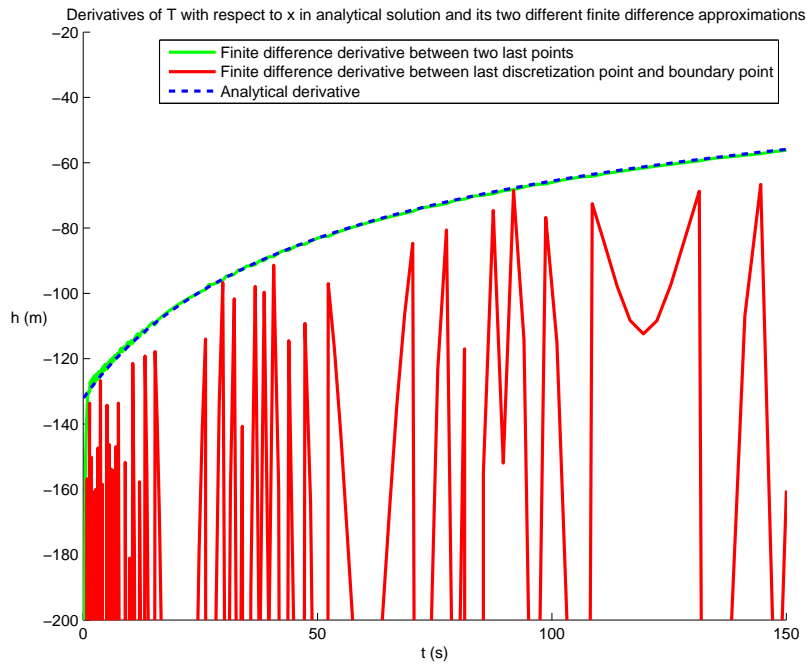


FIG. 4.4: Derivative of temperature with respect to time and its numerical approximations.

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