Questions and comments - Prof. RNDr. Josef Málek, DSc., CSc.

Question 1

Jak se v modelování resp. ve formulaci modelu či v odvození algoritmu projeví druhý zákon termodynamiky? Efektivní metody jsou často takové, které i na diskrétní úrovni druhý zákon termodynamiky splňují. Zdá se, že tento aspekt v práci uvažován není.

How does the modeling and the formulation of the model and derivation of the algorithm reflect the second law of thermodynamics - the entropy principle. Effective methods are usually such that even at the discrete level they satisfy the entropy principle. It appears that this is not considered and taken into account in this work.

- The second law of thermodynamics, the entropy principle (single continuum).

$$\rho\dot{\eta} + \operatorname{div}\vec{s} - \rho b \geq 0$$

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$$\rho\dot{\eta} + \operatorname{div}\left(\frac{\vec{q}}{T}\right) - \rho b \geq 0$$

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$$\rho(T\dot{\eta} - \dot{\varepsilon}) + \boldsymbol{\tau} : \mathbf{d} - \frac{\vec{q} \cdot \operatorname{grad} T}{T} \geq 0$$

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- The second law of thermodynamics, mixture.

$$\sum_{\alpha=1}^{n} \rho_\alpha \grave{\eta_\alpha}^{\alpha} + \sum_{\alpha=1}^{n} r_\alpha \eta_\alpha + \operatorname{div}\left(\frac{\vec{q}}{T}\right) - \frac{Q}{T} \geq 0$$

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$$
\begin{aligned}
0 \quad \geq \quad & \sum_{\alpha=1}^{n} \rho_\alpha \grave{f}_\alpha^{\ \alpha} \ + \ \sum_{\alpha=1}^{n} r_\alpha f_\alpha \ + \ \sum_{\alpha=1}^{n} \rho_\alpha \eta_\alpha \grave{T}^\alpha \ + \ T^{-1} \mathrm{grad}\ T \cdot \vec{q} \\
- \quad & \sum_{\alpha=1}^{n} \mathbf{D}_\alpha : \mathbf{T}_\alpha + \sum_{\beta=1}^{n-1} \vec{k}_\beta \cdot \vec{u}_\beta \ + \ \frac{1}{2} \sum_{\beta=1}^{n-1} r_\beta \vec{u}_\beta^{\,2}
\end{aligned}
$$

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- For the general water-ice mixture model, the entropy principle was fully exploited by the rational-thermodynamics (Truesdell) approach in Souček & Martinec (2001), the shape of the response functionals was derived from a very general form with the use of axioms of constitutive theory, such as objectivity, equipresence, memory, local action and entropy principle by performing a linearisation in the neigborhood of thermodynamic equilibrium and using the representation theorems for isotropic functions.

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- For the single-component model (pure ice), used in the further derivations of the SIA-I algorithm, the entropy principle has also been used in the constitutive theory, but again only in the Truesdell form (entropy production was not specified).

$$
\begin{aligned}
\xi &:= \rho\dot{\psi} - \rho\eta\dot{T} + \boldsymbol{\tau} : \mathbf{d} - \frac{\vec{q}\cdot \operatorname{grad} T}{T} \geq 0 \\
\psi &= \psi(T) \\
\mathbf{d} &= \mathcal{A}(T)\sigma_{II}^{n-1}\boldsymbol{\sigma} \\
\boldsymbol{\tau} &= -p\mathbf{I} + \boldsymbol{\sigma} \\
\vec{q} &= -k\operatorname{grad} T
\end{aligned}
$$

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$$
\begin{aligned}
\xi &= \mathcal{A}(T)\sigma_{II}^{n-1}\boldsymbol{\sigma} : \boldsymbol{\sigma} + k\frac{\operatorname{grad} T \cdot \operatorname{grad} T}{T} \geq 0 \\
\frac{\partial \eta}{\partial T} &= \frac{1}{T}\frac{\partial \varepsilon}{\partial T} \\
k &\geq 0 \\
\mathcal{A}(T) &\geq 0
\end{aligned}
$$

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- The SIA-I algorithm itself doesn't affect the entropy principle, because the limit solution satisfies the rheology equations exactly and these follow the entropy principle already.

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Question 2
Jak je aktivace procesu zakódována do aktivačního parametru Q v rovnici (1.22)? Jsou prováděny výpočty pro vizkozitu závislou na tlaku? Lze charakterizovat/ilustro- vat, jak je v uvažovaném problému podstatná závislost vazkosti na tlaku?

How is the activation of the process contained in the activation parameter Q in equation (1.22)? Are the numerical computations performed for a pressure-dependent viscosity? Is it possible to characterize/illustrate how important is the pressure-dependence of viscosity for the considered problem?

