Analysis of the Stefan Problem: A boundary value problem with a phase boundary moving with time

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(source: http://www.msnbc.msn.com/id/44723746/ns/us_news-environment/t/canadas-arctic-ice-shelves-breaking-fast/#.ULUQZ3lYuQk)

Comment: In this picture of the Ward Hunt Ice shelf, we see a complex example of a moving phase boundary. With Climate Change being a serious issue, analysis of Stefan-type problems, will be crucial in both calculating the melting of artic ice, as well as energy storage in phase change materials such as salt hydrate for clean solar thermal energy.

Abstract: We consider a one-dimensional two-phase Stefan problem, modeling the melting of ice to liquid water. We analyze the error caused by the pseudo-steady state approximation of the temperature profile. The PSS approximation allows estimates for problems with no explicit analytical solution, such as with Newton cooling at the surface. The PSS approximation includes both linear and quadratic shaped temperature profiles.

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Introduction:

The Stefan problem is an example of a free boundary problem, modeling the temperature distribution in a homogenous material undergoing a phase transformation. The heat equation is solved with an intial temperature distribution and a boundary condition called the stefan condition, that conserves energy in and out of the boundary between the two phases.[1]

Joseph Stefan introduced this type of problem around 1890 while studying ice formation. In 1889 Stefan had a paper on ice formation in polar seas that drew attention from scientific community.[2] Stefan was born in Austria in 1835, and is most well known for the Stefan-Boltzmann law, which says that the energy radiated from a blackbody surface is proportional to the fourth power of the body's temperature.

Some background information necessary to understand this problem is the latent heat of fusion for phase changes. The main point to understand about latent heat is that the liquid phase has a higher internal energy than the solid phase. Energy is produced by a liquid when it freezes and consumed by a solid when it melts.[3]

Governing Equations:

We will now discuss the governing equations for the classical Stefan problem with two phases.
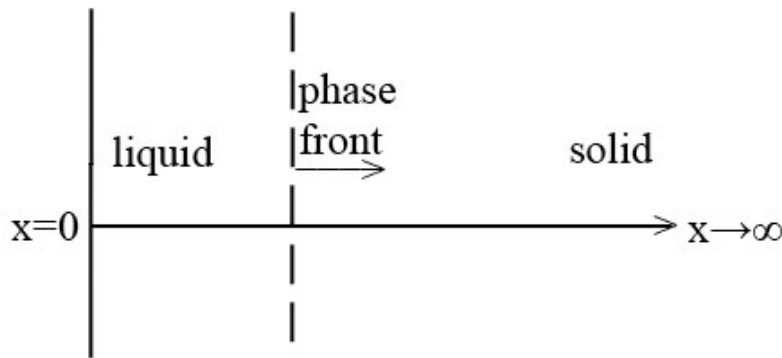
The problem setup consists of a semi infinite half plane, with a material initially solid and at the point of melting. When the surface temperature is rased, melting immediately takes place. Density is assumed to be constant for both phases, therefore no volume change with melting. Values for thermal conductivity, specfic heat, and latent heat of fusion are used.

$$T_L \geq T_1(x,t) \geq T_F \geq T_2(x,t) \geq T_S$$

Where T_L is the temperature at x=0, T_1 is the temperature distribution of the liquid, T_F is the melting temperature, T_2 the tempearture distribution of the ice, and T_S is the temperature of the ice as x goes to infinity.

$$X(0) = 0$$

Where X is the position of the phase boundary, initially at position x=0.

$$\rho_1 c_1 \frac{\partial T_1}{\partial t} = k_1 \frac{\partial^2 T_1}{\partial x^2} \qquad 0 < x < X(t)$$

This equation is for the transient heat condution of the liquid, is it valid from x=0 to x=X(t). Where ρ_1 c_1 and k_1 are the density, specific heat, and thermal conductivity of the liquid phase.

$$T_1(0,t) = T_L$$

This boundary condition says that the temperature T_1 at x=0 stays constant at T_L.

$$\rho_1 c_2 \frac{\partial T_2}{\partial t} = k_2 \frac{\partial^2 T_2}{\partial x^2} \qquad X(t) < x < \infty$$

