RoadSnow Theory Manual

Summary

This document describes the equations/methods used to model the heat exchange and phase transformations in the Road/snow model. One dimensional heat transfer equation is solved using MATLAB (section 1). Primary heat transfer includes: latent heat energy released/absorbed during phase transformation (section 2,3,4), convective heat transfer (section 4), radiation (section 4 and 5), and conduction (section 6,7).

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1. One Dimensional Heat Equation

$$\left(\frac{c_p\rho}{k}\right)\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2} + \frac{q_v}{k}$$
 Eq. 1

Here \boldsymbol{c}_p is heat capacity, k is thermal conductivity, \boldsymbol{u} is temperature, \boldsymbol{q}_v is volumetric heat addition

Boundary Conditions:

$$q_{surf} = -k \frac{\partial u(t, x_{surf})}{\partial x}$$
 Eq. 2

$$u(t, x_{bottom}) = T_{diurnal}$$
 Eq. 3

In MATLAB, pdepe function solves PDEs in the following form [1]:

$$c\left(x, t, u, \frac{\partial u}{\partial x}\right)\frac{\partial u}{\partial t} = x^{-m}\frac{\partial}{\partial x}\left(x^{m} f\left(x, t, u, \frac{\partial u}{\partial x}\right)\right) + s(x, t, u, \frac{\partial u}{\partial x})$$
Eq. 4

From Eq. 1 and Eq. 4,

m = 0

$$c\left(x, t, u, \frac{\partial u}{\partial x}\right) = \frac{c_{p}\rho}{k}$$
Eq. 5
$$f\left(x, t, u, \frac{\partial u}{\partial x}\right) = \frac{\partial u}{\partial x}$$

$$s\left(x, t, u, \frac{\partial u}{\partial x}\right) = \frac{q_{v}}{k}$$

2. Modeling Phase Transformation without Salt Content

For snow without any salt content, the phase transition from ice to water occurs at a temperature equal to 0 degree Celsius, the enthalpy vs. temperature curve is illustrated below:

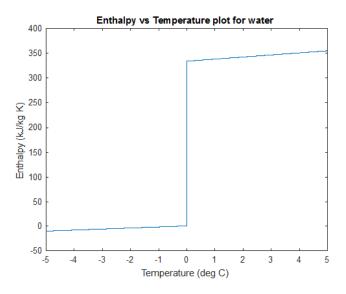


Figure 1 - Enthalpy vs. Temperature curve of water

The Heat Capacity c_p at any temperature is the slope of the curve at that temperature, as shown in the figure above. At temperature close to 0 degree Celsius, the slope of the curve is infinite and therefore c_p is infinite, since we need a numerical value for 0, the curve is modified such that the phase transition occur at a small temperature range $\Delta T = T_2 - T_1$, the onset of melting occurs at T_1 , and complete melting at T_2 . This approach is also used by the other paper and referred to as the effective heat capacity method [2], in the figure below $T_1 = -0.1 \text{ deg C}$ and $T_2 = 0.1 \text{ deg C}$

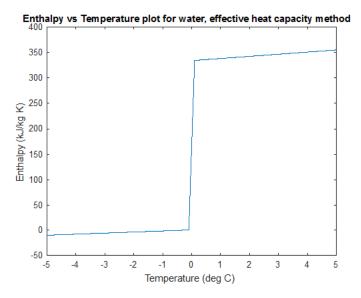


Figure 2 - Enthalpy vs. Temperature curve for water, effective heat capacity method

The heat capacity of snow or ice, is determined based on the layer temperature:

$$c_{p}(T) = \begin{cases} \frac{2090 \text{ for } T < T_{1}}{2} \\ \frac{2090 + 4200}{2} + \frac{334000}{T2 - T1} \text{ for } T_{1} \le T < T_{2} \\ 4200 \text{ for } T \ge T_{2} \end{cases}$$
Eq. 6

3. Modeling Phase Transformation with Salt Content

Salt concentration has a significant effect on the melting point of the water as illustrated by the phase diagram below for varying salt (NaCl) concentration.

