Introduction to the Mars Subsurface Ice Model (MSIM) Program Collection

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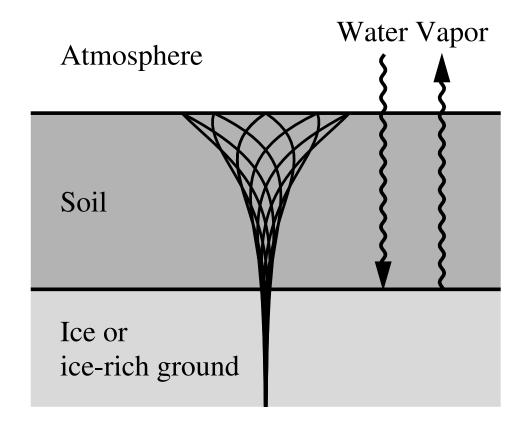
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https://github.com/nschorgh/MSIM/

Ground Ice in Diffusive Contact with Atmospheric Water Vapor



Vapor diffusion in the presence of temperature variations

Mars Subsurface Ice Model (MSIM)

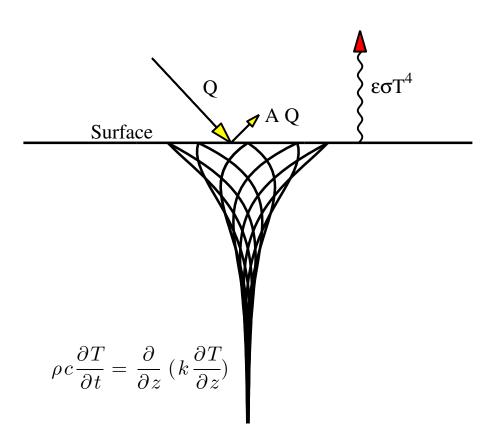
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Component		Typical
		time step
Thermal model	semi-implicit + nonlinear b.c.	15 mins
Microphysical model	diffusion, adsorption, sublimation	seconds
Equilibrium ice table	vapor equilibrium	_
Non-equilibrium ice	net vapor flux & ice content	100 yr

https://github.com/nschorgh/Planetary-Code-Collection/

3D surface energy balance slopes & shadows Megapixels

Subsurface Heat Storage (1D)



Heat equation with nonlinear boundary condition

- 1) Flux-conservative discretization (heat conservation) on irregular grid
- 2) Time-marching scheme that is *not* subject to $\Delta t < \Delta z^2/(2\kappa)$. Semi-implicit solver, $\Delta t \lesssim (\text{Solar Day})/100$

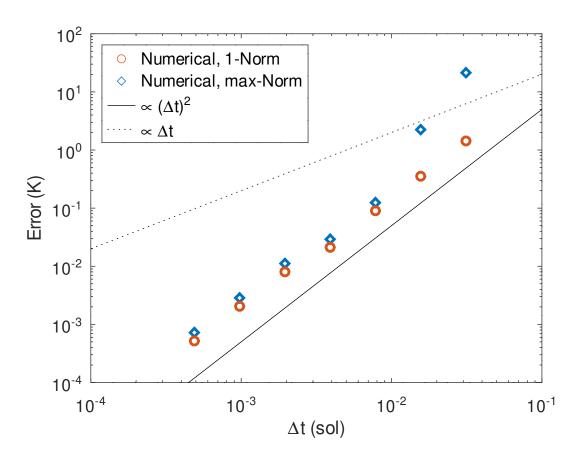
Numerical Solver for Heat Equation

<u>Semi-implicit</u> finite-difference method (Crank-Nicolson)



2nd order

unconditionally stable (for linear b.c.)



Convergence with time step Δt for the Crank-Nicolson method with nonlinear boundary condition.

(Many common Mars thermal models use explicit time steps, which lack both of these advantages.)