This equation is for the transient heat condution of the solid, is it valid from x=X(t) to x goes to finity. Where c_2 and k_2 are the specific heat, and thermal conductivity of the solid phase. Density is constant for both phases, so ρ_1 is used in this equation.
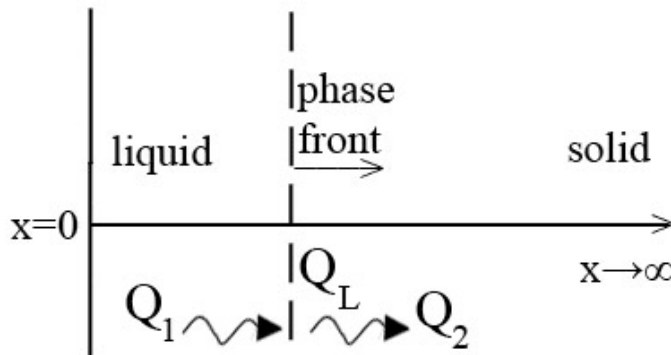
$$T_2(\infty,t) = T_S$$

This boundary condition says that the temperature T_2 at x goes to infinity stays constant at T_S.

$$T_1(X(t),t) = T_2(X(t),t) = T_F$$

This boundary condition says that the temperature T_1 and T_2 at x=X(t) stays constant at T_F.

Conserve thermal energy, using fouriers law, across the phase front, this is known as the stefan condition.

$$Q_1 - Q_2 - Q_L = 0$$

$$-k_1 \frac{\partial T_1(X(t),t)}{\partial x} + k_2 \frac{\partial T_2(X(t),t)}{\partial x} - \rho_1 L \frac{dX}{dt} = 0$$

The speed of the phase front is directly proportional to the jump in heat flux across the boundary.

Solution Methods:

Explicit Solution[4] –

There is an explicit analytical solution for a 2 phase stefan problem when the slab is initial at T_F (Carslaw and Jaeger 1959).

The phase front location is given by

$$X(t) = 2\lambda(\alpha t)^{1/2} \quad \text{where} \quad \alpha \quad \text{is the thermal diffusivity} \quad \alpha = \frac{k_1}{c_1 \rho_1}$$

λ is the root of the transcendental equation $\quad \lambda e^{\lambda^2} erf(\lambda) = St/\sqrt{\pi}$

This means that you need to find the value of λ that makes the left side equal to the right side of the equation.

$$St = c_1(T_L - T_F)/L$$

Is the stefan number, the ratio of sensible heat to latent heat.

$$T(x,t) = T_L - (T_L - T_F)erf(\frac{x}{2(\alpha t)^{1/2}})/erf(\lambda)$$

Is the solution for temperature distribution, where erf() is the error function, a special S-shaped function.

Pseudo Steady State Approximation[5] –

The pseudo steady state approximation is an analytic estimate that assumes the movement of the boundary is slower than the rate of diffusion. In other words the heat diffuses quickly and the distribution is assumed steady state, therefore linear. This allows us to neglect the time partial derivative in the diffusion equation. In the book 1-D Stefan Problems: An Introduction, they provide a derivation for this and other approximations, but the problem is normalized before the derivation, I choose to derive the same expressions, without any normalizing.

Our stefan condition becomes

$$-\frac{\partial T_1(X(t),t)}{\partial x} = \frac{\rho_1 L}{k_1}\frac{dX}{dt}$$

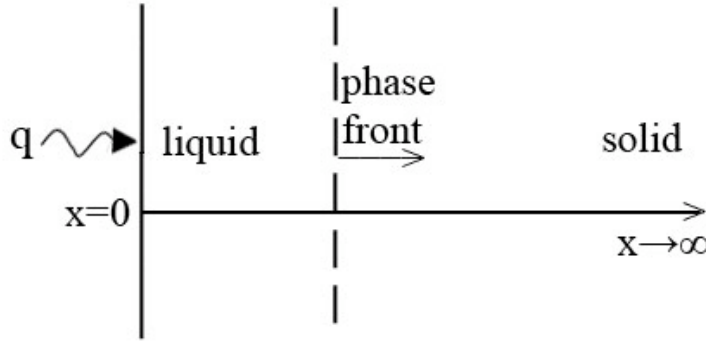because the $k_2\dfrac{\partial T_2(X(t),t)}{\partial x}$ term goes to zero since $T_2 = T_F$ for all x.

Our linear temperature distribution is

$$T_1(x,t) = T_L - x\left(\frac{T_L - T_F}{X(t)}\right)$$

When we combine and integrate we get an expression for the position of the phase front, X(t).

$$\frac{T_L - T_F}{X(t)} = \frac{\rho_1 L}{k_1}\frac{dX}{dt} \qquad \int dt = \frac{\rho_1 L}{(T_L - T_F)k_1}\int XdX \qquad X(t) = \sqrt{\frac{2t(T_L - T_F)k_1}{\rho_1 L}}$$

Pseudo Steady State Approximation with Newton Cooling at x=0 –

Now we will solve the same stefan problem, but instead of a constant temperature at boundary x=0, we will have a heat flux as determined by newton's law of cooling.

