Benchmark test for the heat conduction equation with phase change: two-phase Stefan problem for melting of an ice slab

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1 Heat conduction equation with phase change

The initial-boundary value problem for the heat equation equation with phase (water-to-ice) change reads:

$$\left((\varrho c_p)^{\mathrm{eff}} - \ell\varrho_{\mathrm{IR}}\frac{\mathrm{d}\phi_{\mathrm{I}}}{\mathrm{d}T}\right)\frac{\partial T}{\partial t} - \lambda^{\mathrm{eff}}\Delta T - (\lambda_{\mathrm{IR}} - \lambda_{\mathrm{LR}})\frac{\mathrm{d}\phi_{\mathrm{I}}}{\mathrm{d}T}|\nabla T|^2 = Q_T(\mathbf{x},t) \quad \text{in } \Omega, \tag{1}$$

where $T = T(\mathbf{x},t)$ is the temperature distribution subject to the initial and boundary conditions

$$\begin{cases} T = T_0(\mathbf{x}) & \text{in } \Omega \quad \text{(IC)}, \\ T = T_1(t) & \text{on } \Gamma_D \quad \text{(BC)}. \end{cases} \tag{2}$$

Equation (1) is the extended version of a classical heat conduction equation and is capable of modeling ice formation and melting in saturated porous medium. In the OpenGeoSys documentation it is sometimes termed the "T+freezing" equation.

In (1), on has

$$(\varrho c_p)^{\mathrm{eff}} = (1-\phi)\varrho_{\mathrm{SR}}c_{p\mathrm{S}} + (\phi - \phi_{\mathrm{I}})\varrho_{\mathrm{LR}}c_{p\mathrm{L}} + \phi_{\mathrm{I}}\varrho_{\mathrm{IR}}c_{p\mathrm{I}},$$

$$\lambda^{\mathrm{eff}} = (1-\phi)\lambda_{\mathrm{SR}} + (\phi - \phi_{\mathrm{I}})\lambda_{\mathrm{LR}} + \phi_{\mathrm{I}}\lambda_{\mathrm{IR}},$$

where ϕ is the porosity, function $\phi_{\mathrm{I}} := \phi_{\mathrm{I}}(T) = \phi S_{\mathrm{I}}(T)$ models the ice volume fraction, where, in turn,

$$S_{\mathrm{I}}(T) := \frac{1}{1 + e^{k(T - T_{\mathrm{m}})}}, \quad k > 1,\ T_{\mathrm{m}} = 273.15\,\mathrm{K}, \tag{3}$$

is the so-called ice-fraction indicator function which aims at distinguishing between the liquid and the ice phases of the fluid (values 0 and 1, resp.) within the physical domain

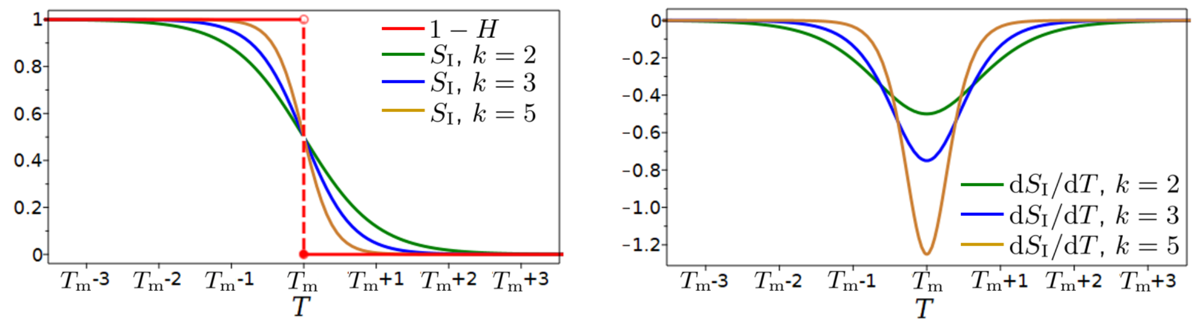

Figure 1: On the left: plots of the Heaviside-like ice-fraction indicator function (denoted as $1-H$) and its regularized counterpart S_I; on the right: plots of the first-order derivative of S_I.

Ω, as well as at tracing these phases evolution in time. It is a regularized counterpart of the corresponding Heaviside-like function, see Figure 1. Also in (1), parameter ℓ is the so-called heat of fusion of ice, whereas all other parameters in (1) are standard ones related to the classical THM modeling of processes in saturated porous medium.

