Boundary integral method for modeling dendritic structures

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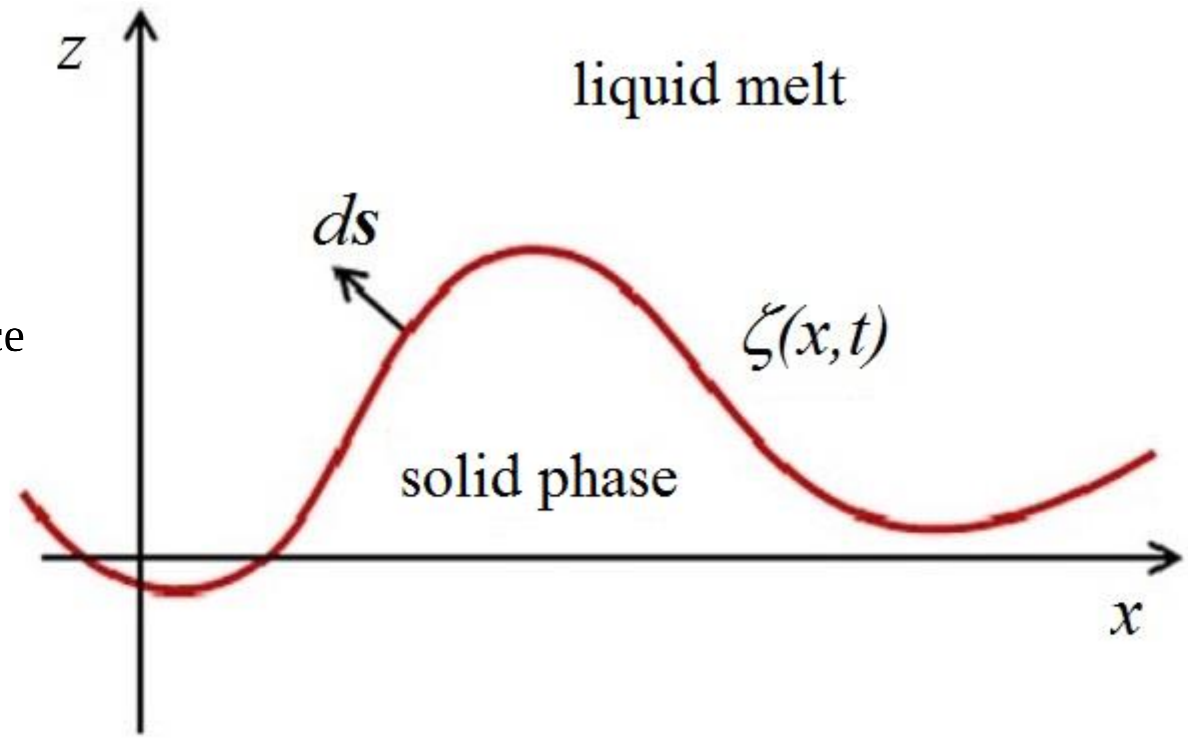
Boundary integral method*

$$\left(D_T\nabla^2 + V\frac{\partial}{\partial z} - \frac{\partial}{\partial t}\right)T = 0$$ Heat transfer equation

$$D_T(\nabla T_s - \nabla T_l)\cdot d\boldsymbol{s} = \frac{Q}{c_p}\left(V + \frac{\partial\zeta}{\partial t}\right)d^2x$$ Heat balance condition

$$T_i = T_0 - \frac{Q}{c_p}d_c(\theta)K - \tilde{\beta}(\theta)V$$ Gibbs-Thomson condition

$$\left(D_T\nabla_1^2 - V\frac{\partial}{\partial z_1} + \frac{\partial}{\partial t_1}\right)G(\boldsymbol{p}|\boldsymbol{p}_1) = -\delta(\boldsymbol{p} - \boldsymbol{p}_1)$$



Green's function is a effect in a point $\boldsymbol{p}$ of point source placed in $\boldsymbol{p}_1$

G.E. Nash, NRL Report 7679 May 1974, 1974.
G.E. Nash, M.E. Glicksman, Acta Metall. 22 (1974) 1291.
J.S. Langer, L.A. Turski, Acta Metall. 25 (1977) 1113.
J.S. Langer, Acta Metall. 25 (1977) 1121
M.N. Barber, A. Barbieri, J.S. Langer, Phys. Rev. A 36 (1987) 3340.
E.A. Brener, V.A. Mel'nikov, Adv. Phys. 40 (1991) 53.
D.A. Kessler, J. Koplik, H. Levine, Adv. Phys. 37 (1988) 255

Thermo-chemical high-speed solidification

$$-\frac{Q}{m_V c_p}\left[\Delta - \frac{d_c(\theta)}{\rho}K - \beta V - I_\zeta^T\right] - C_{l\infty} = I_\zeta^{CH} \quad * \qquad d_c(\theta) = \left(\gamma(\theta) + \frac{d^2\gamma}{d\theta^2}\right)\frac{T_0 c_p}{Q^2}$$

