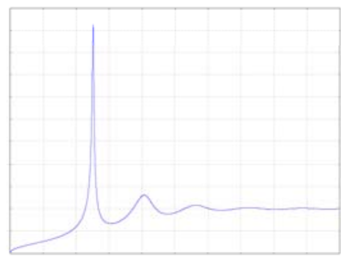
TRANSIENT EFFECTS IN PLANAR SOLIDIFICATION OF DILUTE BINARY ALLOYS



Konstantin Mazuruk and Martin P. Volz

The 21st Conference on Crystal Growth and Epitaxy-West
June 8 - 11, 2008, Stanford Sierra Camp, Fallen Leaf Lake, CA

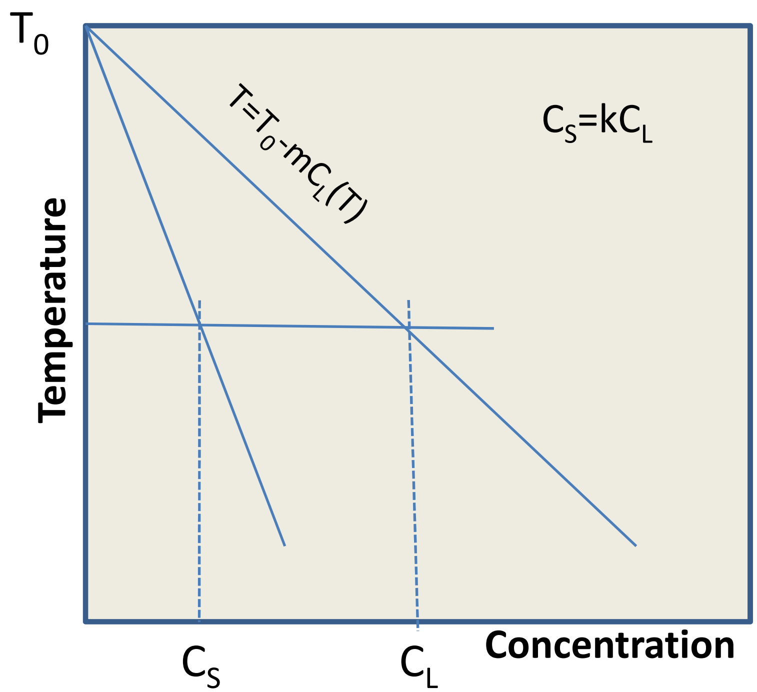
Modeling of Directional Solidification

Diffusion controlled growth

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

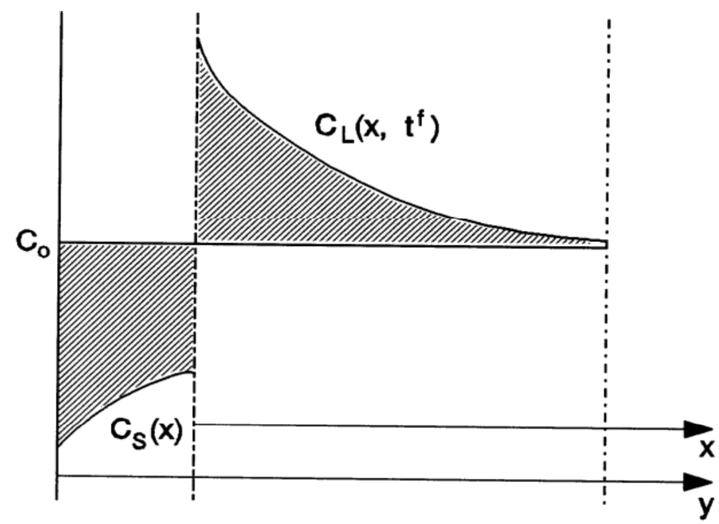
Local equilibrium at interface

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

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

Interface velocity

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

Initial Conditions

At time t=0:

