

TRANSIENT EFFECTS IN PLANAR SOLIDIFICATION OF DILUTE BINARY ALLOYS



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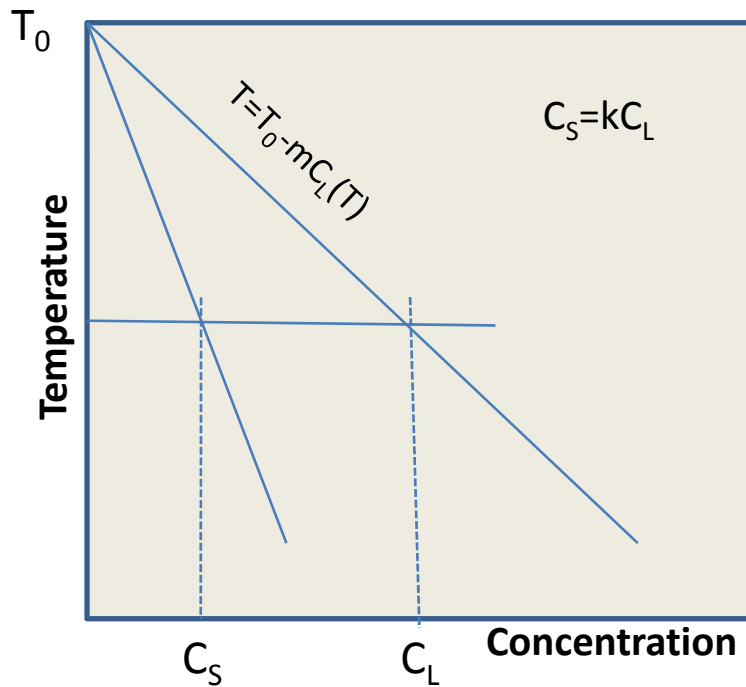
Modeling of Directional Solidification

Diffusion controlled growth

Frozen temperature approximation $T(z)=T_0+G(z-V_0t)$

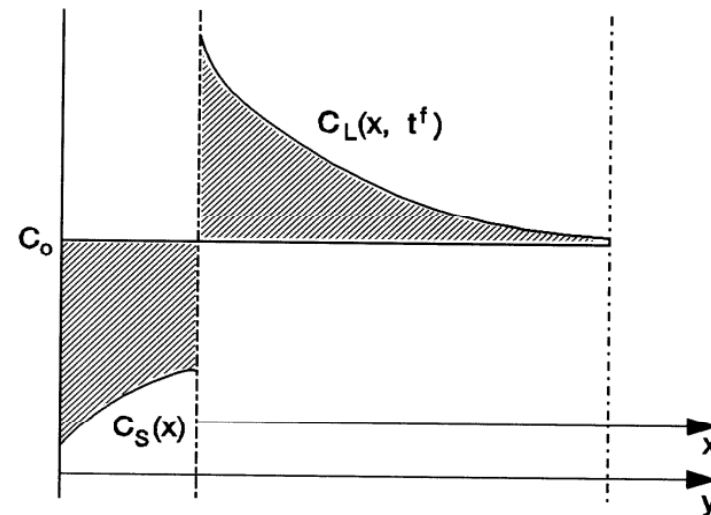
Local equilibrium at interface

One dimensional case - planar interface growth



G – thermal gradient in liquid phase

V_0 – furnace translation rate



Governing Equations

Solute diffusion in liquid phase in the coordinate system co-moving with the interface

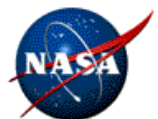
$$\frac{\partial c}{\partial t} - V \frac{\partial c}{\partial z} = D \frac{\partial^2 c}{\partial z^2}$$

Interface boundary condition

$$D \frac{\partial c}{\partial z} = (c_S - c_L)V = -c(1 - k)V$$

Interface velocity

$$V = V_0 + \frac{m}{G} \frac{\partial c}{\partial t}$$



Initial Conditions

At time $t=0$:

Interface velocity is zero

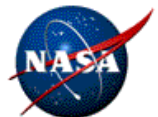
Solute concentration in liquid phase is C_0 everywhere