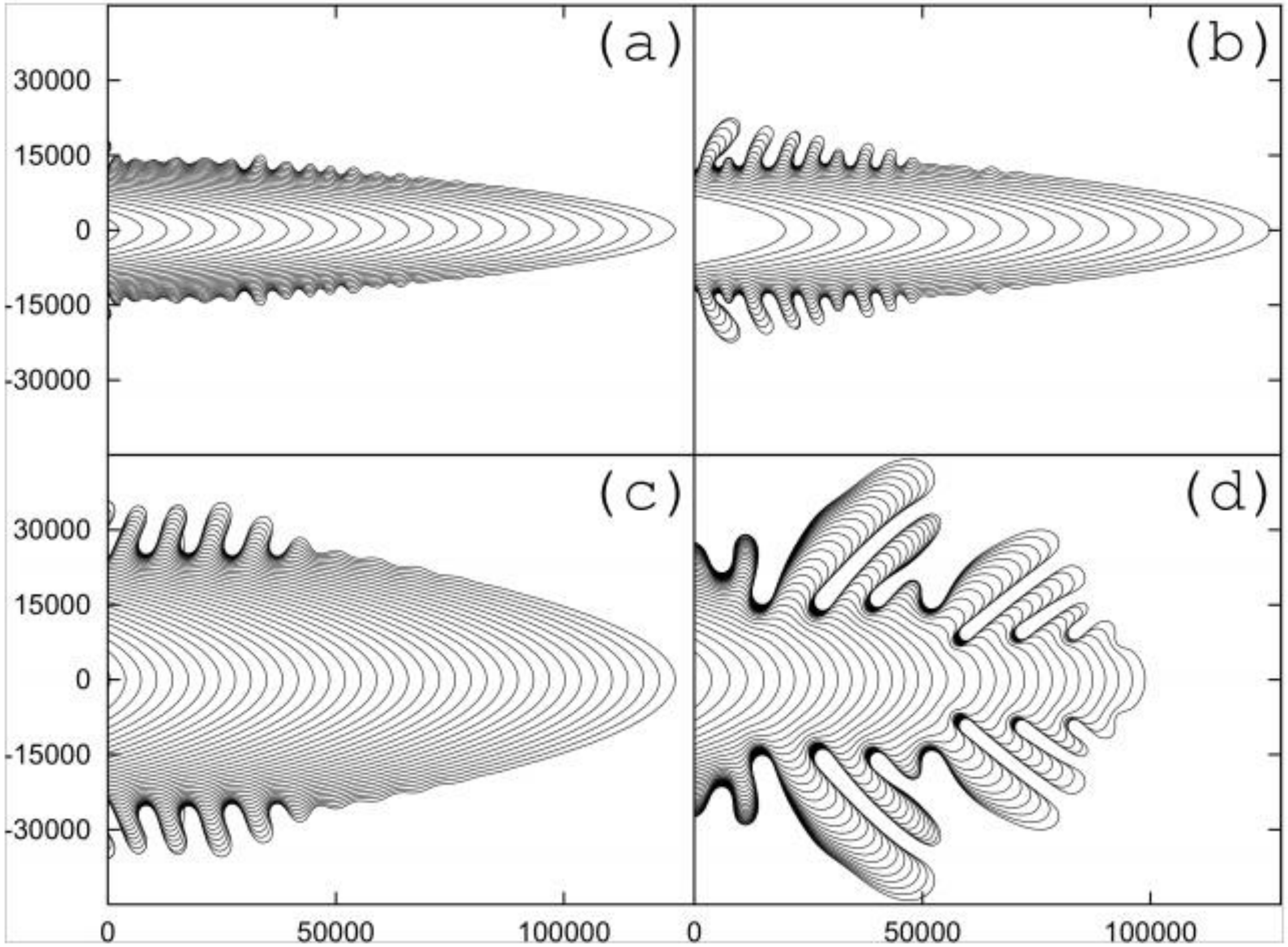
$$I_\zeta^T = 2\left(\frac{P_T}{2\pi}\right)^{3/2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} d^2\boldsymbol{x}_1 \exp\{-P_T[\zeta(\mathbf{x}) - \zeta(\mathbf{x}_1)]\}K_{1/2}\left(P_T\sqrt{b_p}\right)/b_p^{1/4}$$

$$I_\zeta^{CH} = \frac{2(1-k_V)C_i}{\sqrt{1-P_C\tau_*}}\left(\frac{P_C}{2\pi}\right)^{3/2}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} d^2\boldsymbol{x}_1 \exp\left\{-\frac{P_C[\zeta(\mathbf{x}) - \zeta(\mathbf{x}_1)]}{1-P_C\tau_*}\right\}K_{1/2}\left(\frac{P_C\sqrt{b_H}}{1-P_C\tau_*}\right)/b_H^{1/4}$$

$$b_H = (1-P_C\tau_*)|\mathbf{x}-\mathbf{x}_1|^2 + \big(\zeta(\mathbf{x}) - \zeta(\mathbf{x}_1)\big)^2, \qquad b_p = |\mathbf{x}-\mathbf{x}_1|^2 + \big(\zeta(\mathbf{x}) - \zeta(\mathbf{x}_1)\big)^2$$

D. V. Alexandrov and P. K. Galenko, Acta Mater. **137,** 64–70 (2017)

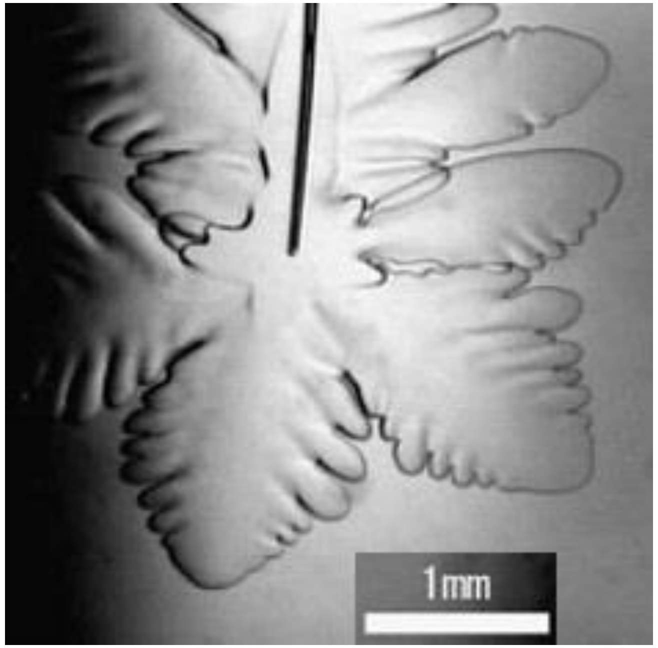
Numerical experiments on selection of dendritic tip