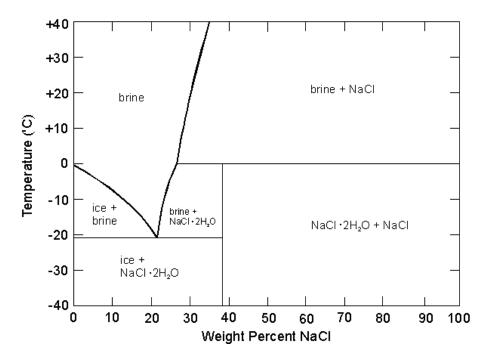


Figure 3 - Water NaCl Phase Diagram [3]

In our application, it is unlikely that salt concentration will exceed 20%, therefore it is not necessary to consider the properties of a brine solution with a salt concentration greater than 23%.

The liquid fraction at a given salt concentration and temperature can be determined using the lever rule on the water NaCl phase diagram.

The phase boundary between ice+brine and brine at concentration from 23% to 0% is determined through interpolation of known data points (Table 1). The interpolated curve, as shown in Figure 4, fits closely with the data points [4] as the R^2 value is very close to 1.

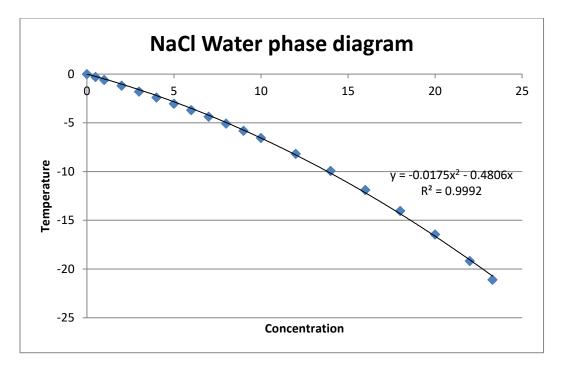


Figure 4 - Phase boundary of NaCl -Water diagram

Concentration	Temperature	Concentration	Temperature
0	0	0.09	-5.81
0.5	-0.3	0.110	-6.56
0.01	-0.59	0.12	-8.18
0.02	-1.19	0.14	-9.94
0.03	-1.79	0.16	-11.89
0.04	-2.41	0.18	-14.04
0.05	-3.05	0.20	-16.46
0.06	-3.7	0.22	-19.18
0.07	-4.38	0.233	-21.1
0.08	-5.08		

 Table 1 Phase boundary of NaCl -Water diagram, Data points [4]

Eq. 7

where T_3 is the temperature when ice starts to form and C is the fractional concentration.

Rearranging Eq. 7:

$$C_{\text{boundary}} = \frac{48.06 - \sqrt{48.06^2 + 4 \times 175 \times (-T)}}{2 \times -175}$$
 Eq. 8

Applying the lever rule, the liquid fraction (LF) at any concentration C (in fractions) and temperature T (degrees Celsius) is

$$LF(C,T) = \frac{C-0}{C_{\text{boundary}} - 0} = \frac{C}{C_{\text{boundary}}} = \frac{-350C}{48.06 - \sqrt{48.06^2 - 700T}}$$
Eq. 9

Eq. 9 only describes the ice+brine region of the phase diagram. At T = -21.1 deg. C, there is a phase transformation in which latent heat energy absorbed with the temperature staying constant at -21.1 degrees, which is similar to the phase transformation of pure water/ice and can therefore be handled in a similar manner.

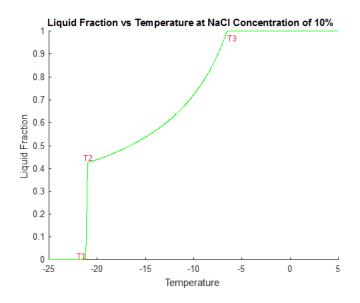


Figure 5 - Liquid Fraction vs. Temperature at NaCl Concentration of 10%

From Figure 5, three temperatures can be defined to describe the curve, T_1 is the temperature when melting initializes, given by $T_1 = -21.1 - \frac{\Delta T}{2}$. T_2 is the end of the first stage of melting, given by $T_2 = -21.1 + \frac{\Delta T}{2}$, thus $T_1 = T_2 = -21.1$.