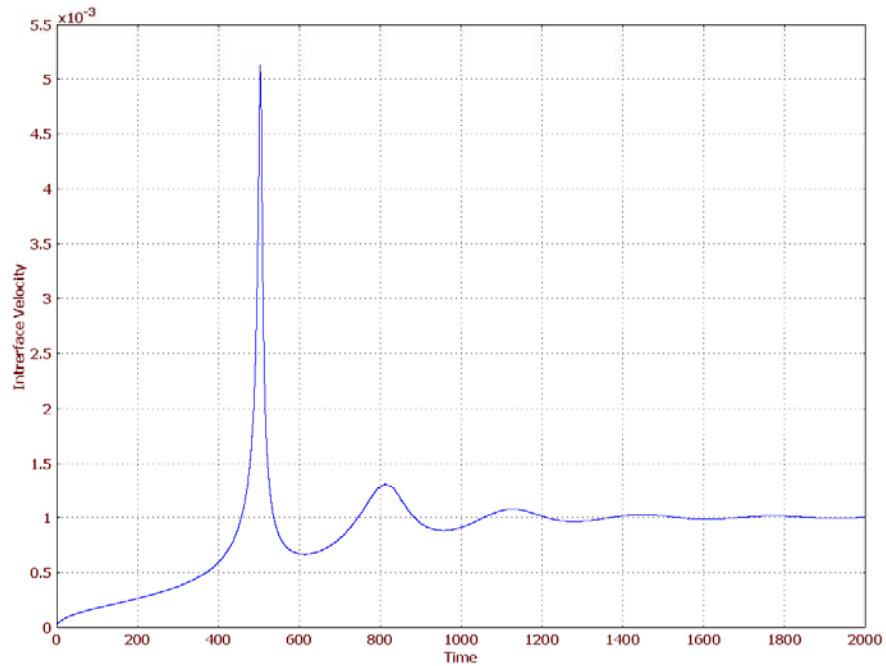
Interface velocity is zero
Solute concentration in liquid phase is C_0 everywhere
Solute concentration in solid is kC_0
Temperature at the interface position z_0 is $T_0 - Gz_0$

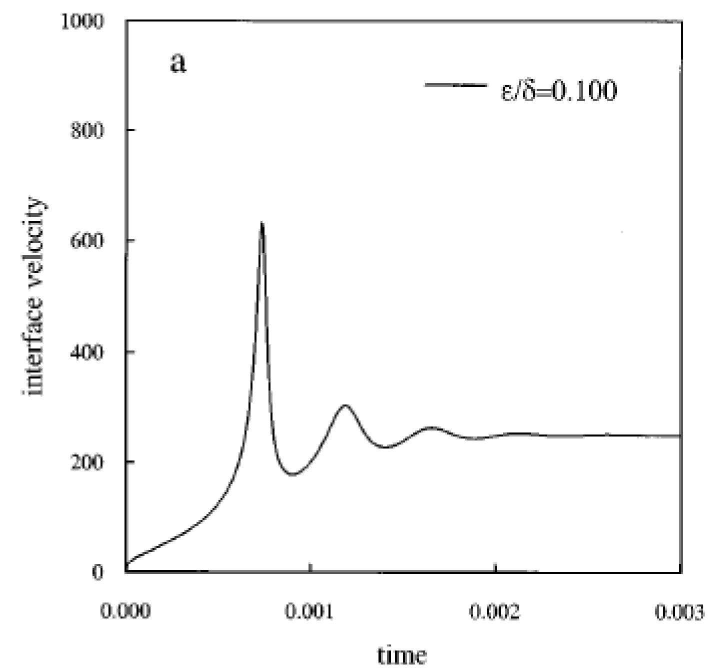
Initial transient during directional solidification was treated by Tiller in 1953. Some recent works include:

- 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

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

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

Here $c_0(t)$ it 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

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

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

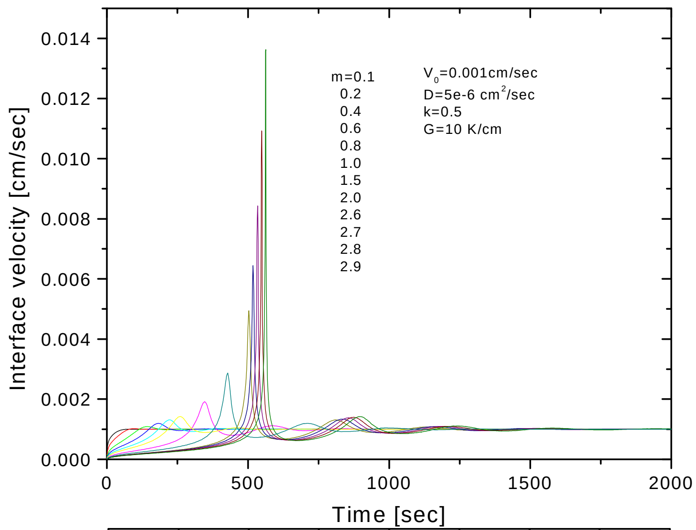
Inverse Laplace recovers Tiller's formula