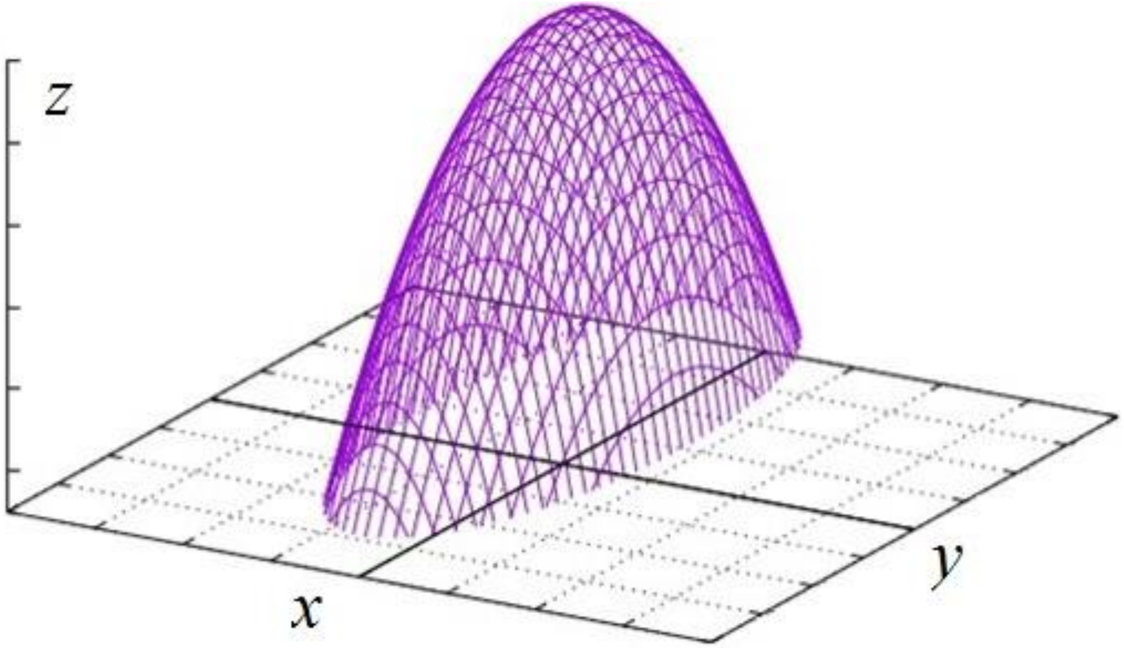


Stroboscopic plots of solidification front positions which show the effect of anisotropy on the dendrite shape selection. Calculations have been made for the constant undercooling, $\Delta T = 23K$, constant kinetic anisotropy, $\alpha_\beta = 0.07$, and various anisotropy of interfacial energy α_d: (a) – 0.100, (b) – 0.085, (c) – 0.055, (d) – 0.040

P. K. Galenko, D. V. Alexandrov, and E. A. Titova, Phil Trans R Soc. A **376**, 20170218 (2017).

Non-axisymmetric dendritic growth





Ice dendrite, $T = -0.4$°C *

Yoshikazu Teraoka, Akio Saito, Seiji Okawa International Journal of Refrigeration 25 (2002) 218–225

$$\zeta(x,y) = -\frac{x^2}{2(\omega-b)} - \frac{y^2}{2(\omega+b)} + \frac{\omega}{2}$$

$$I_\zeta^T = \left(\frac{P_T}{2\pi\rho}\right)^{3/2} \frac{1}{\sqrt{V}} \int_0^\infty \frac{d\tau}{\tau^{3/2}} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \exp\left\{-\frac{P_T}{2\rho V\tau}\left[|x-x_1|^2 + \left(\frac{x_1^2-x^2}{2(\omega-b)} + \frac{y_1^2-y^2}{2(\omega+b)} + \tau V\right)^2\right]\right\} dx_1 dy_1$$