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- Eq. 1.22

$$\mathcal{A}(T, p) = A\exp\left(-\frac{Q}{RT^\star}\right)$$

- $T^\star$ the absolute temperature corrected for the pressure melting point

$$T^\star = (T + C_{Cl}p)$$

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- The word activation is related to the energy required to activate the process of sliding - e.g. single ice grain dislocation. From statistical mechanics, one then obtains probability of realization of such dislocation proportional to $\exp(-\frac{Q}{k_b T})$. Because of pressure dependence of melting temperature, it is necessary to correct the temperature for this effect $T^\star = (T + C_{Cl} p)$.

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- We may evaluate the pressure dependence of the rate factor by considering some realistic values
- Take $\rho = 990\ \mathrm{kg\ m^{-3}}$, $g = 9.81\ \mathrm{m\ s^{-2}}$, $T = 273.15\ K$, $C_{Cl} = 9.7 \times 10^{-8}\ \mathrm{K\ Pa^{-1}}$, $Q = 13.9 \times 10^{4}\ \mathrm{J\ mol^{-1}}$, $A = 1.73 \times 10^{3}\ \mathrm{Pa^{-3}\ s^{-1}}$

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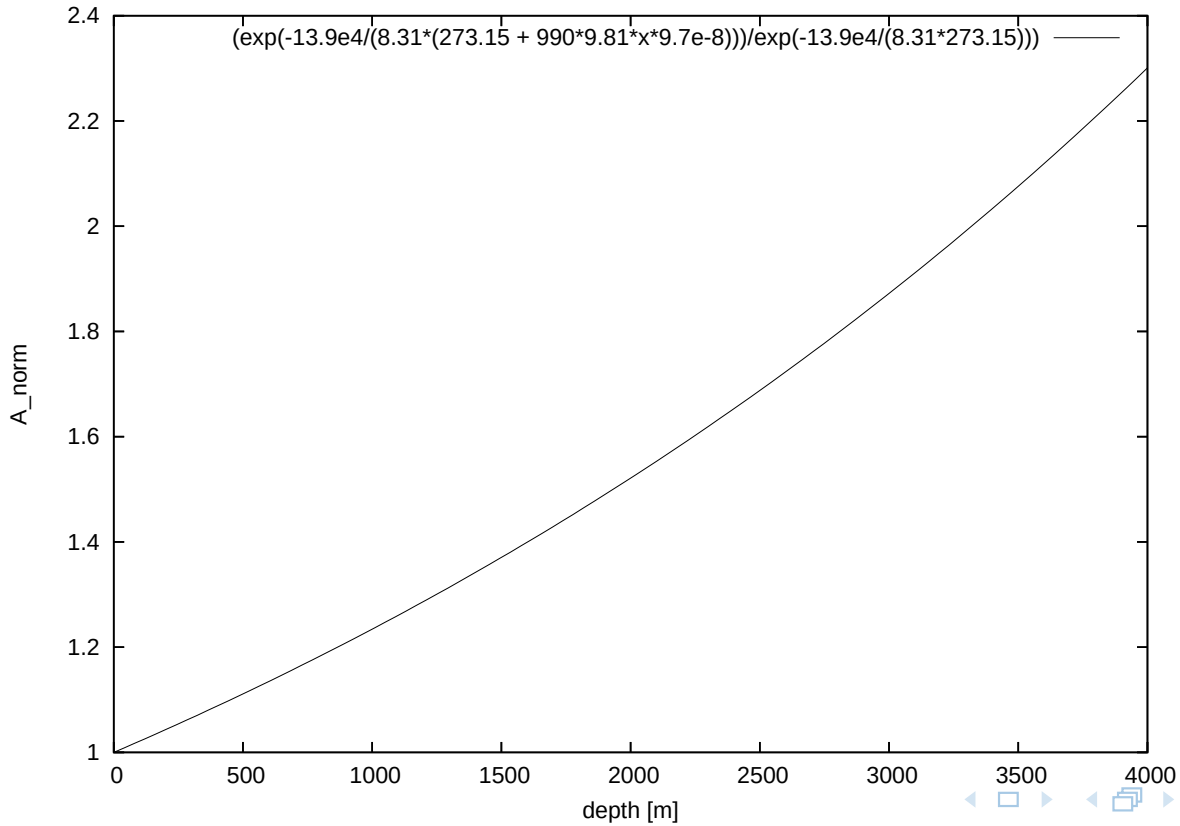
- Effect of pressure on rate-factor $\mathcal{A}$ vs. the temperature effect (linear profile $T_{surf} = -30^{\circ}C$)



