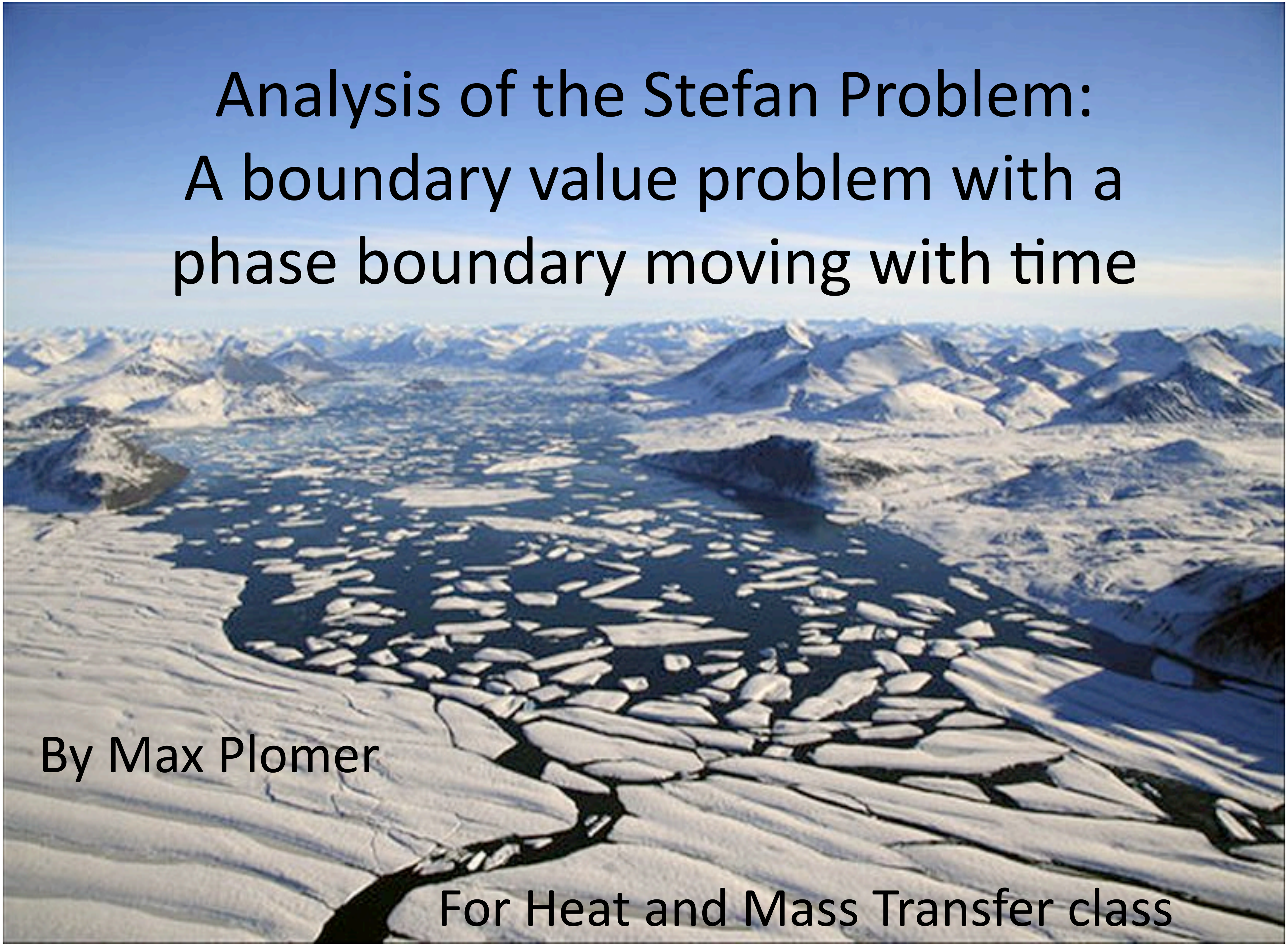
Analysis of the Stefan Problem: A boundary value problem with a phase boundary moving with time