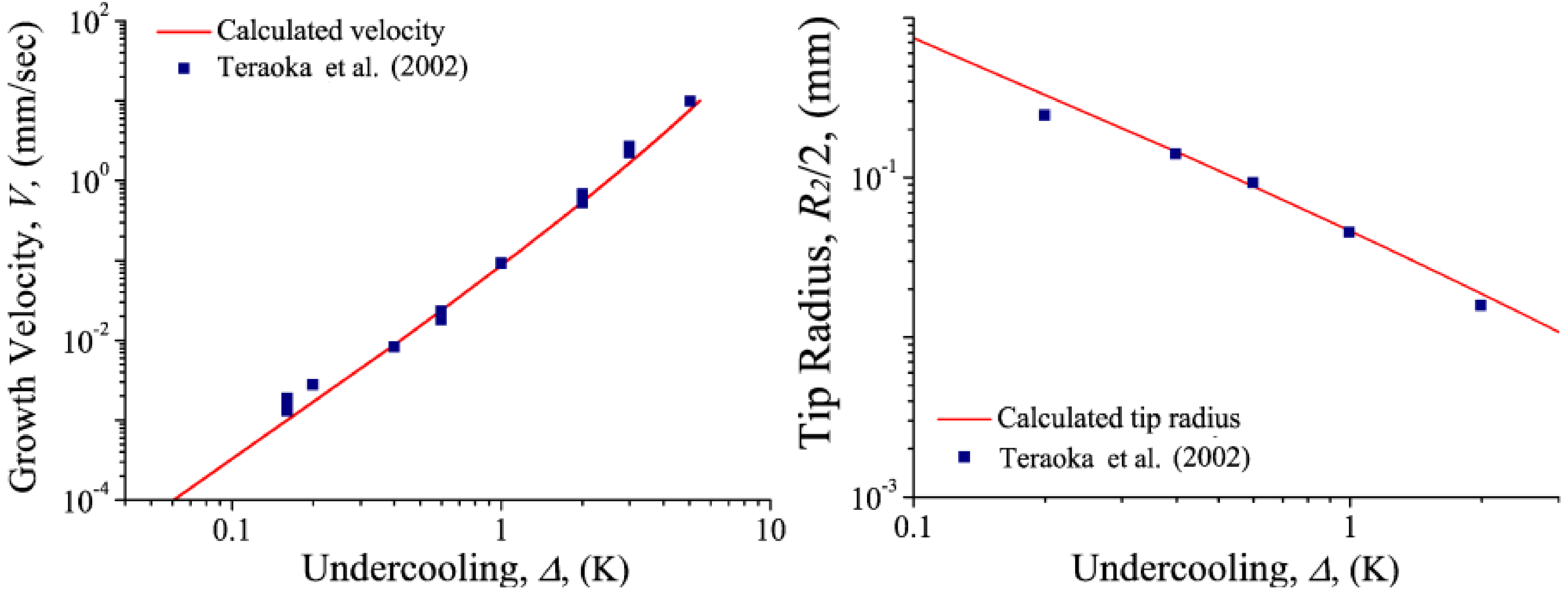
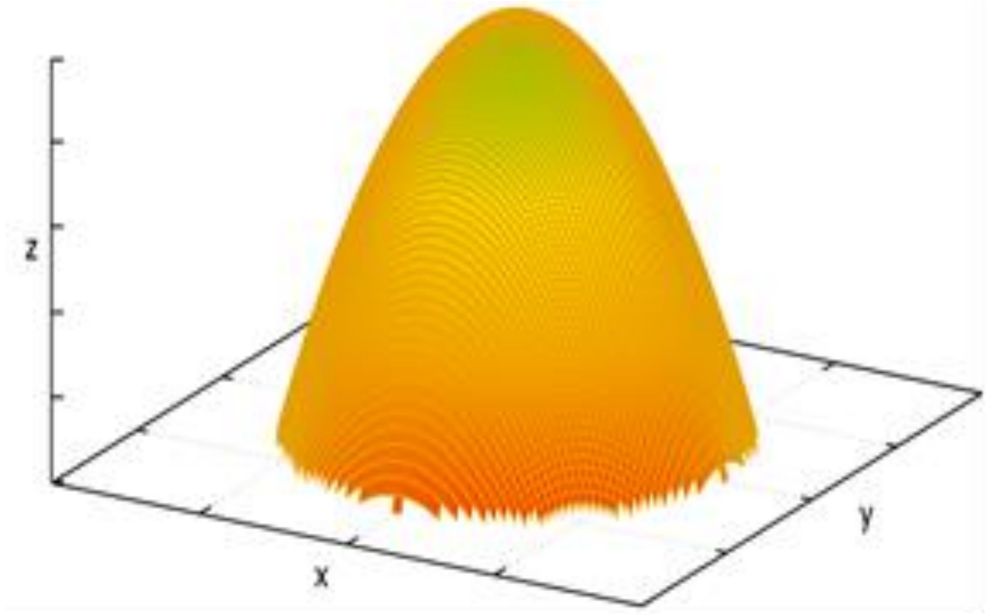
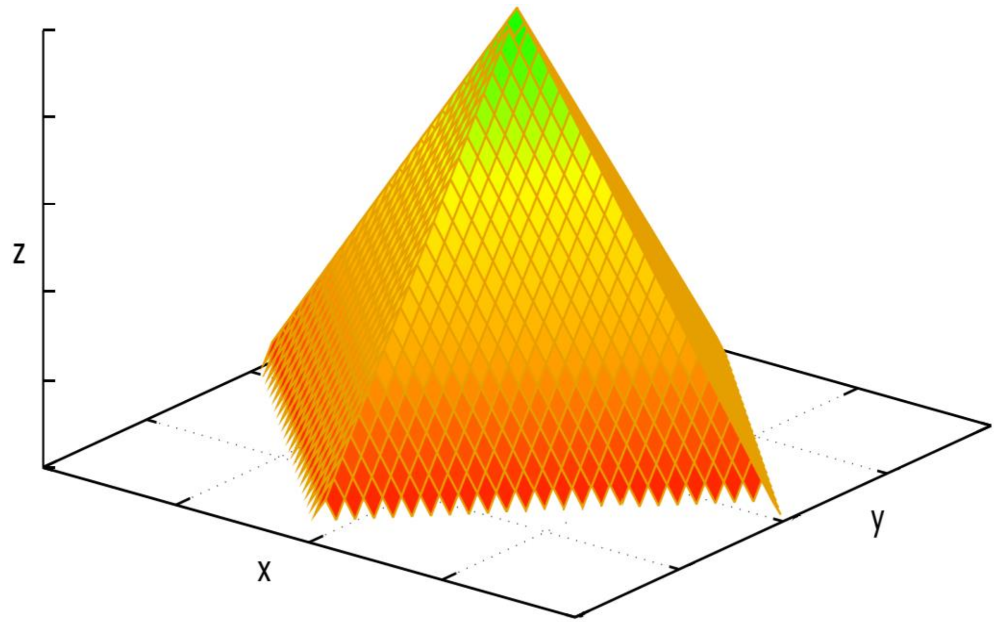


Fig. 3. Calculated dendrite growth velocity (left panel) and dendrite tip radius (right panel) in the main plane at $\alpha_d = 0.04$, $\beta_0 = 0.0012$ and $\sigma_0 = \sigma_{06} = 0.003$ (solid line) in comparison with experimental data [28] (points) obtained for solidification of undercooled H_2O.