In next section, we first consider and detail the so-called two-phase Stefan problem which models melting of a semi-infinite solid slab (in our case, an ice slab), see [1], and for which the closed-from analytical solution in $x \in (0,\infty)$ is available. Then, we apply (1)-(2) to model such melting process and solve the problem in OpenGeoSys.

This is done in the relatively large but finite spacial interval $x \in (0,4)$ by extracting the initial condition as well as the Dirichlet boundary conditions from the reference analytical data. The results obtained in $x \in (0,4)$ at various time-steps for the two modeling approaches are compared.

2 Stefan problem for ice slab melting process

Physically, two-phase Stefan problem models a semi-infinite slab, $0 \le x < \infty$, initially solid at sub-zero temperature $T_\mathrm{I} < T_\mathrm{m}$, which starts melting by imposing a constant positive temperature $T_\mathrm{L} > T_\mathrm{m}$ at $x = 0$. We expect that during melting, an interface between the two phases given by $x = X(t)$ such that $X(0) = 0$ advances to the right. The situation is sketched in Figure 2, where the boundary condition for T at infinity, that is, $\lim_{x\to\infty} T(x,t) = T_\mathrm{I}$ is also depicted (note that the homogeneous Neumann boundary conditions may be also physically appropriate, but the exact analytical solution cannot be derived in this case). Finally, it is assumed that the corresponding phases are characterized by the material parameters $\varrho_\mathrm{LR}, \lambda_\mathrm{LR}, c_{p\mathrm{L}}$ and $\varrho_\mathrm{IR}, \lambda_\mathrm{IR}, c_{p\mathrm{I}}$.

We skip the detailed mathematical formulation of the problem, only referring to the solution equations[1]. Thus, the temperature evolution during the process is described as

[1]A comprehensive treatment is available in [1].

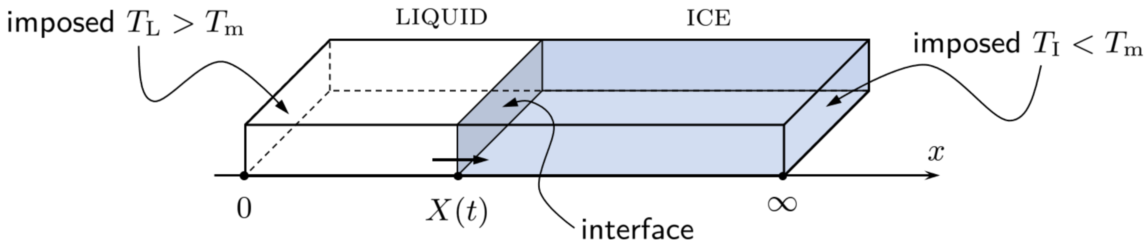

Figure 2: Sketch of a semi-infinite melting slab as a physical situation modelled by the two-phase Stefan problem.

follows:

$$T(x,t) := \begin{cases} T_{\rm L} - (T_{\rm L} - T_{\rm m}) \dfrac{\operatorname{erf}\left(\frac{x}{2\sqrt{\alpha_{\rm L} t}}\right)}{\operatorname{erf}(\Lambda)}, \quad 0 < x \le X(t),\ t > 0 & (\textsc{Liquid}), \\ T_{\rm I} + (T_{\rm m} - T_{\rm I}) \dfrac{\operatorname{erfc}\left(\frac{x}{2\sqrt{\alpha_{\rm I} t}} - (1-\varrho^\star)\alpha^\star\Lambda\right)}{\operatorname{erfc}(\varrho^\star\alpha^\star\Lambda)}, \quad X(t) \le x < \infty,\ t > 0 & (\textsc{Ice}), \end{cases} \tag{4}$$

where $\alpha_{\rm L} := \frac{\lambda_{\rm LR}}{\varrho_{\rm LR} c_{p\rm L}}$ and $\alpha_{\rm I} := \frac{\lambda_{\rm IR}}{\varrho_{\rm IR} c_{p\rm I}}$ are thermal diffusivity of the corresponding phases, $\varrho^\star := \frac{\varrho_{\rm LR}}{\varrho_{\rm IR}}$ and $\alpha^\star := \sqrt{\frac{\alpha_{\rm L}}{\alpha_{\rm I}}}$ are dimensionless parameters, $X(t) := 2\Lambda\sqrt{\alpha_{\rm L} t}$, $t > 0$ is the position of a melt front (an interface), and $\Lambda > 0$ is the root of the transcendental equation