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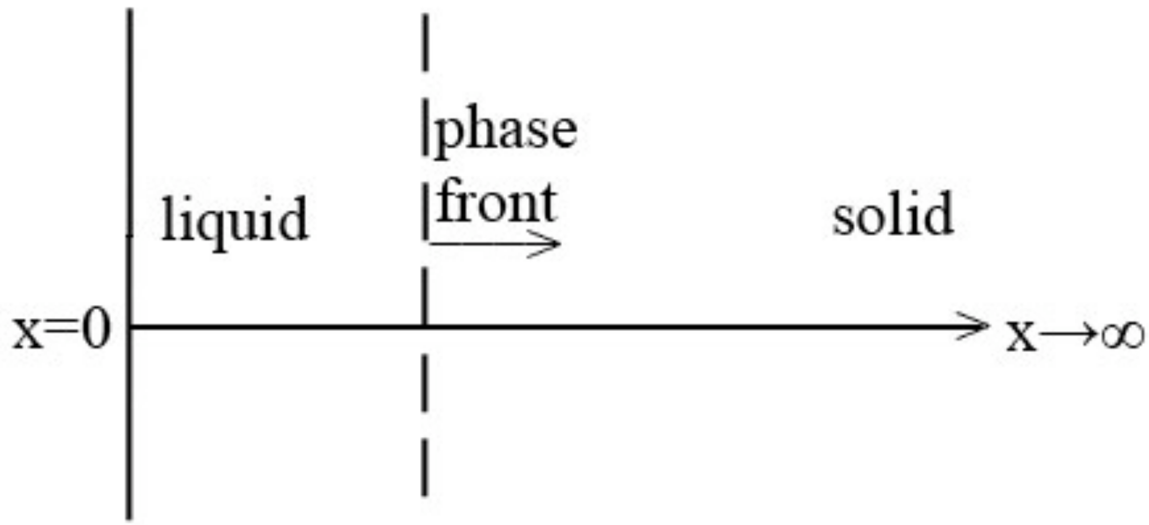
For Heat and Mass Transfer class

Contents of Talk

Background

- Joseph Stefan introduced 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.[1]
- Enthalpy of fusion
  "The liquid phase has a higher internal energy than the solid phase. This means energy must be supplied to a solid in order to melt it and energy is released from a liquid when it freezes, because the molecules in the liquid experience weaker intermolecular forces and have a larger potential energy."[2]

Problem Setup and Properties Used



- Semi infinite half plane
- Initially solid at point of melting, $T_{Solid}=T_{Fusion}$
- When surface temp raised melting immediately takes place
- Properties used: Density (assume constant for both phases, no volume change w/ melting), thermal conductivity and specific heat of phases, latent heat of fusion

Classical Stefan Problem 2 phase

$$T_L \geq T_1(x,t) \geq T_F \geq T_2(x,t) \geq T_S \qquad X(0) = 0$$

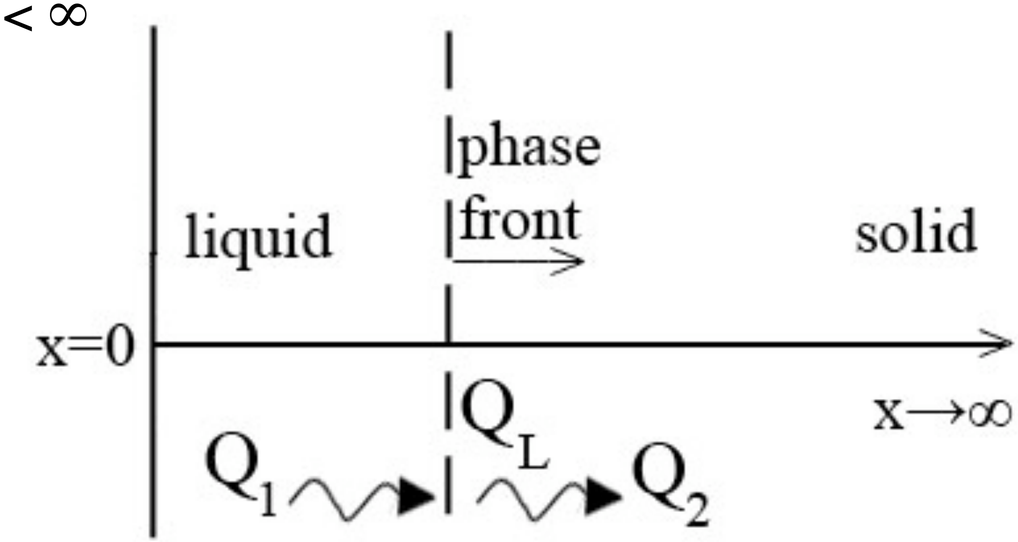
$$\rho_1 c_1 \frac{\partial T_1}{\partial t} = k_1 \frac{\partial^2 T_1}{\partial x^2} \qquad 0 < x < X(t)$$