[28] Yoshikazu Teraoka, Akio Saito, Seiji Okawa International Journal of Refrigeration 25 (2002) 218–225





$$\zeta(\mathbf{x}) = \zeta(x, y) = a\left(x^2 + y^2\right) + b(x + y) + c,\ \ a < 0.$$

$$\zeta(x, y) = a\left(|x| + |y|\right) + b,\ \ a < 0.$$

$$I_\zeta^T = \frac{-P_T}{2a}\exp\left(-\frac{P_T}{2a}\right)\int_1^\infty \frac{\exp\left(P_T\eta/(2a)\right)}{\eta}d\eta.$$

$$I_\zeta^T = \frac{1}{\pi\sqrt{1+a^2}}\int_0^\infty \frac{d\omega}{\omega}\int_0^\infty \exp\left(-\omega\left[1 + \frac{\chi^2(x_1,\omega)}{a^2}\right]\right)\mathrm{erfc}(-\chi\sqrt{\omega})dx_1$$

$$\Delta - \frac{d_c(\theta)}{\rho}K - \beta V = I_\zeta^T$$

Alexandrov D V and Galenko P K 2020 Phil. Trans. R. Soc. A 378 20190243

Interface shape in large Peclet number limit

$$-\frac{Q}{m_V c_p}\left[\Delta - \frac{d_c}{\rho}\mathrm{K} - \beta V - I_\zeta^T\right] - C_{l\infty} = I_\zeta^{CH} \qquad P_T = \frac{\rho V}{2D_T} \gg 1, \qquad P_C = \frac{\rho V}{2D_C} \gg 1$$

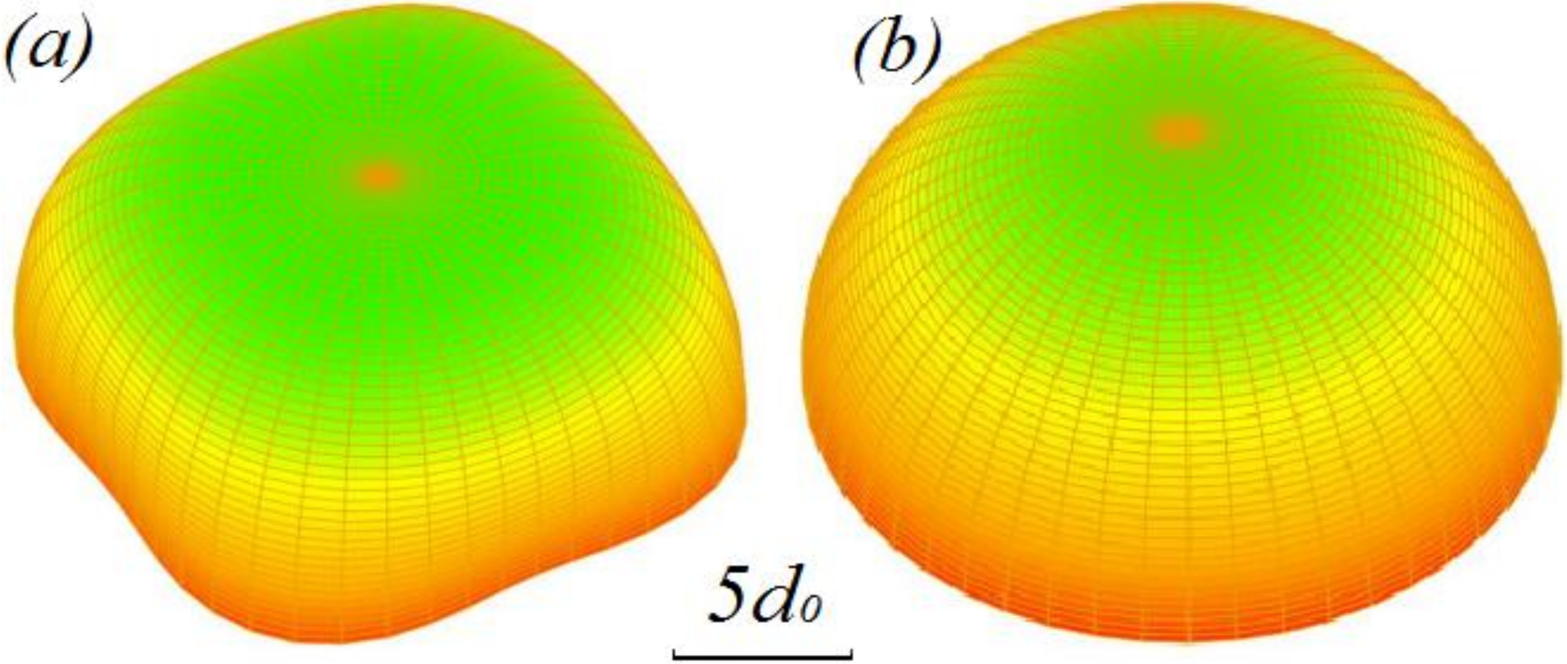
$$I_\zeta^{CH} = \frac{(1-k_V)C_i}{\sqrt{1-P_C\tau_*}}\frac{P_C}{\pi}\int_{-\infty}^{\infty}\exp\{-\lambda[\zeta(x)-\zeta(x_1)]\}K_0\left(\lambda\sqrt{b_H}\right)dx_1, \qquad K_0\left(\lambda\sqrt{b_H}\right) \approx \sqrt{\frac{\pi}{2\lambda}}\frac{\exp\left(-\lambda\sqrt{b_H}\right)}{b_H^{1/4}}$$