$$\frac{St_{\rm L}}{\Lambda \exp(\Lambda)^2 \operatorname{erf}(\Lambda)} - \frac{St_{\rm I}}{\varrho^\star\alpha^\star\Lambda \exp(\varrho^\star\alpha^\star\Lambda)^2 \operatorname{erfc}(\varrho^\star\alpha^\star\Lambda)} = \sqrt{\pi}, \tag{5}$$

where, in turn, $St_{\rm L} > 0$ and $St_{\rm I} > 0$ are the so-called Stefan numbers defined as

$$St_{\rm L} := \frac{c_{p\rm L}(T_{\rm L} - T_{\rm m})}{\ell}, \quad St_{\rm I} := \frac{c_{p\rm I}(T_{\rm m} - T_{\rm I})}{\ell}, \tag{6}$$

with, finally, ℓ being a latent heat of fusion.

To calculate all the induced quantities in (4)–(6), we use the material parameters presented in Table 1. In this case, $\Lambda \approx 0.3933292421$ and the corresponding temperature evolution within the melting process of slab given by equations (4) can be visualized, see Figure 3. In the plots, T is depicted at time-steps $t \in \{4\,\text{h}, 12\,\text{h}, 28\,\text{h}, 60\,\text{h}, 124\,\text{h}, 240\,\text{h}\}$ and in the finite intervals $x \in [0, 4\,\text{m}]$ (the left plot) and $x \in [0, 1\,\text{m}]$ (the right plot). The former case intends to illustrate that the problem boundary condition at the infinity, $\lim_{x\to\infty} T(x,t) = T_{\rm I}$ is indeed fulfilled, whereas the latter one is only the zoom in into the region in which the comparison between the analytical and the OGS numerical results will later be performed.

liquid phase	ice phase
$\varrho_{\rm LR} = 1000$ kg/m^3	$\varrho_{\rm IR} = 920$ kg/m^3
$c_{p\rm L} = 4190$ J/(kg K)	$c_{p\rm I} = 2090$ J/(kg K)
$\lambda_{\rm LR} = 0.58$ W/(m K)	$\lambda_{\rm IR} = 2.2$ W/(m K)
	$\ell = 3.34 \cdot 10^5$ J/kg
$T_{\rm L} = 35$ °C (308.15 K)	$T_{\rm I} = -10$ °C (263.15 K)
Melting temperature, $T_{\rm m} = 0$ °C (273.15 K)	

Table 1: Material properties and parameters for Stefan problem.

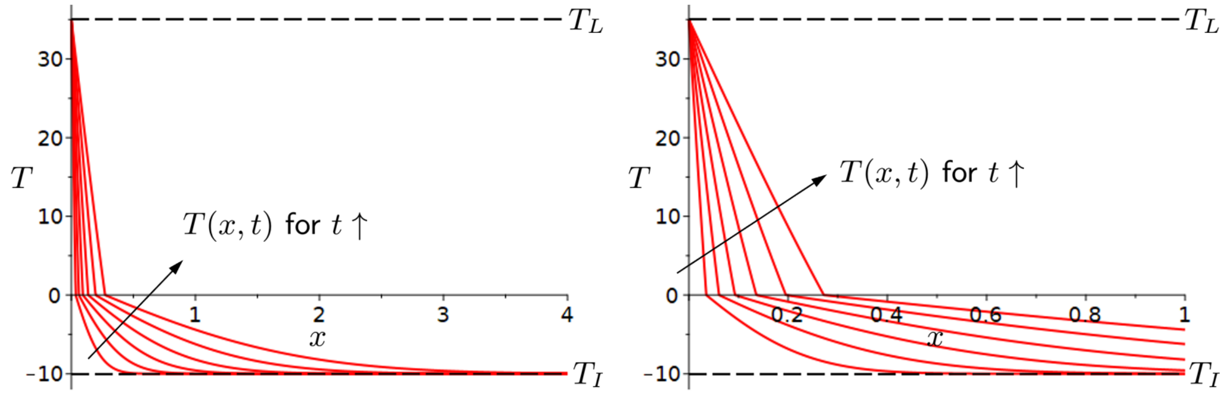

Figure 3: Solution (4) at time-steps $t \in \{4\,\mathrm{h}, 12\,\mathrm{h}, 28\,\mathrm{h}, 60\,\mathrm{h}, 124\,\mathrm{h},\ 240\,\mathrm{h}\}$ in the intervals $x \in [0, 4\,\mathrm{m}]$ (on the left) and $x \in [0, 1\,\mathrm{m}]$ (on the right); dashed lines depict the prescribed $T_{\rm L}$ and $T_{\rm I}$ in degrees Celsius.