The boundary condition becomes

$$-k_1 \frac{\partial T_1}{\partial x}(0,t) = h[T_0 - T_1(0,t)]$$

Where T_0 is the temperature of the air.

Our linear temperature will now be of the form

$$T_1(x,t) = T_1(0,t) - x\left(\frac{T_1(0,t) - T_F}{X(t)}\right)$$

From these two equations we obtain

$$-\left(\frac{T_1(0,t) - T_F}{X(t)}\right) = \frac{h}{k_1}[T_1(0,t) - T_0]$$

and then

$$T_1(0,t) = \frac{\dfrac{T_F k_1}{X(t)h} + T_0}{1 + \dfrac{k_1}{X(t)h}}$$

Now combine the stefan condition, our linear temperature profile, and our expression for $T_1(0,t)$ and integrate.

$$\frac{\left(\dfrac{\dfrac{T_F k_1}{X(t)h} + T_0}{1 + \dfrac{k_1}{X(t)h}}\right) - T_F}{X(t)} = \frac{\rho_1 L}{k_1}\frac{dX}{dt}$$

$$\frac{(T_0 - T_F)h}{X(t)h + k_1} = \frac{\rho_1 L}{k_1}\frac{dX}{dt}$$

To accomplish this algebraic simplifcation in the above step I used symbolic variables and the simple() matlab function, in file max_plomer_heatmassmatlabcode2.m .

$$\frac{(T_0 - T_F)hk_1}{\rho_1 L} \int dt = \int (X(t)h + k_1) dX$$

$$\frac{(T_0 - T_F)hk_1}{\rho_1 L} t = \frac{1}{2} X(t)^2 h + k_1 X(t) + C \qquad \text{where C=0 because X(0)=0}$$

Note: for the case of black body radiation, the boundary condition at x=0 becomes

$$-k_1 \frac{\partial T_1}{\partial x}(0,t) = \sigma_1 E[T_0^{\ 4} - T_1(0,t)^4]$$

<u>Pseudo Steady State Approximation with Quadratic temperature profile</u> –

We assume a solution of the form

$$T_1(x,t) = T_F + A_1(t)(x - X(t)) + A_2(t)(x - X(t))^2$$

We take the boundary condition $T_1(X(t),t) = T_F$ and differentiate with respect to time, using the definiton of the total derivative. We obtain

$$\frac{\partial T_1}{\partial t}(X(t),t) + \frac{\partial T_1}{\partial x}(X(t),t)\frac{dX}{dt} = 0$$

From this equation, the stefan condition, and equation for heat conduction in liquid phase we obtain

$$\left(\frac{\partial T_1(X(t),t)}{\partial x}\right)^2 = \frac{L}{c_1}\frac{\partial^2 T_1}{\partial x^2}(X(t),t)$$

By taking the derivative of our quadratic solution form, $\dfrac{\partial T_1(X(t),t)}{\partial x} = A_1$ and

$\dfrac{\partial^2 T_1}{\partial x^2}(X(t),t) = 2A_2$, and subsituting into the above equation, we obtain an expression relating A_1 and A_2.

$$A_2 = \frac{c_1 A_1(t)^2}{2L}$$

Then we substiute this equation and the surface condition, $T_1(0,t) = T_L$, back into the quadratic solution form.

$$\frac{c_1}{2L} A_1(t)^2 X(t)^2 - A_1(t)X(t) + (T_F - T_L) = 0$$

Taking the negative root of the quadratic equation ensures $T \geq T_F$

$$A_1(t) = \left[1 - \sqrt{1 - 2\frac{c_1}{L}(T_F - T_L)}\right] \div \left(\frac{c_1}{L} X(t)\right)$$

Now we can obtain X(t) from the Stefan Condition and our expression for A_1, this is called Megerlin's Method.

$$A_1 = -\frac{\rho_1 L}{k_1}\frac{dX}{dt} \qquad \left[1 - \sqrt{1 - 2\frac{c_1}{L}(T_F - T_L)}\right]\int dt = -\frac{\rho_1 c_1}{k_1}\int X(t)dX$$

$$\left[1 - \sqrt{1 - 2\frac{c_1}{L}(T_F - T_L)}\right]t = -\frac{\rho_1 c_1}{2k_1}X(t)^2 + C \qquad \text{where C=0 because X(0)=0}$$

Enthalpy Method for Numerical Simulation[4] –

I also explored an enthalpy method for numerical simulation of the Stefan problem. The results are not presented here, I received a significant error as compared to the analytical solution. The Numerical method would over predict the phase front location by a factor of 2. Within the time frame of this paper I could not confirm whether this was due to a code error, parameter error (delta x, delta time), scheme error (perhaps semi implicit would work better), an issue with material properties (stefan number, thermal diffusivity), or an issue with determining location of phase front (more difficult because numerial solution contains a mushy zone while analytical doesn't). I would like to continue to debug and validate the code for this problem, presented in file max_plomer_heatmassmatlabcode_finiteelement.m, in future work.