Solute concentration in solid is kC_0

Temperature at the interface position z_0 is $T_0 - Gz_0$

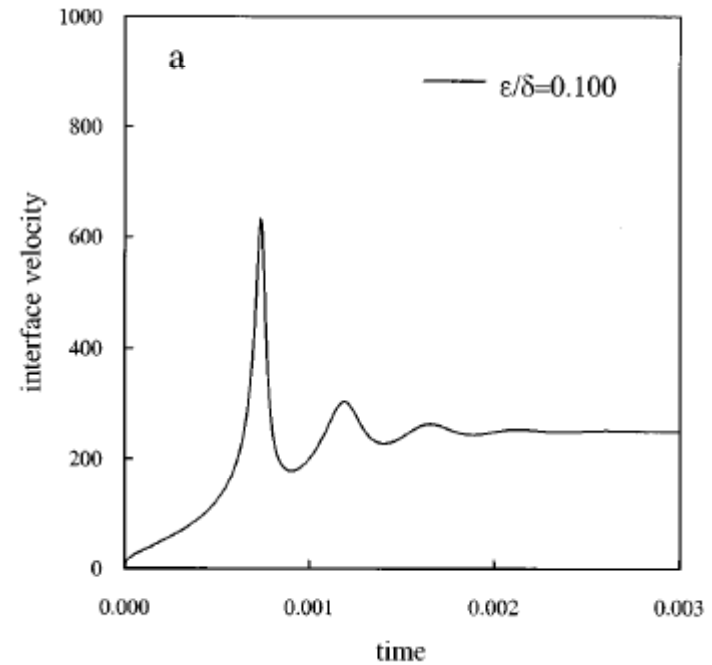
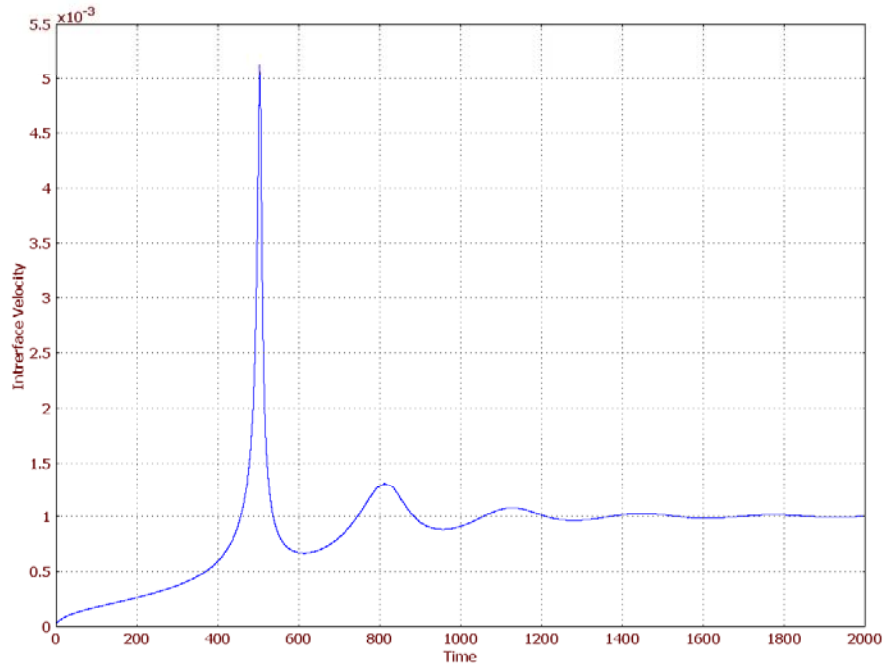
Initial transient during directional solidification was treated by Tiller in 1953. Some recent works include:

- W. Huang et al, J.Cryst.Growth 182 (1997) 212-218.
- D. Ma et al, J. Cryst.Growth 169 (1996) 170-174.
- A. Karma, A. Sarkissian, Phys.Rev. E 47,(1993) 513-533.
- B. Caroli et al, J.Cryst. Growth 132 (1993) 377-388.
- Majchrzak et al, J. Mater. Proc. Techn. 78 (1998) 122-127.
- Ch. Charach et al, Phys. Rev. E 54 (1996) 588-598.
- M.Conti, Phys.Rev. E 60 (1999) 1913-1920.