The latent heat absorbed in a layer can be described using the change of the liquid fraction

$$\frac{dE}{dt} = \rho L_e \frac{d(LF)}{dt}$$
 Eq. 10

Where ρ is the density, L_e is the latent heat of fusion (-334kJ/kg) and LF is the liquid fraction. For $T < T_1$:

$$\frac{d(LF)}{dt} = 0$$
 Eq. 11

For $T_1 \leq T < T_2$

$$\frac{4.23577}{T2 - T1} \left(\frac{dC}{dt} (T - T1) + C \frac{dT}{dt} \right)$$
 Eq. 12

For $T_2 \leq T < T_3$

$$\frac{d(LF)}{dt} = \frac{\left(0.808417 - 1.6821\sqrt{0.230976 - 0.07T} - 0.245T\right)\frac{dC}{dt} + 0.1225C\frac{dT}{dt}}{\left(0.4806 - \sqrt{0.230976 - 0.07T}\right)^2\sqrt{0.230976 - 0.07T}}$$
Eq. 13

For $T \ge T_3$

$$\frac{d(LF)}{dt} = 0$$
 Eq. 14

Notice

$$\frac{d(LF)}{dt} = f_1\left(C, T, \frac{dC}{dt}\right) + f_2(C, T)\frac{dT}{dt}$$
 Eq. 15

where f_1 and f_2 are functions of C and T and $\frac{dC}{dt}$, f_1 account for energy absorption due to change of salt concentration, and f_2 accounts for energy absorption due to change of temperature. Note that f_2 is a term to be added to the c variable in pdepe, while f_1 is a term for the s variable

$$c\left(x, t, u, \frac{\partial u}{\partial x}\right) = \frac{c_p \rho}{k} - f_2 \frac{\rho L_e}{k}$$
Eq. 16

$$s\left(x, t, u, \frac{\partial u}{\partial x}\right) = s_{other \ sources} + f_1$$
 Eq. 17

Salt concentration change can be approximated using the semi-infinite model of 1 dimensional diffusion [5]

$$C = \begin{cases} C_s - (C_s - C_0) \operatorname{erf}\left(\frac{d}{2\sqrt{t \cdot D}}\right), t \neq 0 \\ C_0, \quad t = 0 \end{cases}$$
Eq. 18

where d is the depth from surface, C_s is the constant surface concentration, C_0 is the initial layer concentration, t is time, D is diffusion coefficient.

In order to ensure that the change in salt concentration in each snow/water layer is continuous, it was assumed that each layer have a constant coordinate or depth, even after some layer has melted and the total thickness has reduced, the depth of each layer was set at the beginning of the simulation and will stay the same throughout the simulation, this is important because any discontinuity in salt concentration will result in discontinuity in the internal energy of the layer, so that a layer might suddenly melt without absorbing any energy.

$$d = \frac{\text{total thickness of layers above } \times \text{ averge density of layers above}}{\text{density of water}}$$
Eq. 19

The derivative of salt concentration with respect to time is then

$$\frac{dC}{dt} = \begin{cases} (Cs - C0) \frac{D \cdot d}{2\sqrt{\pi} \exp\left(\frac{d^2}{4D \cdot t}\right) (D \cdot t)^{\frac{3}{2}}}, t \neq 0\\ 0, \quad t = 0 \end{cases}$$
Eq. 20

4. Surface Energy Exchange

There are three type of energy exchange at the surface of the snow, including:

- 1. Sensible Heat Flux
- 2. Latent Heat Flux
- 3. Long wave radiation

Total surface heat exchange is the superposition these three effects.

$$q_{surf} = q_h + q_e + q_{lw}$$
 Eq. 21

Sensible heat flux at the surface can be determined using Eq. 22 [6]:

$$q_h = h_c * (T_{air} - T_{surf})$$
 Eq. 22

Where q_h is the sensible heat convection in W/m², h_c is the convective heat transfer coefficient in W/(m² K) and $T_{air} - T_{surf}$ is the difference between air temperature far away and the surface temperature.