$$\lambda = \frac{P_C}{1-P_C\tau_*} = \frac{P_C}{1-V^2/V_D^2} \gg 1$$

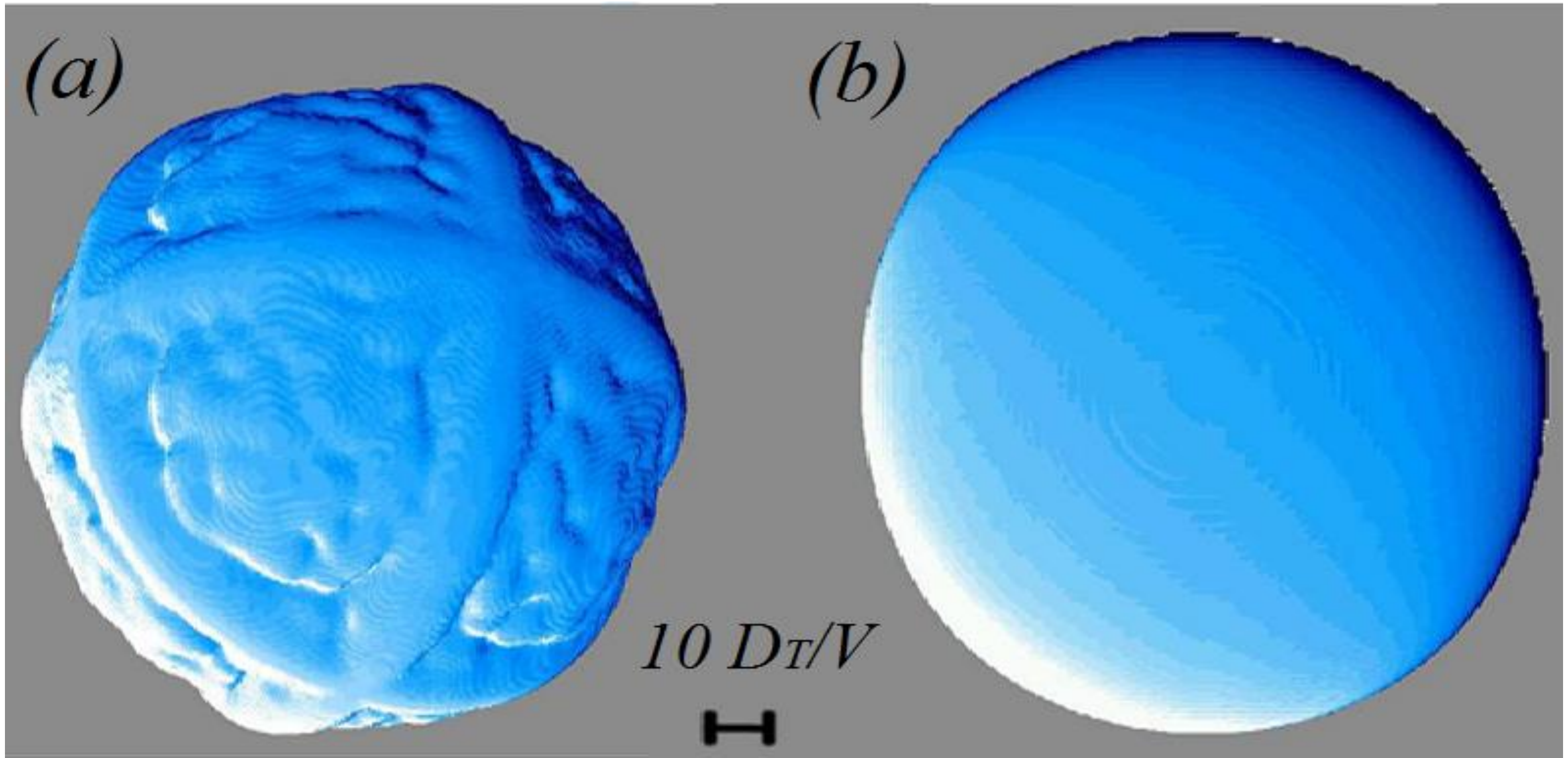
$$I_\zeta^{CH} \approx \frac{(1-k_V)C_i\sqrt{P_C}}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\frac{\exp\{\lambda S_C(x,x_1)\}}{b_H^{1/4}}dx_1$$