Numerics

Numerical solution by COMSOL 3.3 and FLEXPDE 5



M. Conti, Phys Rev. E (1999)

Volterra Integral Equation

$$\int_0^t dt' \int_{z(t')}^{\infty} G(t, z, t', \xi) \left[D \frac{\partial^2 c}{\partial \xi^2} - \frac{\partial c}{\partial t'} \right] d\xi = 0 \quad G(t, z; t', z') = \frac{1}{\sqrt{4\pi D(t-t')}} \exp\left(-\frac{(z-z')^2}{4D(t-t')}\right)$$

$$c_0(t) = -\frac{1}{\sqrt{\pi D}} \int_0^t e^{-\frac{(z-z')^2}{4D(t-t')}} \left[\frac{V(kc_0 - (1-k)c_\infty)}{\sqrt{(t-t')}} - \frac{c_0(z-z')}{2((t-t'))^{3/2}} \right] dt'$$

Here $c_0(t)$ is the interface concentration, $z(t)$ is the interface position, $V(t)$ is the interface velocity, C_∞ is the concentration in the liquid far from interface

Analytic Analysis

Tiller's case of a constant growth rate $V=V_0$

$$c_0(t) = -\frac{V}{\sqrt{\pi D}} \int_0^t \frac{e^{-\frac{V^2(t-t')}{4D}}}{\sqrt{(t-t')}} \left(kc_0 - (1-k)c_\infty - \frac{c_0}{2} \right) dt'$$

Laplace transform technique

$$c(s) = -\frac{V}{\sqrt{\pi D}} \left[c(s) \left(k - \frac{1}{2} \right) - \frac{c_\infty (1-k)}{s} \right] L(K)$$

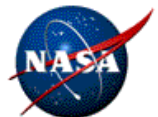
$$L(K) = \sqrt{\frac{\pi}{s + \frac{V^2}{4D}}} \quad c(s) = -\frac{c_\infty \sqrt{D}}{kV} \left[\frac{1}{\sqrt{s+a+b}} + \frac{b}{s} - \frac{\sqrt{s+a}}{s} \right] \quad a = \frac{V^2}{4D} \quad b = \frac{V(k-1/2)}{\sqrt{D}}$$