Surface Energy Balance

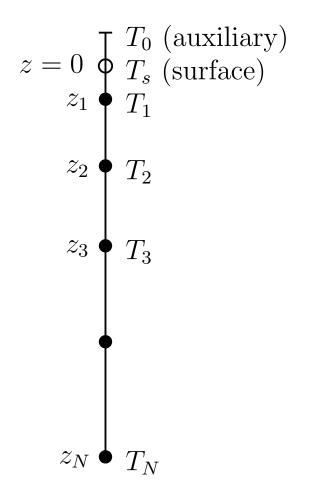
Surface energy balance:

$$k\frac{\partial T}{\partial z} = \epsilon \sigma T^4 - Q(t)$$

nonlinear boundary condition, because dependence on T itself (superposition fails)

- In MSIM, Stefan-Boltzmann term is linearized, so it can be incorporated into implicit method (Schorghofer & Khatiwala 2004)
- Nonlineary implies fully-implicit and semi-implicit schemes are no longer unconditionally stable (Williams & Curry 1977)
 For Mars and flat ground, stability is not an issue;
 For airless bodies and slopes, this can be a common issue at sunrise

Grid Spacing



 $z = 0 \begin{tabular}{l} \hline T_0 (auxiliary) \\ T_s (surface) \\ T_1 \end{tabular} \begin{tabular}{l} \bullet & Flux is defined in between grid points, so surface boundary condition should be imposed there too. \end{tabular}$

$$\Rightarrow (z_1 - 0) = \frac{1}{2}(z_2 - z_1)$$

Otherwise grid-spacing is arbitrary

Thermal Model Performance

Full surface energy balance:

$$\underbrace{(1-A)Q_0\sin\theta}_{\text{direct insolation}} + Q_{\text{sky}} + \underbrace{k\frac{\partial T}{\partial z}}_{\text{subsurf.}} = \underbrace{\epsilon\sigma T^4}_{\text{Stefan-Boltzmann}} - \underbrace{L\frac{dm_{CO_2}}{dt}}_{\text{latent heat of seasonal CO}_2}$$

Benchmark (3.6 GHz Intel Xeon E5-1650, gfortran 11.4.0): 10 Mars years (6686 sols), 100 steps/sol (15 mins), 80 grid points: only 1.1 seconds (with 2nd order accuracy)

For example, 1 million thermal model runs over 10 Mars years on a 10-core (20 threads) CPU take 15 hours, hence feasible on a simple workstation.

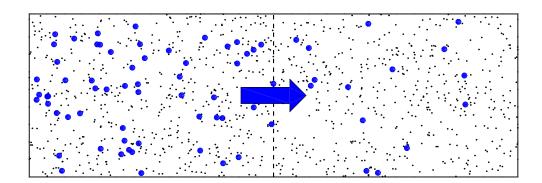
Vapor Transport in Non-Isothermal Sublimation Environments

Phases of H_2O incorporated: vapor, adsorbed H_2O , and ice

Vapor flux in non-isothermal environment (Landau & Lifshitz):

$$\vec{J} = -D\rho_{\text{atm}} \vec{\nabla} \left(\frac{\rho_v}{\rho_{\text{atm}}} \right) + (\text{exotic terms}) + (\text{advection}) \approx -D \vec{\nabla} \rho_v$$

 \vec{J} ...vapor flux; D...diffusion coefficient; ρ_v ... H_2O vapor density



Vapor diffuses along gradient of **absolute humidity** (kg/m³), not necessarily along gradients of relative humidity. E.g., diffusion from warm unsaturated to cold saturated region

Microphysical Model Equations

Diffusion of water vapor in porous medium with phase transitions (adsorption and sublimation) on 1-dimensional irregular grid

Governing Equations

Conservation of mass:
$$\frac{\partial}{\partial t}(\bar{\rho}_v + \bar{\rho}_f + \bar{\rho}_a) + \frac{\partial \bar{J}}{\partial z} = 0$$