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

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

$$T_2(\infty,t) = T_S$$

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



Conserve Thermal Energy
(using Fouriers Law)

$$Q_1 - Q_2 - Q_L = 0$$

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

Explicit solution and Pseudo-Steady State Approximation

- Explicit Solution[3] (Carslaw and Jaeger 1959) slab initially at T_F

$$X(t) = 2\lambda(\alpha t)^{1/2} \qquad \alpha = \frac{k_1}{c_1\rho_1}$$

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

$$St = c_1(T_L - T_F)/L \qquad T(x,t) = T_L - (T_L - T_F)erf\left(\frac{x}{2(\alpha t)^{1/2}}\right)/erf(\lambda)$$

- PSSA[4] – analytic estimate that assumes movement of boundary slower than rate of diffusion, neglect time partial derivative in diffusion equation

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

Combine and integrate

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

Matlab Code for PSSA Validation

```
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/m3]
alpha1= k1/(c1*rho1);  % thermal difusivity of phase 1
St=c1*(Tl-Tf)/L;       % one form of the stefan #

f=@(x) x*exp(x^2)*erf(x) - St/sqrt(pi);
lambda=fzero(f,2);

%analytical stefan solution
f2=@(t) 2*lambda*sqrt(alpha1*t);
f3=@(x,t) Tl-(Tl-Tf)*erf(  x/(2*sqrt(alpha1*t))  )/erf(lambda);

%PSS aproximation stefan solution
f4=@(t) sqrt( 2*t*(Tl-Tf)*k1/ (rho1*L));
f5=@(x,t) Tl - x*(Tl-Tf)/f4(t);

time=1e29;
f2(time)
f4(time)

error=abs(f2(time)-f4(time))/max(f2(time),f4(time))
```

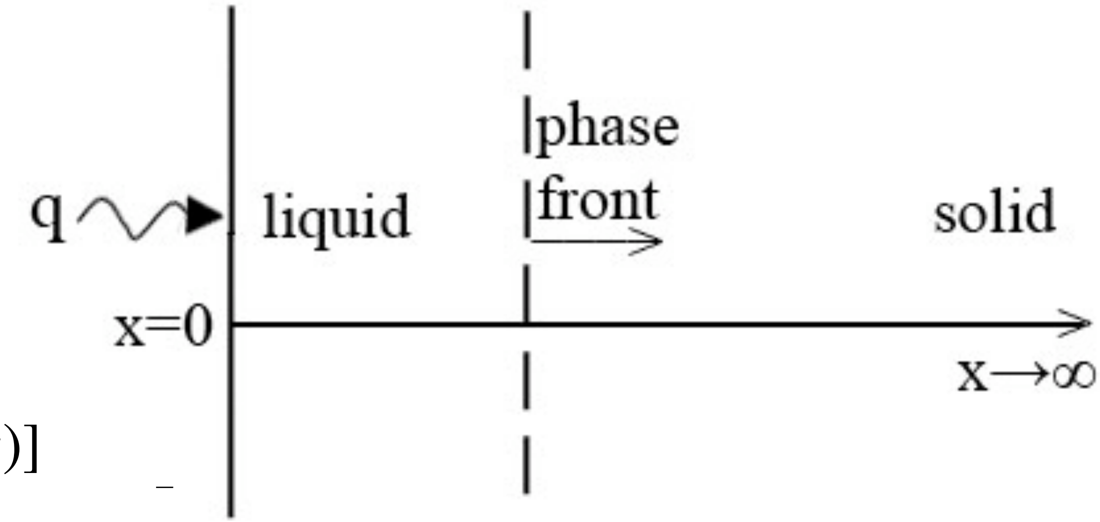
Output:

```
ans =

     9.185934201751227e+10


ans =

     9.667466711145732e+10


error =

   0.049809585466619
```

