

Physical Properties Models use in Permafrost Thermal Hydrological Models

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1 Notation and Units

Temperature is denoted T and is in units of Kelvin.

2 Saturated Vapor Pressure

Sonntag (1990) gives the following fit for the range $173.15 \text{ K} < T < 373.15 \text{ K}$:

$$p_{sat}(T) = 100 \exp(a_0 + a/T + bT + cT^2 + d \ln T) \quad (2.1)$$

where

$$a_0 = 16.635764 \quad (2.2)$$

$$a = -6096.9385 \quad (2.3)$$

$$b = -2.711193 \times 10^{-2} \quad (2.4)$$

$$c = 1.673952 \times 10^{-5} \quad (2.5)$$

$$d = 2.433502 \quad (2.6)$$

Note these fits are for saturated vapor over ice below 273.15 K and saturated vapor over liquid for $T \geq 273.15 \text{ K}$. Since the permafrost model presumes that unfrozen liquid water films occlude ice, it is more appropriate to use saturated vapor pressure over supercooled water (to be done). The fits of saturated vapor pressure over ice are from Marti and Mauersberger 1993. The fits of saturated vapor pressure over water are from the CRC Handbook (2000 edition).

3 Internal Energy

The specific internal energy [J/mol] is defined relative to that of water at 273.15 K .

3.1 Mixtures of air and vapor

Treating mixtures of air and water vapor as ideal gas, the internal energy may be calculated as

$$u_{gas} = (1 + 0.622 \omega) C_{v,dry}(T - 273.15) + \omega \Delta H_{vaporization} \quad (3.1)$$

The specific heat capacity of dry air $C_{v,air}$ is approximately 720 J/kg-K or 13.0 J/mol-K (CRC Handbook). The heat of vaporization for water $\Delta H_{vaporization}$ is approximately independent of temperature at low temperatures and approximately $4.065 \times 10^4 \text{ J/mol}$. Here ω is the mole fraction of water vapor or ratio of vapor partial pressure to total pressure.

3.2 Liquid Water

The specific heat capacity of water at 0 C is 4.2170 J/g-K (ref) or approximately 76 J/mol-K . Thus,

$$u_{liq} = 76.0(T - 273.15) \quad (3.2)$$

with T in Kelvin and u_{liq} in J/mol.

3.3 Ice

Specific heat capacity of ice varies with temperature. The following fit was found to be accurate in the range -60 to 0 C.

$$C_p = a + b(T - 273.15) \quad (3.3)$$

with

$$a = 37.7841 \quad (3.4)$$

$$b = 0.131932 \quad (3.5)$$

$$(3.6)$$

with C_p in units of J/mol-K and T in Kelvin. Results of that fitting are shown in the Figure.

Integrating from zero C to T and assigning the internal energy at 0 C the value $-\Delta H_{fusion}$

$$u_{ice} = -\Delta H_{fusion} + a(T - 273.15) + b(T - 273.15)^2 \quad (3.7)$$

with u_{liq} in J/mol and

$$a = 37.7841 \quad (3.8)$$

$$b = 0.0659661 \quad (3.9)$$

$$(3.10)$$

and the heat of fusion of water is $\Delta H_{fusion} = 33.34 \text{ J/g} = 600.787 \text{ J/mol}$.

4 Densities

4.1 Liquid Water

Mass density of water (kg/m³) at 1 bar varies with temperature as

$$\rho_{liq}(1 \text{ bar}) = a + b(T - 273.15) + c(T - 273.15)^2 + d(T - 273.15)^3 \quad (4.1)$$

with

$$a = 999.915 \quad (4.2)$$

$$b = 0.0416516 \quad (4.3)$$

$$c = 0.0100836 \quad (4.4)$$

$$d = 0.000206355 \quad (4.5)$$

Taking the compressibility of liquid water to be independent of temperature at low temperatures,

$$\frac{\rho_{liq}(T, P)}{\rho_{liq}(1 \text{ bar})} = 1 + \alpha(P - P_0) \quad (4.6)$$

where $\alpha = 5 \times 10^{-10} \text{ Pa}^{-1}$ and $P_0 = 10^5 \text{ Pa}$.

4.2 Ice

Mass density of water ice (kg/m^3) at 1 bar varies with temperature as

$$\rho_{ice}(1 \text{ bar}) = a + b(T - 273.15) + c(T - 273.15)^2 \quad (4.7)$$

with

$$a = 916.724 \quad (4.8)$$

$$b = -0.147143 \quad (4.9)$$

$$c = -0.000238095 \quad (4.10)$$

Assuming the compressibility to be independent of temperature,

$$\frac{\rho_{ice}(T, P)}{\rho_{ice}(1 \text{ bar})} = 1 + \alpha(P - P_0) \quad (4.11)$$

where $\alpha \approx 1 \times 10^{-10} \text{ Pa}^{-1}$ (CRC) and $P_0 = 10^5 \text{ Pa}$.

5 Viscosity

The following fit is from the CRC Handbook:

$$\mu = 0.001 \times 10^\xi \quad (5.1)$$

The ξ function is given as different values above and below $T_1 = 20^\circ\text{C} = 293.15 \text{ K}$. Below T_1 ,

$$\xi = 1301.0(1/A - 1/a) \quad (5.2)$$

$$A = a + b(T_1 - T) + c(T_1 - T)^2 \quad (5.3)$$

$$a = 998.333 \quad (5.4)$$

$$b = -8.1855 \quad (5.5)$$

$$c = 0.00585 \quad (5.6)$$

For $T \geq T_1$

$$\xi = \frac{A}{T - 168.15} \quad (5.7)$$

$$A = b(T_1 - T) + c(T_1 - T)^2 \quad (5.8)$$

$$b = 1.3272 \quad (5.9)$$

$$c = -0.001053 \quad (5.10)$$

where viscosity is in units of Pa-s and T is in Kelvin.

6 Diffusion Coefficient

(Note: Dusty gas model is a better model. Possibly update at some point. Not important for now)
The following model is used in TOUGH2

$$D_g = D_0 \frac{P_{ref}}{P} \left(\frac{T}{273.15 \text{ K}} \right)^a \quad (6.1)$$

$$a = 1.8 \quad (6.2)$$

$$D_0 = 2.13 \times 10^{-5} \quad (6.3)$$

$$P_{ref} = 10^5 \text{ Pa} \quad (6.4)$$

D_g has units of m^2/s .

A model is also needed for tortuosity as a function of porosity and gas saturation.

$$\tau_g = \tau_0 \phi^\beta s_g^{\beta_1} \quad (6.5)$$

Typical values for the constant and exponents are $\tau_0 = 1$, $\beta = 1/3$ and $\beta_1 = 7/3$ (consistent with Millington and Quirk, 1971, but looks different because of a different definition of the diffusion coefficient).

(Note: that the Millington and Quirk fit was not developed for frozen soils. We should check sensitivity and modify if needed. Earth permafrost is unlikely to be sensitive to this process.)

7 References

Marti, J. and Mauersberger, K. 1993 A survey and new measurements of ice vapor pressure at temperatures between 170 and 250 K. *Geophys. Res. Lett.*, 20, 363-366

FRANK J. MILLERO, RICHARD W. CURRY, and WALTER DROST-HANSEN, Isothermal Compressibility of Water at Various Temperatures, *JOURNAL OF CHEMICAL AND ENGINEERING DATA*, 14(4), OCTOBER 1969