The convective heat transfer coefficient is a strong function of wind speed, for wind speed>2m/s [6]

$$h_c = 10.45 - V + 10V^{0.5}, \quad V > 2 m/s$$
 Eq. 23

For Wind Speed less than 2m/s, linear interpolation of the curve above is used, assuming that continuity of the function and its first derivative

hc = hc(2) - V * hc'(2) = 17.5210 + V
$$\left(\frac{5}{\sqrt{2}} - 1\right)$$
, V ≤ 2 m/s Eq. 24

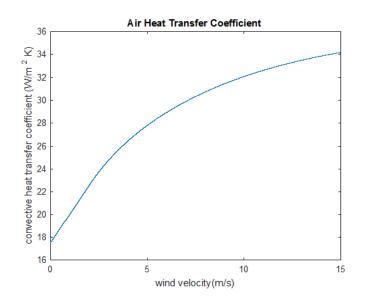


Figure 6 - Air Heat Transfer Coefficient vs. Wind Velocity

Latent Heat Flux can be approximated using the relationship [7]:

$$qe = 0.622 \rho_{air} L_e K_e V (e_{air} - e_{surf}) / P_{atm}$$
 Eq. 25

Where ρ_{air} is density of air, L_e is latent heat of vaporization, K_e is dimensionless transfer coefficient for water vapor, V is wind velocity, e_{air} is air partial vapor pressure, e_{surf} is saturation pressure at snow/water/ice surface, and P_{atm} is atmospheric pressure

Assuming that air is ideal gas, the density of air is [8]

$$\rho_{air} = \frac{P_{atm}}{0.287 \text{ kPa} \cdot \text{m}^3/(\text{kg} \cdot \text{K}) \cdot (\text{T}_{air} + 273.15\text{K})}$$
Eq. 26

Latent heat of vaporization at 0.1 degree Celsius

$$L_e = 2500500 \text{ J/kg}$$
 Eq. 27

Transfer coefficient for water vapor is constant:

$$K_e = 0.0023$$
 Eq. 28

The saturation water vapor partial pressure is a function of temperature [9]

$$P_{\text{saturated}}(T) = P_0 \exp\left(\frac{\text{Le}}{R}\left(\frac{1}{T_0} - \frac{1}{T}\right)\right)$$
Eq. 29

Here T_0 is reference temperature $T_0 = 273.25$ K, R is ideal gas constant for water vapor R = 0.462 kPa \cdot m³/(kg \cdot K), and P₀ is reference saturation pressure P₀ = 0.61173 kPa

$$e_{air} = P_{saturated}(T_{air}) \times RH$$
 Eq. 30

and

$$e_{surf} = P_{saturated}(T_{surf})$$
 Eq. 31

Where RH is relative humidity

Long wave radiation heat transfer is the difference between outgoing long wave radiation and incoming long wave radiation

$$q_{lw} = q_{lw_{in}} - q_{lw_{out}}$$
 Eq. 32

Incoming long wave radiation is approximated using the Eq. 33 [10]

$$q_{lw_{in}} = 1.24 \cdot \left(\frac{e_{air}}{T_{air}+273.15K}\right)^{\frac{1}{7}} \cdot (1 + 0.44RH - 0.18\tau) \cdot \sigma(T_{air} + 273.15K)^{4}$$
 Eq. 33

 σ is Boltzmann constant, τ is the atmospheric transmissivity for shortwave radiation, and it typically ranges from 0 to 0.75 and inversely proportional to cloud cover [10], therefore, τ is approximated using cloud cover data from input file

$$\tau = 0.75(1 - cc)$$
 Eq. 34

Ea 35

Where cc is the cloud cover

Outgoing long wave radiation can be determined through Stefan-Boltzmann law

$$q_{lw_{out}} = \epsilon \sigma (T_{surf} + 273.15K)^4 + (1 - \epsilon)q_{lw_{in}}$$