PSSA Newton Cooling at surface x=0

- No explicit analytical solution exists
- Boundary condition becomes:

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



Linear temp profile:

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

From these equations we obtain:

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

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

PSSA Newton Cooling at surface x=0 continued

$$-\frac{\partial T_1(X(t),t)}{\partial x} = \frac{\rho_1 L}{k_1}\frac{dX}{dt} \qquad T_1(x,t) = T_1(0,t) - x\left(\frac{T_1(0,t) - T_F}{X(t)}\right) \qquad T_1(0,t) = \frac{\dfrac{\dfrac{T_F k_1}{X(t)h} + T_0}{}}{1 + \dfrac{k_1}{X(t)h}}$$

Combine equations and integrate

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

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

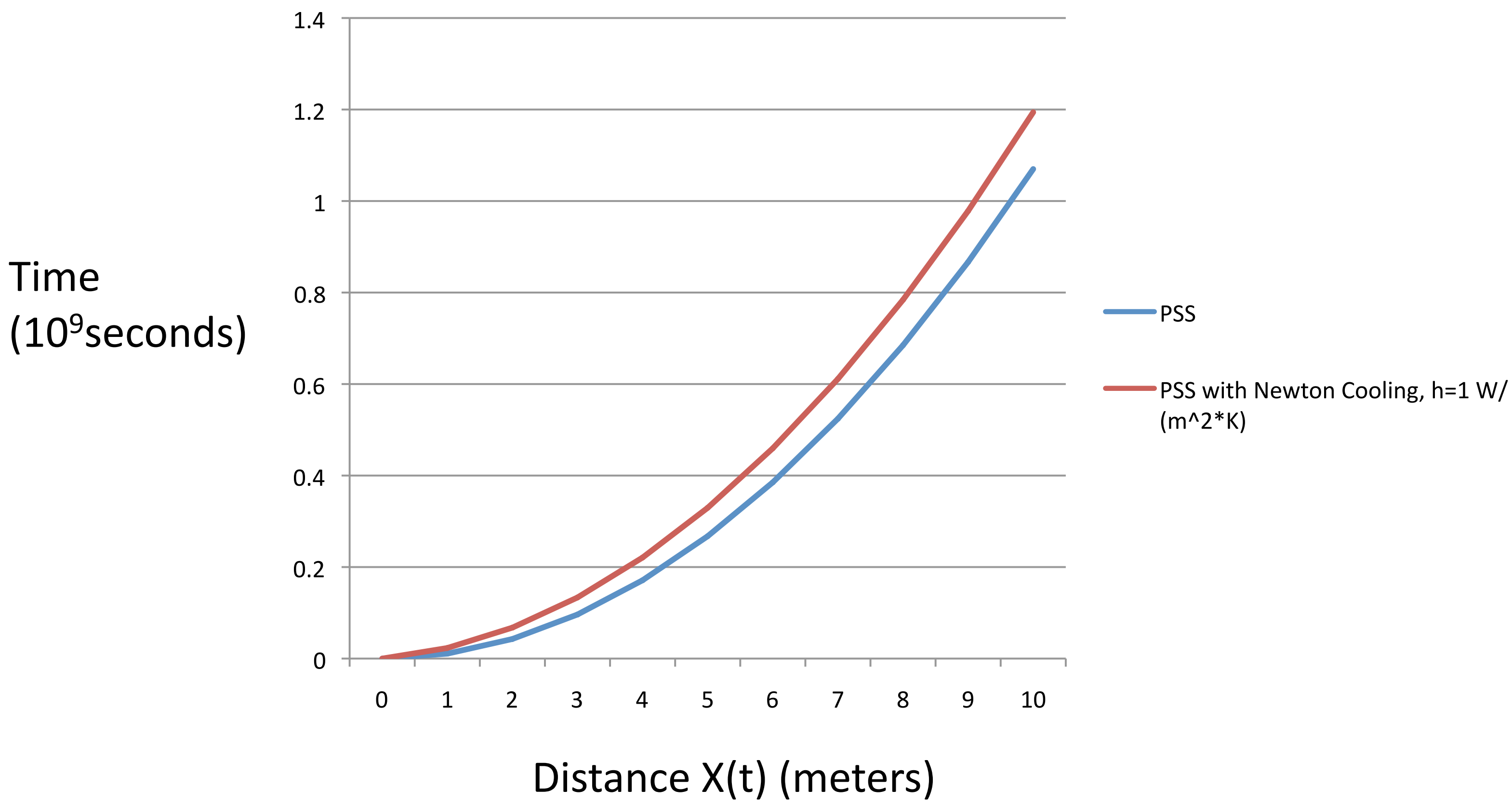
$$\frac{(T_0 - T_F)hk_1}{\rho_1 L}\int dt = \int (X(t)h + k_1)dX$$