We now model the slab melting process using our IBVP for the T+freezing equation (1) implemented in the OGS package and compare the simulated results with the analytical ones presented in Figure 3. In the computations for (1), we restrict ourselves to the interval $x \in [0, 4\,\mathrm{m}]$. The boundary condition for the unknown T^h at $x = 0$ is $T_{\rm L}$. At $x = 4\,\mathrm{m}$, we set $T^h := T(4,t)$, where $T(4,t)$ is the ice-phase part of the Stefan solution in (4) evaluated at $x = 4$. Imposing the initial condition is a bit more involving, as the direct use of the original one $T_{\rm I}$ at $t = 0, x \geq 0$ – given its incompatibility with the boundary condition $T_{\rm L}$, $x = 0, t \geq 0$, as well as that we deal here with a problem with a (strong) boundary layer – will result in the convergence issues at the first time step of computations. Therefore, in our solution process, we opt for taking $t_0 := 3600\,\mathrm{s}$ as the initial moment and the initial condition for T^h is hence taken to be the Stefan solution $T(x, t_0)$. The simulation time interval is $t \in [3600\,\mathrm{s}, 864000\,\mathrm{s}] = [1\,\mathrm{h}, 240\,\mathrm{h}]$, and the time-step increment $\Delta t := 36\,\mathrm{s}$. The special discretisation of $x \in [0, 4\,\mathrm{m}]$ is uniform and uses $\Delta x = 0.005\,\mathrm{m}$. Finally, we set the porosity $\phi = 1$ and compute two cases in terms of the Sigmoid functions coefficient k, namely, $k := 2$ (Case 1) and $k := 5$ (Case 2).

The results obtained with the OGS for both cases at time steps $t \in \{4\,\mathrm{h}, 12\,\mathrm{h}, 28\,\mathrm{h}, 60\,\mathrm{h}, 124\,\mathrm{h}, 240\,\mathrm{h}\}$ are depicted in Figure 4, where we restrict the solution plots to the interval

$[0, 1\,\mathrm{m}]$. The melting temperature T_m is also plotted to make the interface visible. It can be seen that the general trend of temperature evolution in the slab in either simulated case is the same as the reference one in Figure 3, right. For the lager k (Case 2), the temperature 'kink' at the interface became sharper, as expected, since (to recall) k governs the steepness of S_I in the transition zone and thus, the induced spacial thickness of this zone.