Inverse Laplace recovers Tiller's formula

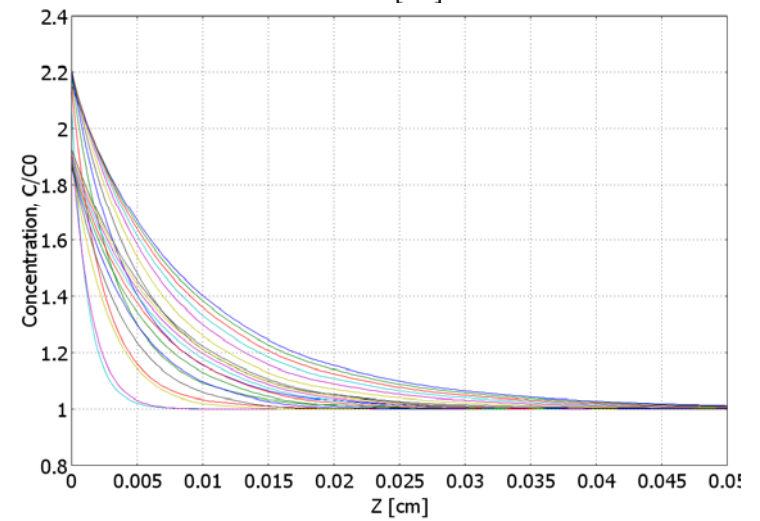
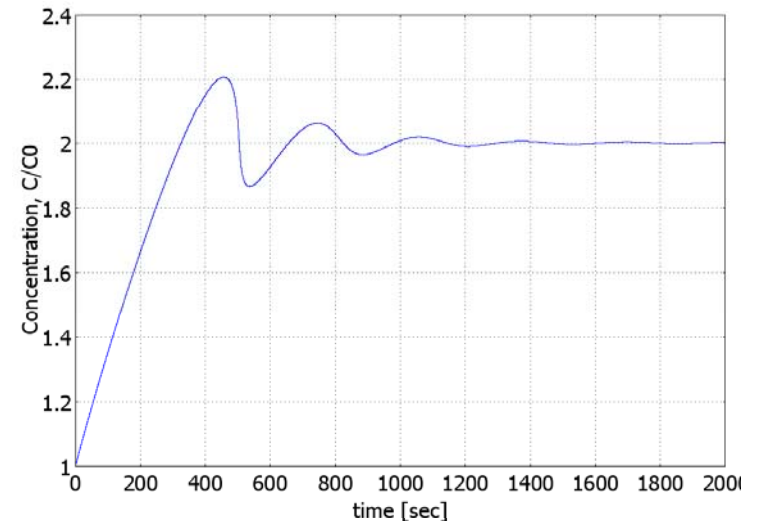
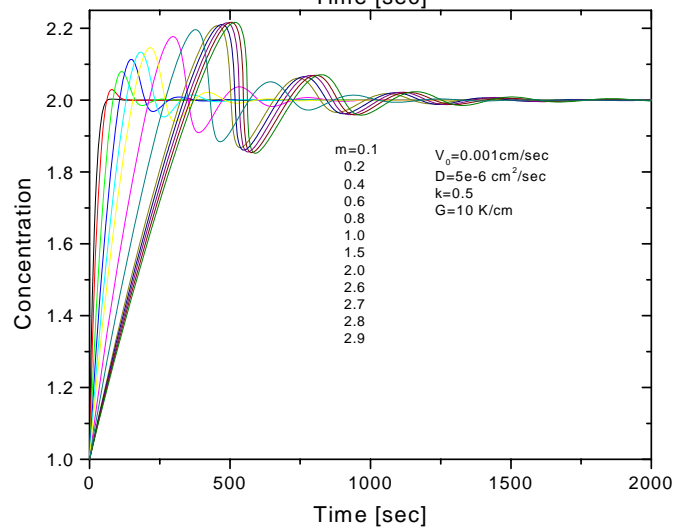
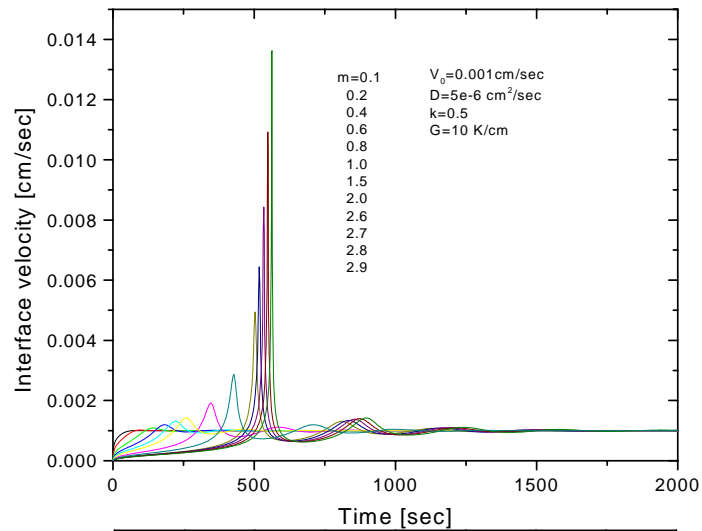
$$L^{-1} [] = b - b \operatorname{erfc}(b\sqrt{t}) e^{(b^2-a)t} - \sqrt{a} \operatorname{erf}(\sqrt{at})$$

Small time asymptotics

$$V = -\frac{2V_0}{mc_\infty(1-k)} \sqrt{\frac{Dt}{\pi}} \quad c = -\frac{t}{b} + \frac{4t^{3/2}}{3b^2\sqrt{\pi}(k-1)}$$

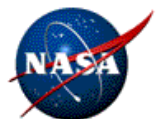


Results



Conclusions

- Strong spikes in growth velocity are obtained for the simplest, physically sound, start-up model of directional solidification.
- Spikes are sensitive to the flow in the system and to the latent heat.
- Integral equation approach can be managed numerically easier than the Finite Elements/Volume methods.
- The spike phenomenon is not uniquely related to the phase field model of the solidification.



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