The idea behind the numerical simulation is the enthalpy method, which conserves enthalpy between elements on a mesh.

Liquid has an enthalpy $h \geq L$ (L is latent heat)

Solid has an enthalpy $h \leq 0$

For thermal conductivity of material with enthalpy 0<h<L we use

k(h) = (k_1+k_2)/2   0<h<L

Relations between temperature and enthalpy

$$T = T_F + h/c_2 \qquad h \leq 0$$

$$T = T_F \qquad 0 < h < L$$

$$T = T_F + (h - L)/c_1 \qquad h \geq L$$

Conservation of energy and Fouriers Law

$$\rho\frac{\partial h}{\partial t} + \frac{\partial q}{\partial x} = 0 \qquad q = -k(h)\frac{\partial T}{\partial x}$$

The procedure provided in the phase transformations book is an explicit finite difference scheme.

$$\rho\big[h(x,t+\Delta t)-h(x,t)\big]/\Delta t+\big[q(x+\Delta x/2,t)-q(x-\Delta x/2,t)\big]=0$$

$$q(x+\Delta x/2,t)=-\big[k(x+\Delta x,t)+k(x,t)\big]\big[T(x+\Delta x,t)-T(x,t)\big]/(2\Delta x)$$

with stability requiring $\qquad \alpha\Delta t \le (\Delta x)^2/2$

Results:

PSSA Validation –

A matlab code was developed, file max_plomer_heatmassmatlabcode1.m, that calulates the error in X(t) for a given time for both the analytical and pseudo steady state approximation. Matlab function fzero() is used to find λ.

For the following parameters:

| Parameter	Value	Meaning	Units
c1	4.1818	heat capacity of water	J/(g*K) water at 20 deg C
Tl	300	temperature of liquid at x=0	K
Tf	273.15	temperature of melting	K
L	334	latent heat of fusion	J/g of water
k1	0.58	thermal conductivity of liquid water	W/(m*K)
rho1	0.99777e6	density (constant for both phases)	g/m^3

We found Error in X(t) = 4.98% for all time.

Which is an expected behavior, since both the analytical and PSSA solutions are functions of the square root of time. The PSSA solution is expected and does overpredict X(t) for a given time, since assuming steady state assumes more heat is transferred to the boundary.

Using error equation: $error = \dfrac{abs(S_1 - S_2)}{\max(S_1, S_2)}$

PSS vs PSS with Newton Cooling –

The values for the following graph are generated in file max_plomer_heatmassmatlabcode3.m, and then graphed in excel. Using same parameters as already mentioned.
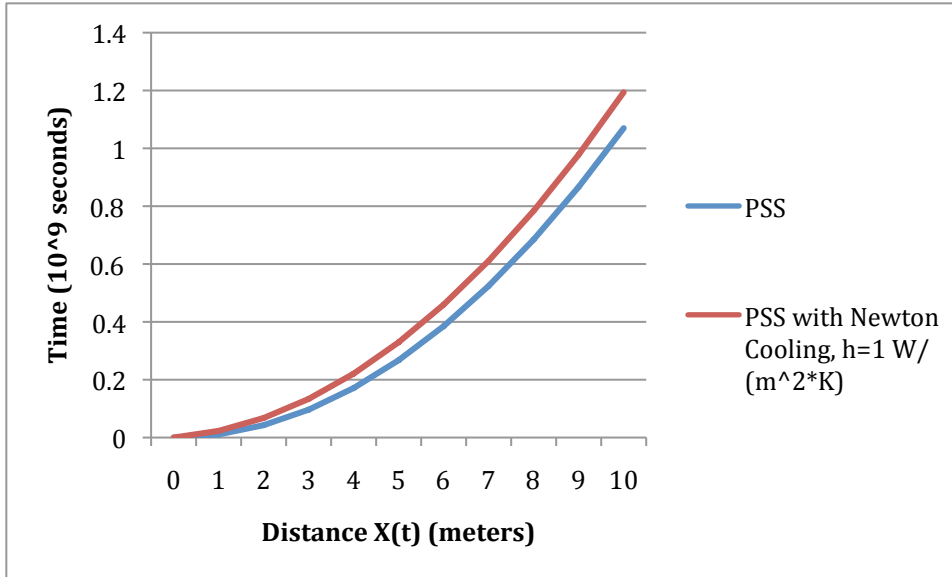
Comment: As expected the effect of newton cooling causes the phase change front to move more slowly.