$x_1 = x_0$ - point of maximum for S_C

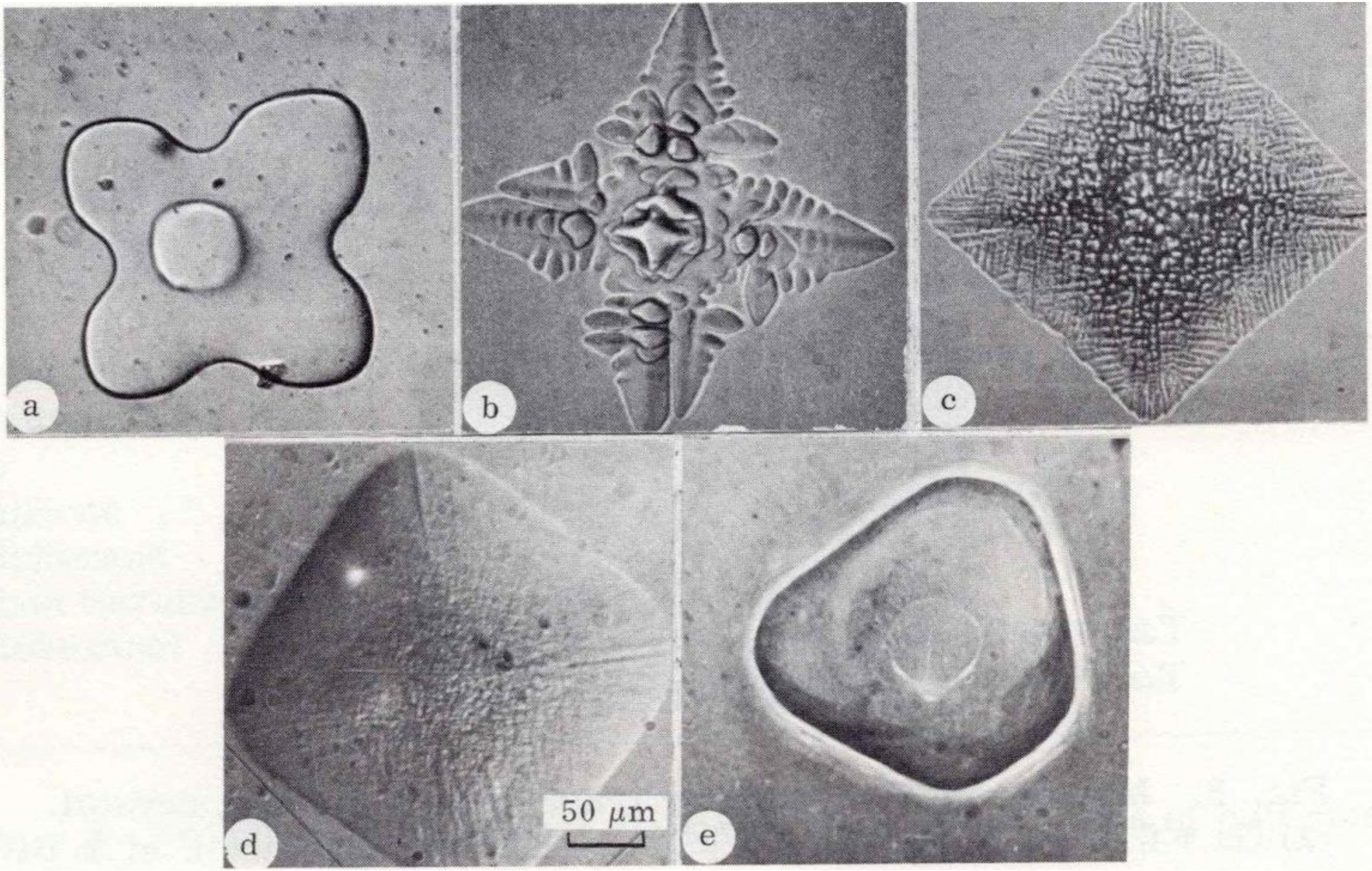
Alexandrov DV, Titova EA, Galenko PK. 2019 A shape of dendritic tips at high Péclet numbers. *J. Cryst. Growth* **515**, 44–47.



A globular form of dendritic tips growing from Ti-Al melt at the kinetically-limited regime, dimensionless undercooling $\Delta = 1.0$; growth Péclet number $P_T = 1$ and with (a) anisotropic interface and (b) isotropic interface.



Globular shapes of crystals from article Galenko PK, Herlach DH. 2006 In: *Complexus mundi: Emergent patterns in nature*, New Jersey, World Scientific, pp. 199–208 obtained by the phase field model of Karma and Rappel. Computations were made for nickel crystals growing with (a) the anisotropic interface at the dimensionless undercooling $\Delta = 1.1$ and (b) the isotropic interface at the $\Delta = 1.2$.



Interfacial shape of cyclohexane crystal at different values of undercooling:

(a) ΔT = 0.3°C;
(b) ΔT = 0.45°C;
(c) ΔT = 2.35°C;
(d) ΔT = 3.5°C;
(e) ΔT = 10.25°C;

Ovsienko DE, Alfintsev GA 1986 Pecularities of melt growth of crystals with different entropies of melting. Growth of Crystals, Vol. 13, 137–146

Convective boundary integral

$$\int_{-\infty}^{t+\varepsilon}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} G(\boldsymbol{p}|\boldsymbol{p}_1)\left[2+\dot{\zeta}\right] dt_1\, dx_1 dy_1 - 2\lambda I_c = \Delta$$

$$G(\boldsymbol{p}|\boldsymbol{p}_1) = \left(\frac{1}{4\pi(t-t_1)}\right)^{3/2} \exp\left(-\frac{|x-x_1|^2 + [(z-z_1)+2(t-t_1)]^2}{4(t-t_1)}\right)$$

Green's function for a heat diffusion problem without convection

$$I_c = \int_{-\infty}^{t+\varepsilon}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{\zeta(\boldsymbol{p}_1)}^{\infty} G(\boldsymbol{p}|\boldsymbol{p}_1)\,(\boldsymbol{v}\cdot\nabla T) dt_1 dx_1 dy_1 dz_1$$