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

For case of black body radiation, boundary condition becomes:

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

Graph of X(t) for PSS vs. PSS with Newton Cooling



As expected the affect of Newton cooling causing the phase change front to move more slowly.

Quadratic approximations

Approx solution of the form: $T_1(x,t) = T_F + A_1(t)(x - X(t)) + A_2(t)(x - X(t))^2$

Differentiate wrt t: $T_1(X(t),t) = T_F \longrightarrow \dfrac{\partial T_1}{\partial t}(X(t),t) + \dfrac{\partial T_1}{\partial x}(X(t),t)\dfrac{dX}{dt} = 0$

$$\rho_1 c_1 \frac{\partial T_1}{\partial t} = k_1 \frac{\partial^2 T_1}{\partial x^2} \qquad -\frac{\partial T_1(X(t),t)}{\partial x} = \frac{\rho_1 L}{k_1}\frac{dX}{dt} \longrightarrow \left(\frac{\partial T_1(X(t),t)}{\partial x}\right)^2 = \frac{L}{c_1}\frac{\partial^2 T_1}{\partial x^2}(X(t),t)$$

Take derivative of quad approx: $\dfrac{\partial T_1(X(t),t)}{\partial x} = A_1 \qquad \dfrac{\partial^2 T_1}{\partial x^2}(X(t),t) = 2A_2 \longrightarrow A_2 = \dfrac{c_1 A_1(t)^2}{2L}$