Vapor transport:
$$J = -D \frac{\partial \rho_v}{\partial z}$$

Adsorption: $\bar{\rho}_a = \bar{\rho}_a(p,T)$ reversible and not kinetically-limited

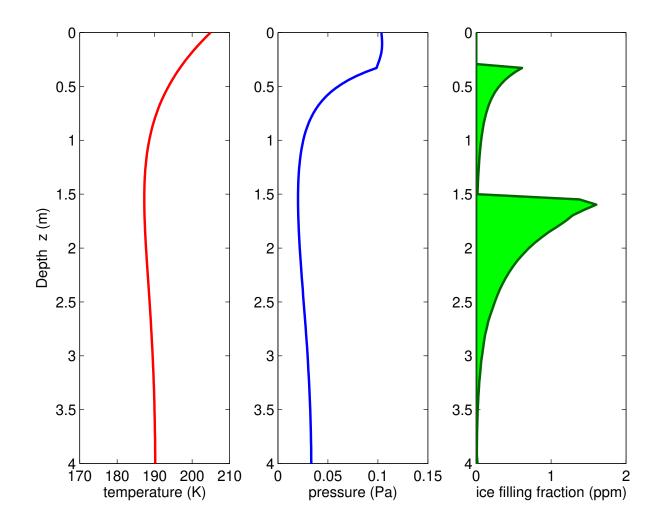
Sublimation: $p \leq p_{sv}(T)$ excess vapor converted to ice

Indices: v ... vapor, f ... ice, a ... adsorbed water $\bar{\rho}$... mass per total volume, \bar{J} ... vapor flux per total area

Microphysical Model Numerics

- Flux-conservative discretization on irregular 1d grid (there are several options)
- Threshold for phase transition implies problem is non-linear
 ⇒ forward-time discretization (explicit time step)

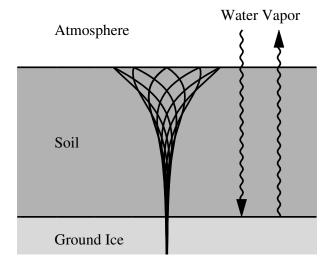
Accumulation of Subsurface Ice



Snapshot of temperature cycles that pump atmospheric humidity into the ground; movie is on GitHub

Time-Averaging of Transport Equations

Microphysics is complicated, but time averages can help us.



$$J = -D \frac{\partial \rho_v}{\partial z}$$

J ... vapor flux; D ... diffusion coefficient ρ_v ... H_2O vapor density; z ... vertical coordinate

Time average over period $P: \qquad \langle X \rangle = \frac{1}{P} \int_0^P X \, dt$

$$\langle J \rangle = -\left\langle D \frac{\partial \rho_v}{\partial z} \right\rangle \approx -\left\langle D \right\rangle \left\langle \frac{\partial \rho_v}{\partial z} \right\rangle = -\left\langle D \right\rangle \frac{\partial \left\langle \rho_v \right\rangle}{\partial z}$$

The **time-averaged flux** is given by the gradient of the **time-averaged vapor density**. \Rightarrow Net vapor flux can be calculated without microphysical processes. \Rightarrow "Fast" computational methods for subsurface ice evolution.

Boundary-Value Formulation

If averaging period is one solar year, time-average of ρ_v is determined by the boundary values at the surface and the ice table.