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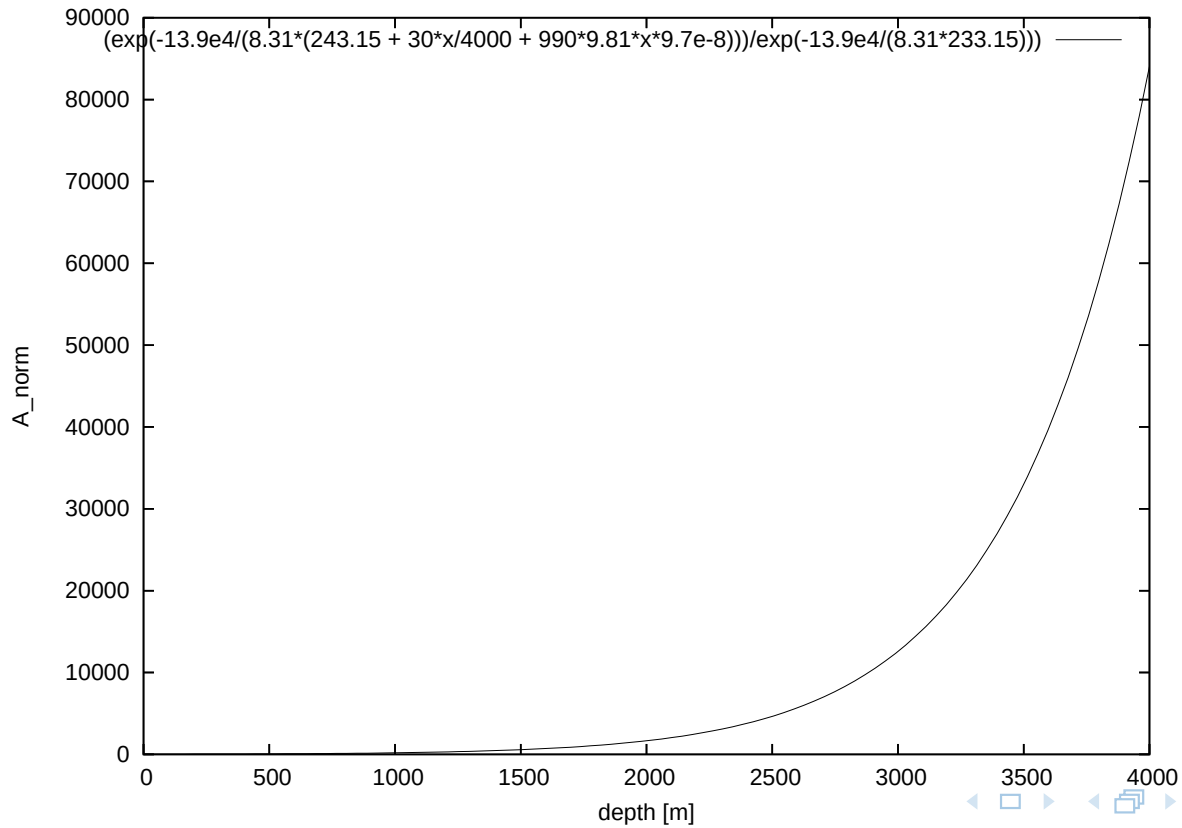

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Question 3

Proč jste nevyužil pro diskretizaci SI-aproximace metodu konečných prvků a zvolil raději metodu konečných diferencí?

Why didn't you use the finite-element method for discretization of the SI approximation, but rather chose a finite-difference method?

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- The SIA is traditionally numerically developed in as a finite-difference numerical scheme.
- The reason is that SIA is a semi-local method requiring only horizontal spatial derivatives and vertical quadratures of the field quantities.
- Advantage: simplicity, finite-difference grids also allow to use a staggered grid approach which substantially improves numerical stability
- Disadvantage: Difficult implementation of non-uniform grids, which would be much more suitable - better resolution in ice-streams, etc., lower resolution in the inland regions without much dynamics.
- Most existing large-scale models SIA-based (Ritz, Greve, Huybrechts, ...) are FD-models, but FEM SIA models exist (MacAyeal)
- FEM technique is often used for higher-order models (Larour, Gagliardini,...)

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Question 4

Nechybi v (1.83) ρ v definici barycentricke rychlosti?

Isn't there missing a ρ variable in (1.83) in the definition of barycentric velocity.

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Question 4
Nechybi v (1.83) ρ v definici barycentricke rychlosti?

Isn't there missing a ρ variable in (1.83) in the definition of barycentric velocity.

- Yes it is a misprint.

$$\vec{v}_b := \rho_1 \vec{v}_1 + \rho_2 \vec{v}_2$$

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