 ϵ is the emissivity, for a snowpack surface, the emissivity is approximately 0.9875[11]

5. Shortwave radiation

Incident short wave radiation I_{sw} is a function of longitude, latitude, date of the year, time of the day and cloud cover. Clear sky shortwave radiation is approximated using the code adapted from AIR_SEA TOOLBOX (version 2.0: 8/9/99) by Rich Pawlowicz, and data taken from Appendix E in the 1978 edition of Almanac for Computers, Nautical Almanac Office, U.S. Naval Observatory

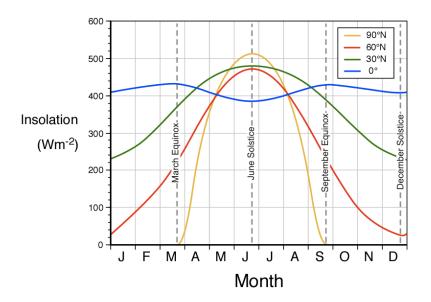


Figure 7 - Daily average of incoming short wave radiation at different latitude[13]

Shortwave radiation that is available to be absorbed/reflected by the snow/water layers can be determined from clear sky short wave radiation and cloud cover:

$$I_{sw} = I_{swclear\,sky} * (1 - cc)$$
 Eq. 36

cc is the cloud cover fraction.

Most of the shortwave radiation will be absorbed by the first few centimeters of the snow pack, when the thickness of snow is small or there is a soot layer present near the surface of the snow, melting will accelerate since the reflectivity of the soot layer or the road surface is much smaller comparing to snow. Figure 8 shows the approach used to model the short-wave radiation. The snowpack is broken down into two layers, a layer of water/ice with thickness d_{water} , and a layer of snow with thickness d_{snow} .

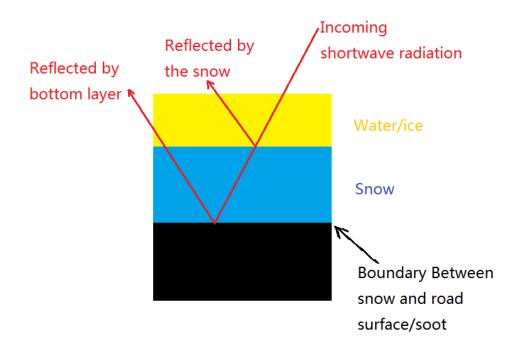


Figure 8 - Model for short wave radiation in the snowpack

At a given layer, the total radiation absorbed is [14]

$$I_a = I_t - I_t e^{-\kappa x} Eq. 37$$

Where I_t is transmitted radiation, κ is the extinction coefficient of that layer and x is the depth.

The transmitted radiation can be determined from the albedo of the layer [14]

$$I_t = I_0(1 - \alpha)$$
 Eq. 38

Where I_0 is the incident radiation to the layer that is available for transmission and reflection, α is the albedo of the layer

The volumetric flux at a given depth can be determined by taking the derivative of the total absorbed radiation

$$q_{v_{sw}} = \frac{dI_a}{dx} = \kappa I_0 (1 - \alpha) e^{-\kappa x}$$
 Eq. 39

And the volumetric flux will be added to the s varible in pdepe

$$s\left(x, t, u, \frac{\partial u}{\partial x}\right) = s_{other \ sources} + \frac{q_{v_{sw}}}{k}$$
 Eq. 40

The extinction coefficient for water is $\kappa_{water} = 6 \text{ m}^{-1}$, for snow is $\kappa_{snow} = 57 \text{ m}^{-1}$, and for soot is is $\kappa_{soot} = 3838 \text{ m}^{-1}$ [14]