(mass conservation)
$$\frac{\partial (\rho_v + \rho_{ads} + \rho_{ice})}{\partial t} + \frac{\partial J}{\partial z} = 0 \quad \Rightarrow \quad \left\langle \frac{\partial J}{\partial z} \right\rangle = 0$$

 $\langle J \rangle$ is constant with depth; $\langle \rho_v \rangle$ is linear with depth; solid lines are microphysics simulation; dotted line connects boundary values

0.05

0.1

Pressure (Pa)

180 190 200

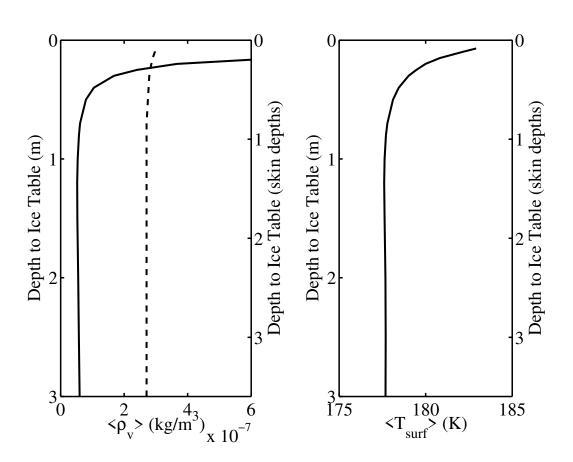
Temperature (K)

 $\langle \rho_{v} \rangle (kg/m^{3})_{v}^{6}$

Equilibrium Ice Table $\langle J \rangle = 0$

Depth of equilibrium ice table:

$$\langle \rho_v(\text{surface}) \rangle = \langle \rho_v(\text{ice table}) \rangle$$

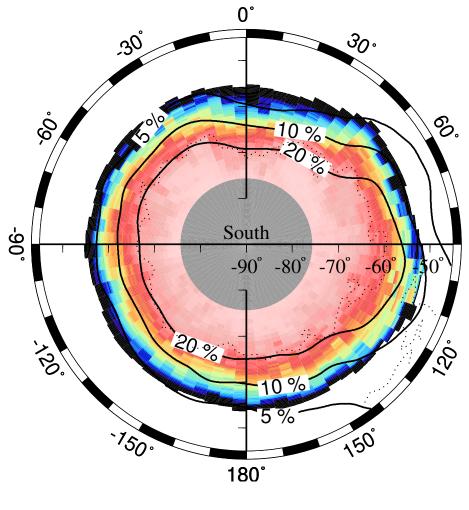


For each depth to ice table, thermal model was equilibrated and $\langle \rho_v \rangle$ was calculated for the last Mars year.

Depth to equilibrium ice table: **Nonlinear root-finding**

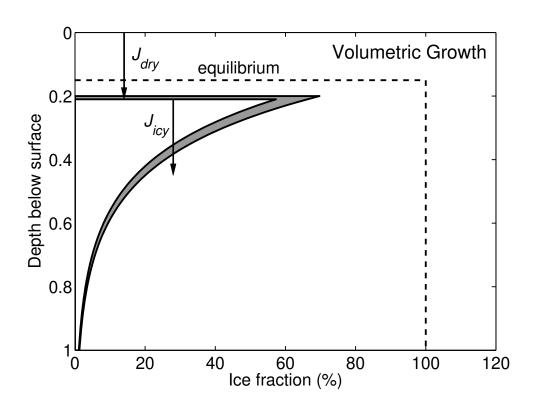
I usually use bisection method, and turn off geothermal heat to avoid missing a root.

Example Result



0 20 40 60 80 100 120 140 Ice Burial Depth (g/cm²) Depth to equilibrium ice table (colors) in the south polar region of Mars compared to results from nuclear spectroscopy (solid contours). Schorghofer & Aharonson (2005)

Beyond Equilibrium: Recharge of Subsurface Ice



- Subsurface ice can be sequestered from atmospheric vapor (Mellon & Jakosky 1993)
- Interface is below equilibrium depth
- Interface is sharp
- Interface is moving (i.e., between grid points)

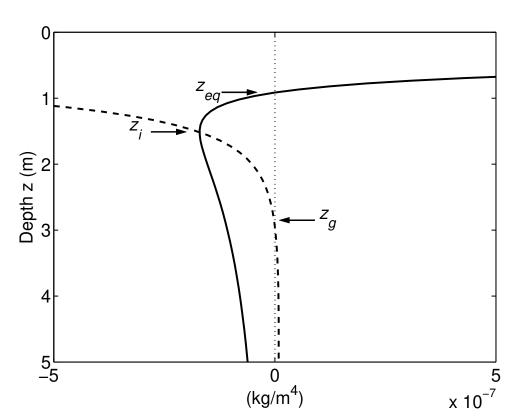
Gray area shows incremental ice growth. Ice fraction is relative to pore volume.

