Changing Temperature to Pressure.

The heat equation fully explained the change in temperature between the bottom and top of the ice given the boundary conditions and initial conditions used. However, the observation from a lyophilizer is pressure. We need an equation that relates ice interface pressure and and ice interface temperature. That equation was provided by Classius and Clapeyron.

$$P(t) = \xi \cdot e^{\frac{-\Delta H_{sub}}{R \cdot T}}$$

where ξ = a constant with units of pressure.

for water vapor pressure in Pascals, $\xi = 3.493 \cdot 10^{12} \cdot Pa$

$$\Delta H_{sub} := 51027 \frac{J}{mol}$$

What I have is an expression for temperature throughout the entire ice cylinder from bottom (x=0) to top (x=L) What I want is only the temperture at the interface(top, x=L).

$$u(x,t) = T1 + \sum_{n=1}^{\infty} \left[c_n \cdot \left[e^{\frac{-(2n-1)^2 \cdot \pi^2 \cdot \alpha^2 \cdot t}{4 \cdot L^2}} \right] \cdot \sin\left[\frac{(2n-1) \cdot \pi \cdot x}{2 \cdot L} \right] \right]$$

let x = L for temperature at the interface. "Change u(x,t) to $T_i(t)$ and change x to L

$$T_i(t) = T1 + \sum_{n=1}^{\infty} \left[c_n \cdot \left[e^{\frac{-(2n-1)^2 \cdot \pi^2 \cdot \alpha^2 \cdot t}{4 \cdot L^2}} \right] \cdot \sin\left[\frac{(2n-1) \cdot \pi}{2} \right] \right]$$

$$c_n = (T1 - T2) \cdot 4 \cdot \frac{2 \cdot \cos(\pi \cdot n) + 2 \cdot \pi \cdot \sin(\pi \cdot n) \cdot n - \pi \cdot \sin(\pi \cdot n)}{\pi^2 \cdot (2 \cdot n - 1)^2}$$

Substitute Ti(t) into the Classius Equation and we have an time varying expression for the interface pressure rise caused by temperature. It is worth looking back to see that T1 represents the temperature at the bottom and T2 represents the temperature at the top of the ice.

$$P2(t) = \xi \cdot e^{\frac{-\Delta H_{sub}}{R \cdot \left[T1 + \sum_{n=1}^{\infty} \left[c_n \cdot \left[e^{\frac{-(2n-1)^2 \cdot \pi^2 \cdot \alpha^2 \cdot t}{4 \cdot L^2}} \right] \cdot \sin\left[\frac{(2n-1) \cdot \pi}{2} \right] \right] \right]}}$$

Remembering that the first term derived for <u>chamber</u> pressure as a function of time was

$P1(t) = P_i - \left(P_i - P_0\right) \cdot e^{-k \cdot t}$ where P1(t) was chamber pressure and P_0 was chamber pressure at time zero.

Since the pressure terms are additive,

$$P1(t) = P_i - (P_i - P_0) \cdot e^{-k \cdot t} + P2(t)$$