Convective contribution

$$\lambda = \frac{U_\infty}{V},$$

$U_\infty -$ Unperturbed flow velocity

D. A. Saville and P. J. Beaghton, Phys Rev. A **37** 3423–3430 (1988)

Convective boundary integral for a needle dendrite

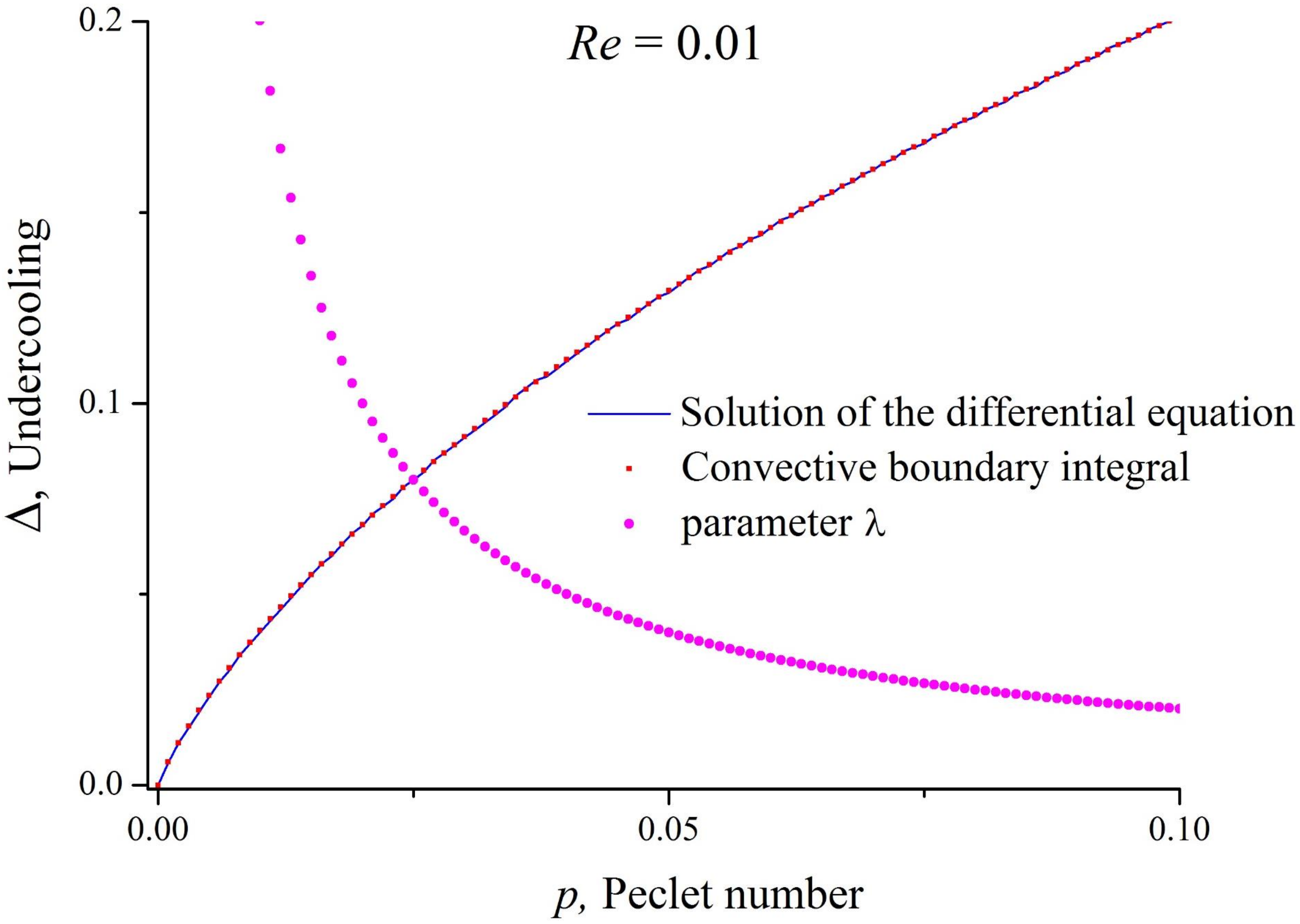
$$\Delta = p\exp(p)\int_{p}^{\infty}\frac{\exp(-x)}{x}dx + \frac{2\lambda p\exp\big(p(1+\lambda)\big)}{E_1(Re/2)}\int_{1}^{\infty}\frac{A(w)I_\Delta(w)}{w}dw$$

$$A(w) = \left(\frac{1}{4\pi}\right)^{3/2}\left(\frac{2}{w\,Re}e^{-\frac{Re}{2}} - e^{-\frac{Re}{2}w} - E_1\,(Re/2) + E_1\,(Re\,w/2)\right)\times$$

$$\exp\left\{-pw(1+\lambda) + \frac{2p\lambda}{Re\,E_1(Re/2)}\left[\int_{\frac{Re}{2}}^{\frac{Re}{2}w_1} E_1(x)dx - E_1\left(\frac{Re}{2}\right) + E_1\left(\frac{Re\,w}{2}\right)\right] + \frac{we^{-\frac{Re}{2}}\ln w}{Re\,E_1(Re/2)}\right\}$$

$$I_\Delta(w_1) = \int_0^\infty \frac{d\tau}{\tau^{3/2}}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\exp\left(\frac{-\{(x-x_1)^2 + (y-y_1)^2 + [z(x,y) - z(x_1,y_1) + 2\tau]^2\}}{4\tau}\right)dy_1dx_1$$

Comparison of convective integral solution and solution of differential problem



Conclusion

- Using the boundary integral method, we can find the temperature and solute concentration distributions in the vicinity of a dendrite with a given shape (including interface temperature and concentration);
- Analysis of the stability of the boundary integral equation allows to select stable forms of dendrite growth. This leads to the condition of microscopic solvability, which allows to obtain a selection criterion for defining the parameters of the tip of a growing dendrite;
- The boundary integral equation can be analytically solved in the limiting cases of small and large Peclet numbers;
- The boundary integral method allows to numerically determine the shape of the solid/liquid interface, with or without the presence of convection.