Location of z_{eq} , z_i , and z_g

 z_{eq} ... equilibrium depth

 z_i ... interface depth

 z_g ... geothermal limit



solid line ...
$$\frac{\langle \rho_{sv} \rangle(z) - \langle \rho(0) \rangle}{z}$$
 dash line ... $\partial \langle \rho_{sv} \rangle / \partial z$

All three of these depths migrate with changing ice content.

for realistic Mars subsurface temperatures at 60°N.

Numerics of Interface Retreat

Depth of uppermost ice z_p , might or might not cross grid-point during advance

Mass conservation:

$$\frac{dz_p}{dt}f(z_p)\Phi_0\rho_{\text{ice}} = -\langle J\rangle = \eta D \frac{\Delta \langle \rho_v\rangle}{z_p}$$

 z_p ... shallowest depth with pore ice; f ... fraction of pore filled with ice; Φ_0 ... ice-free porosity; $0 \le \eta \le 1$... constriction of diffusion

Integrate over one time step Δt_B :

$$\int_{z_p(0)}^{z_p(\Delta t_B)} f(z)zdz = \int_0^{\Delta t_B} \frac{1}{\Phi_0} \frac{\eta D}{\rho_{\text{ice}}} \Delta \langle \rho_v \rangle dt$$

$$\sum_{j=0}^{z_p} f(z_j) z_j \Delta z_j = \frac{1}{\Phi_0} \frac{\eta D}{\rho_{\text{ice}}} \Delta \langle \rho_v \rangle \Delta t_B$$

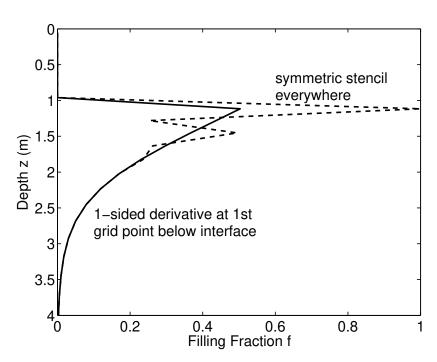
To find $z_p(\Delta t_B)$, sum until this equality is exceeded.

Numerics with Partial Pore Filling

We have to deal with $\sigma(z,t)$, not just depth-to-ice-table $z_T(t)$. σ ... ice density; Mass change for interstitial ice:

$$\frac{\partial \sigma}{\partial t} = \frac{\partial}{\partial z} \left(\eta D_{\text{icefree}} \frac{\partial \langle \rho_{sv} \rangle}{\partial z} \right)$$

 η ... constriction of diffusion (discontinuous at interface) This involves 2nd spatial derivative of ρ_{sv} (difficult near interface \Rightarrow one-sided finite-differences from below)