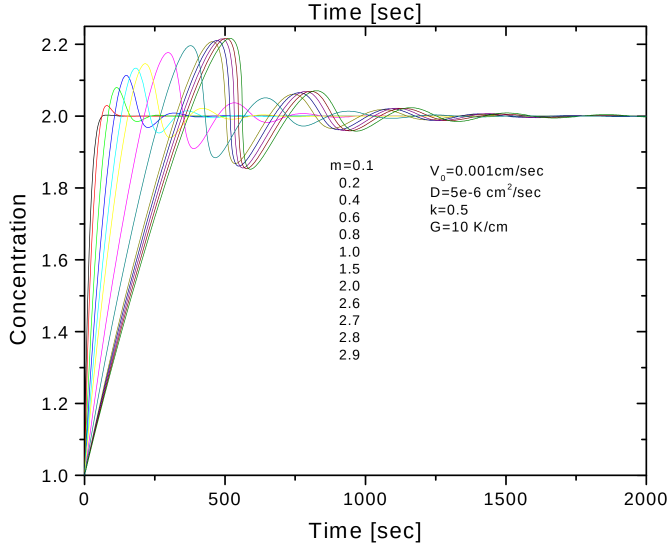
$$L^{-1}[\ ] = b - b\,\mathrm{erfc}\left(b\sqrt{t}\right) e^{\left(b^2-a\right)t} - \sqrt{a}\,\mathrm{erf}\left(\sqrt{at}\right)$$

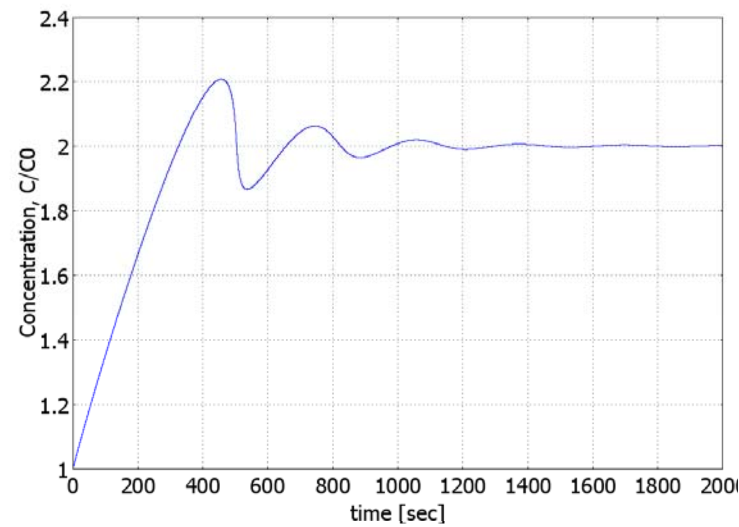
Small time asymptotics

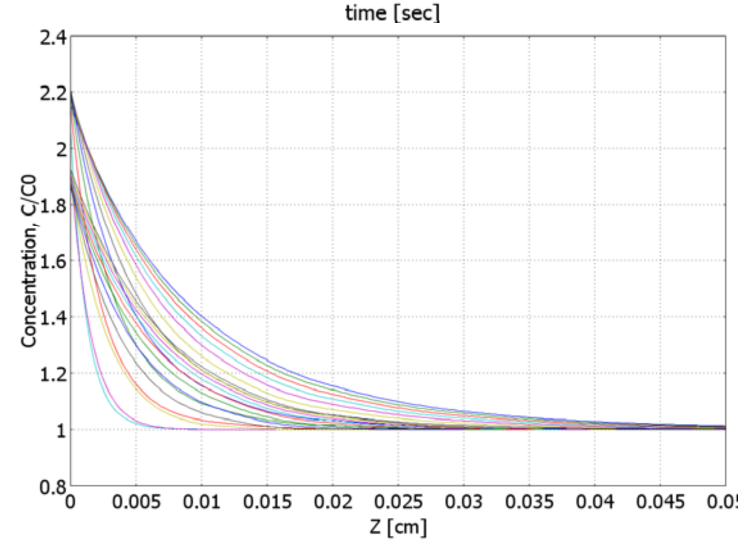
$$V = -\frac{2V_0}{mc_\infty (1-k)} \sqrt{\frac{Dt}{\pi}} \qquad c = -\frac{t}{b} + \frac{4t^{3/2}}{3b^2 \sqrt{\pi} (k-1)}$$

Results


Interface velocity [cm/sec]
Time [sec]
m=0.1
0.2
0.4
0.6
0.8
1.0
1.5
2.0
2.6
2.7
2.8
2.9
V_0=0.001cm/sec
D=5e-6 cm^2/sec
k=0.5
G=10 K/cm


Concentration
Time [sec]
m=0.1
0.2
0.4
0.6
0.8
1.0
1.5
2.0
2.6
2.7
2.8
2.9
V_0=0.001cm/sec
D=5e-6 cm^2/sec
k=0.5
G=10 K/cm


Concentration, C/C0
time [sec]


Concentration, C/C0
Z [cm]

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.