The incident radiation that is available for reflection and absorption in each layer is:

$$I_{0 \text{ water/ice layer}} = I_{sw}$$

$$I_{0 \text{ snow layer}} = I_{sw} \exp(-\kappa_{water} d_{water})$$

$$Eq. 41$$

$$I_{0 \text{ soot/road surface}} = I_{sw} \exp(-\kappa_{water} d_{water})(1 - \alpha) \exp(-\kappa_{snow} d_{snow})$$

The albedo of the snow layer is approximated with Eq. 41 [15]

$$\alpha = \left(1 - e^{-\frac{d}{d^*}}\right)\alpha_{ds} + e^{-\frac{d}{d^*}}\alpha_{ss}$$
 Eq. 42

where d is snow thickness, d^{*} is scaling length which was optimized to be 2.4cm, α_{ds} and α_{ss} are two estimations of the snow albedo with different thickness range [15]

$$\alpha_{ds} = 0.713 - 0.112 \log_{10} T_a$$

Eq. 43

 a_u and T_a are albedo of road surface and daily accumulated temperature respectively, T_a is set to be 0.0237 for reasonable predictions of albedo at any snow layer thickness.[14]

6. Modeling Heat Conduction below the ground surface

To obtain accurate heat transfer through the snow/road surface boundary, conductive heat transfer below the road surface must be considered. At one meter below the ground, daily oscillation in temperature is negligible [14] and can be estimated using the date of the year (doyr). For example, May 29th of 2016 is the 149th day of the year.

The temperature 1m below the ground surface can be approximated using a sinusoidal curve, to define the curve, the average temperature and the amplitude of the temperature fluctuation is required for any specific location.

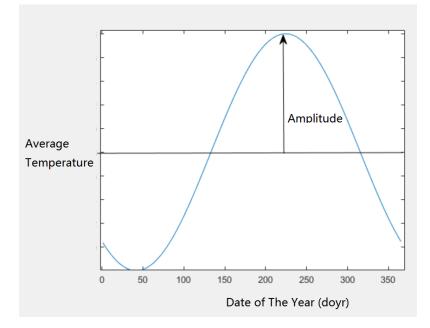


Figure 9 - Modeling the fluctuation of the temperature 1 meter below the ground

$$T_{g} = T_{g_{Amplitude}} \sin\left(\frac{2\pi(doyr - 133)}{365}\right) + T_{g_{Average}}$$
Eq. 44

In the Eq. 43, T_g is the temperature 1 meter below the ground, $T_{g_{Amplitude}}$ is the amplitude of the annual fluctuation in temperature 1 meter below the ground, and $T_{g_{Average}}$ is the average of temperature 1 meter below the ground.



Figure 10 - Typical layers below the ground surface

In Figure 10, the typical material below the road surface is shown [14], these layers are the default road properties. The temperature at the bottom layer of the sand is assumed to be only dependent on the date of the year.

7. Heat Conduction

When pdepe calculates heat conduction transfer for each individual layer, thermal conductivity and heat capacity property of snow, ice or water layer will be evaluated every time based on the layer property, temperature and salt content. Other layers including asphalt or sand will have constant heat capacity and thermal conductivity regardless of the temperature change.

The thermal conductivity of snow is estimated based on its density using the Djachkova's formula [16]

$$k_{snow} = 0.0442 * \exp(0.005181\rho)$$
 Eq. 45

Where ρ is density in kg/m³

For water or ice [17][18]

$$k_{water} = 0.6 \frac{W}{mK}$$
 Eq. 46

$$k_{ice} = 2.25 \frac{W}{mK}$$

For mixture of water and ice:

$$k_{mixture} = k_{water} * liquid fraction + k_{ice}(1 - liquid fraction)$$
 Eq. 47

The heat capacity of water, ice and mixture are [18]:

$$c_{p_{water}} = 4200 \frac{J}{kgK}$$

$$c_{p_{ice}} = 2090 \frac{J}{kgK}$$
Eq. 48

 $c_{p_{mixture}} = c_{p_{water}} * \text{liquid fraction} + c_{p_{ice}}(1 - \text{liquid fraction})$

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