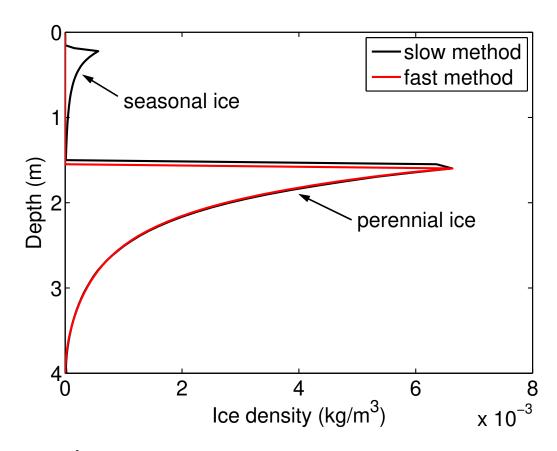


Comparison between

Fast and Slow Method

slow ... microphysical model

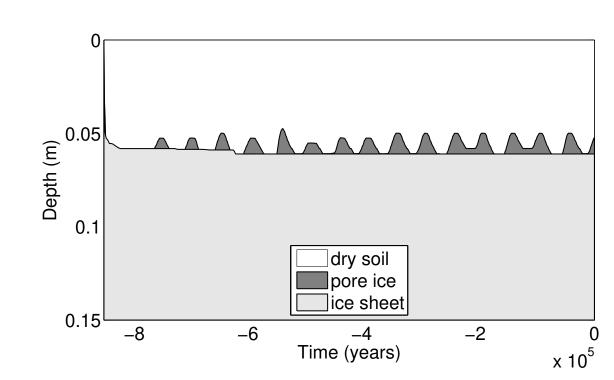
fast ... time-averaged transport equations



Speedup is $\sim 10^4$ -fold! About same speed as a thermal model. Fast method does not resolve diurnal and seasonal cycle.

Example: Phoenix Landing Site

massive ice sheet formed 863 ka ago (local obliquity maximum)



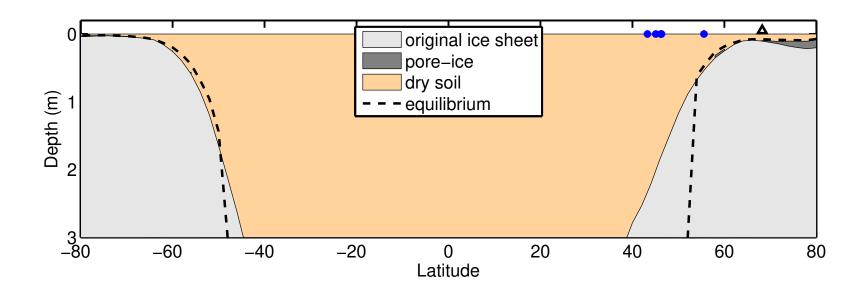
(Schorghofer & Forget 2012)

Filling fraction is always 100% (vertical growth mode).

Present-day thickness of pore ice layer is only 9 mm.
Phoenix observed mostly pore-ice, while neutron spectroscopy reveals massive ice.

Example: Present-day Ice Distribution

Scenario: Massive ice sheet formed 1 Ma ago



consistent with: MONS geographic boundary, MONS burial depths, MONS ice content, pore ice at Phoenix Landing Site, midlatitude icy impact sites (Schorghofer & Forget 2012)

Summary

- 1. MSIM includes a powerful subsurface thermal model (semi-implicit, 2nd order accurate, stabilized)
- 2. MSIM also includes microphysical model for vapor transport and adsorption, but it is computationally slow.
- 3. Method for fast subsurface ice modeling: **Solve time-averaged transport equations**
- 4. Non-equilibrium model with partial pore filling is fast but complex (whereas retreat or growth with full pores is easy)
- 5. MSIM is publicly available at https://github.com/nschorgh/MSIM/

References

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Methods:

- 1. https://github.com/nschorgh/MSIM/blob/main/MSIM_Methods.pdf
- 2. Thermal model: Schörghofer & Khatiwala, PSJ (2024) (most of it was written 2001–2003)
- 3. Fast non-equilibrium model: Schörghofer, Icarus (2010)

Science Applications:

- 1. Vapor diffusion: Schorghofer & Aharonson, JGR (2005)
- 2. Equilibrium ice table: Schorghofer & Aharonson, JGR (2005), Aharonson & Schorghofer, JGR (2006)
- 3. Non-equilibrium ice evolution: Schorghofer, Nature (2007), Schorghofer & Forget, Icarus (2012), Vos et al., JGR (2022, 2023)