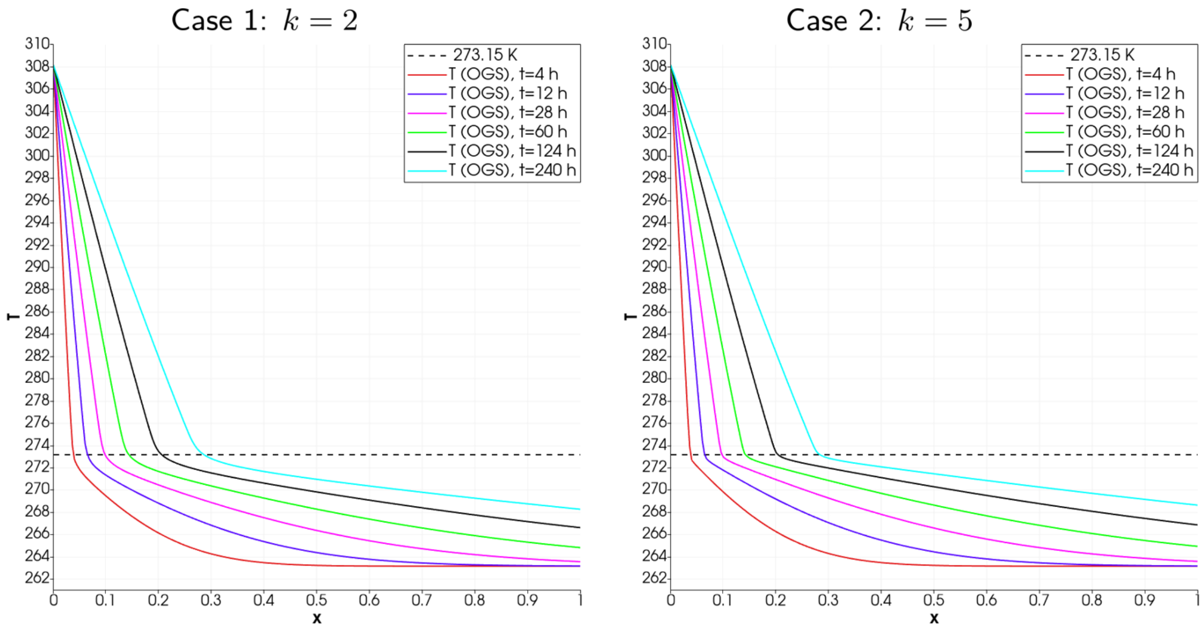

Figure 4: The OGS solution of the IBVP for the T+freezing equation (1) at time-steps $t \in \{4\,\mathrm{h}, 12\,\mathrm{h}, 28\,\mathrm{h},\ 60\,\mathrm{h}, 124\,\mathrm{h}, 240\,\mathrm{h}\}$ in the interval $x \in [0, 1\,\mathrm{m}]$ for the two cases of k; temperature is given in kelvins.

Figure 5 presents comparison of the analytical solution (4) of Stefan problem and the OGS solution of the IBVP for the T+freezing equation (1) obtained in two cases of k in the interval $x \in [0, 4\,\mathrm{m}]$. Again, both representations are restricted to $x \in [0, 1\,\mathrm{m}]$. We observe that despite the fact we have applied two different modeling approaches to the very same physical problem of slab melting – the original two-phase Stefan problem and the one given by the T+freezing equation, and hence, neither can be taken as a reference one – the quantitative discrepancy of the results is minor, especially in Case 2, with the increased magnitude of k.

References

[1] V. Alexiades and A.D. Solomon. Mathematical Modeling of Melting and Freezing Processes. Hemisphere Publishing Corporation, Washington, 1993.

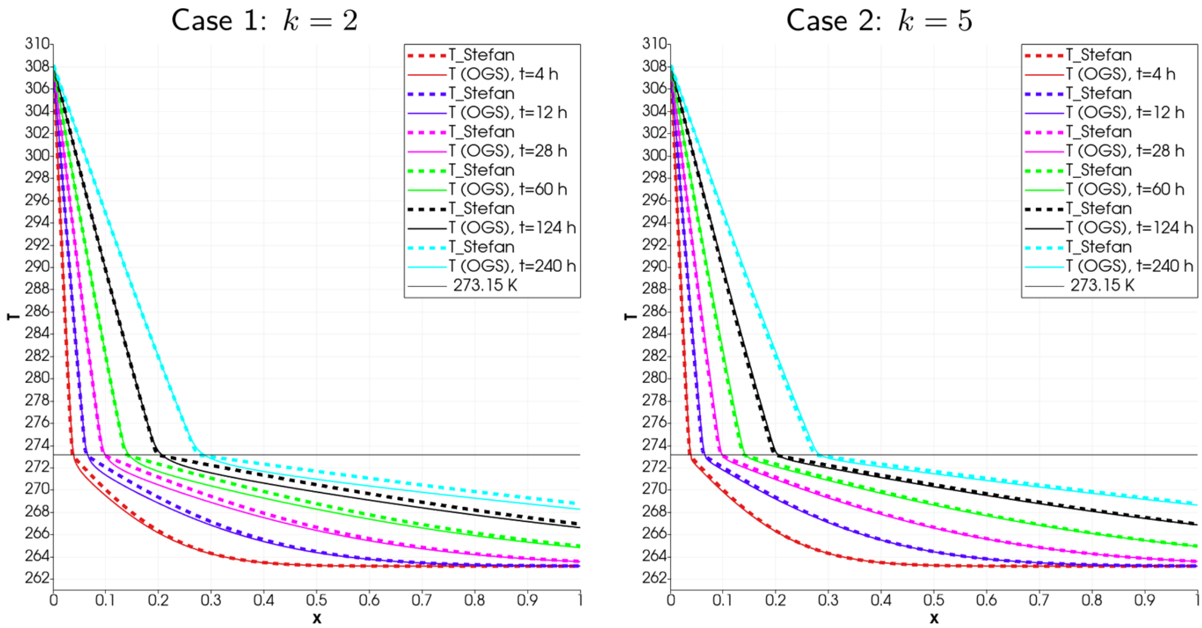

Figure 5: Comparison of the analytical solution (4) to the two-phase Stefan problem and the OGS solution to IBVP for for the T+freezing equation (1) obtained in two cases of k; the temperature is given in kelvins.