PSS vs PSS with Quadratic Temperature Profile vs Analytical Solution –

The values for the following graph are generated in file max_plomer_heatmassmatlabcode4.m, and then graphed in excel. Using same parameters as already mentioned.
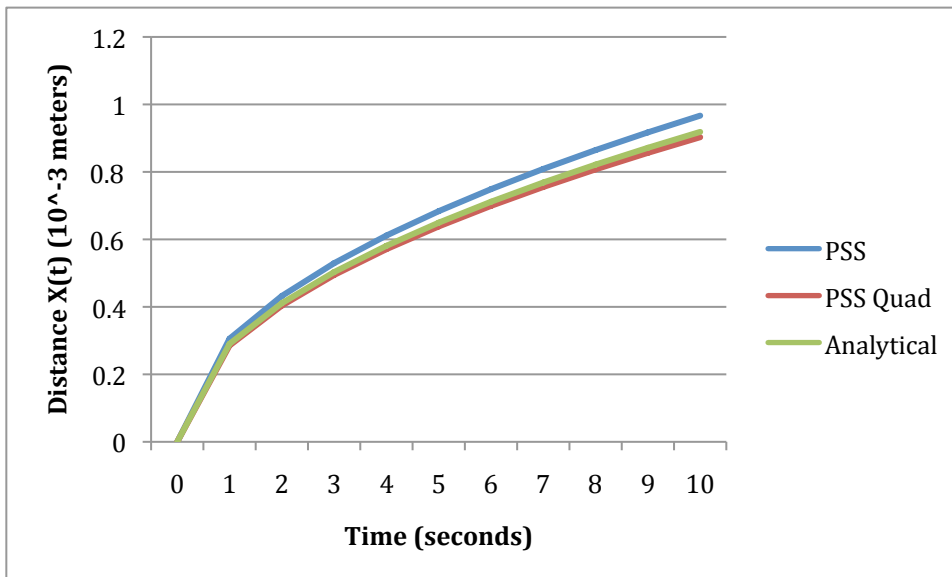
Comment: As expected the PSS solution is greater than the analytical, the PSS with quadratic approximation has much less error and is slightly less than the analytical solution.

Conclusion:

The PSSA method proved to be very useful in solving stefan problems.

The pseudo steady state approximation technique was validated and found to have an error of about 5% in position of the phase front at a given time for the given parameters.

Newton Cooling was added to the problem, which has no analytical solution, and the results compared to PSS without newton cooling agreed with the expected trend that newton cooling would slow the progress of the phase front.

Then we explored assuming the temperature distribution has a quadratic form. This greating increased accuracy, but also added a level of complexity. A next step would be finding a solution for newton cooling with a quadratic temperature distribution. And also do a linear combination of newton cooling and radiation heat transfer to get a more accurate model of artic sea ice.

In future work I would like to explore more finite difference methods for this problem, and also extend these principals to other problems than can be solved using a stefan type solution, such as energy storage in a solar thermal plant.

References:

1. http://en.wikipedia.org/wiki/Stefan_problem
2. http://ta.twi.tudeln.nl/nw/users/vuik/wi1605/opgave1/stefan.pdf
3. http://en.wikipedia.org/wiki/Enthalpy_of_fusion
4. Phase Transformations. Aifantis, Elias C. ; Gittus, John (1986)
5. One-dimensional Stefan problems: An introduc:on. Hill, J.M. (1987)

Descriptions of Matlab Files:

File	Description
max_plomer_heatmassmatlabcode1.m	calulates the error in X(t) for a given time for both the analytical and pseudo steady state approximation
max_plomer_heatmassmatlabcode2.m	simplifies the polynomial for the newton cooling pseudo-steady state aproximation stefan problem
max_plomer_heatmassmatlabcode3.m	compares X(t) for PSS, and PSS w/ newton cooling
max_plomer_heatmassmatlabcode4.m	compares the analytical stefan problem to the pseudo-steady state approximation, both linear and quadratic
max_plomer_heatmassmatlabcode_finiteelement.m	finite element stefan problem

	using the enthalpy method in book "Phase Transformations"