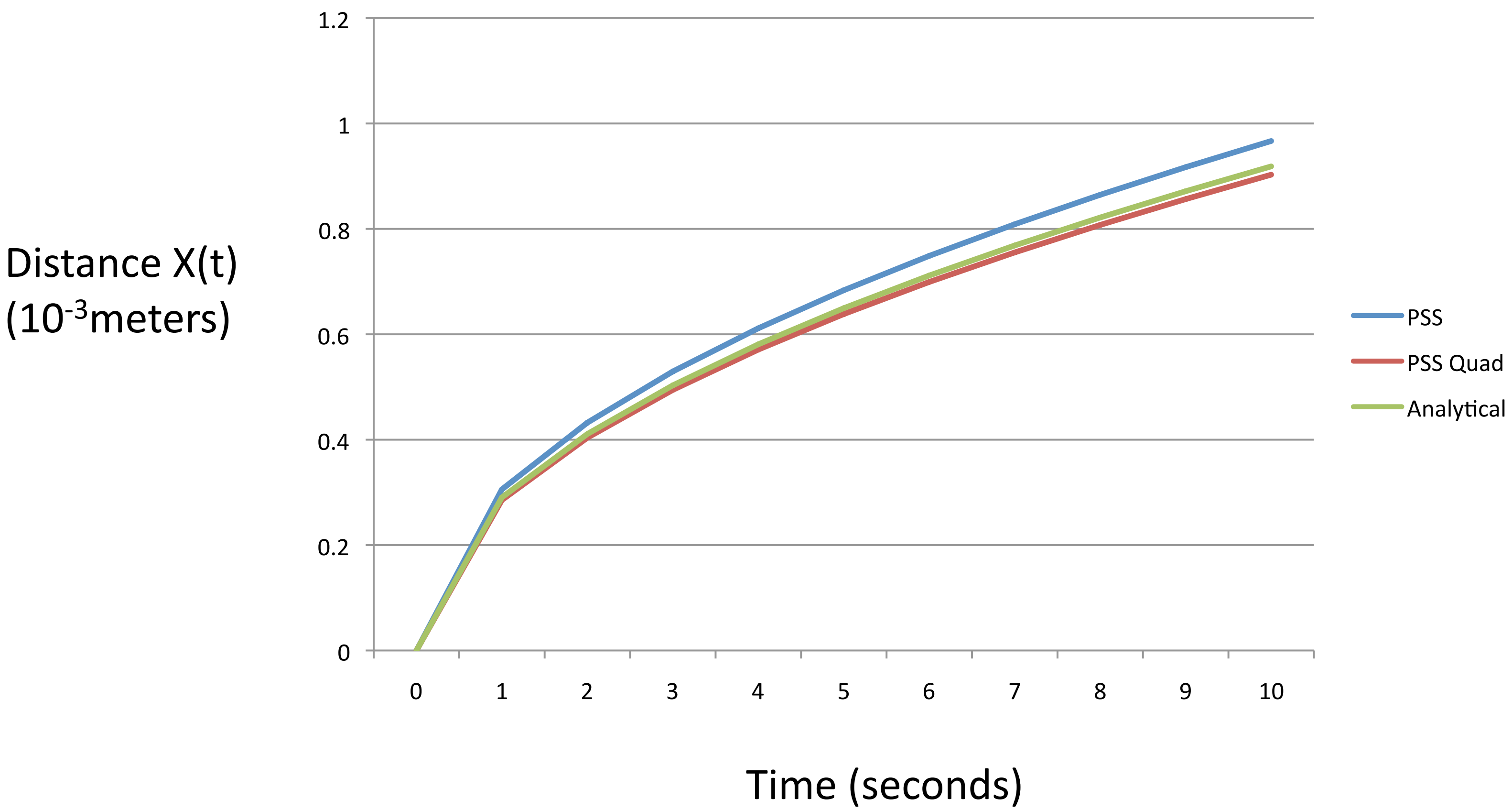
From surface condition $T_1(0,t) = T_L \longrightarrow \dfrac{c_1}{2L}A_1(t)^2 X(t)^2 - A_1(t)X(t) + (T_F - T_L) = 0$

Negative root ensures T ≥ T_F $\qquad A_1(t) = \left[1 - \sqrt{1 - 2\dfrac{c_1}{L}(T_F - T_L)}\right] \div \left(\dfrac{c_1}{L}X(t)\right)$

Megerlin's Method: Obtain X(t) from Stefan Condition $\qquad A_1 = -\dfrac{\rho_1 L}{k_1}\dfrac{dX}{dt}$

$$\left[1 - \sqrt{1 - 2\frac{c_1}{L}(T_F - T_L)}\right]\int dt = -\frac{\rho_1 c_1}{k_1}\int X(t)\,dX \qquad \left[1 - \sqrt{1 - 2\frac{c_1}{L}(T_F - T_L)}\right]t = -\frac{\rho_1 c_1}{2k_1}X(t)^2 + \cancelto{0}{C}$$

Graph of X(t) for PSS vs. PSS with Quadratic approximation



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.

Citations

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