EFFECT OF CONVECTION ON THE MICROSTRUCTURE OF A LAMELLAR EUTECTIC GROWING WITH A STEPPED INTERFACE

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ABSTRACT

This paper describes a two-dimensional model developed to study the influence of convective flow on the concentration field ahead of a growing lamellar eutectic, when one phase projects out into the melt creating a stepped interface. The two dimensional convective flow field, which is periodic in the horizontal direction, was computed numerically using the software FLUENT. The velocity field generated due to the flow of melt over the steps was then incorporated into a finite difference scheme employed to solve the concentration field. The average interfacial composition was calculated and converted to lamellar spacing using the Jackson and Hunt minimum supercooling criterion. It was found that a stepped interface is more sensitive to convection than a planar interface.

1. INTRODUCTION

The primary motivation for this work arises from experiments on eutectic solidification in the reduced gravity environment of space. Some space-grown samples exhibited marked structural differences from identically processed earth-grown samples [1,2]. For example, when the MnBi/Bi eutectic was solidified in space the average fiber spacing λ was half of what was obtained on earth [3]. The difference has been attributed to the absence of convective currents at low g as compared to conditions on earth. The application of a magnetic field to suppress convection showed the same effect on the MnBi/Bi microstructure as solidification in space [10].

As a result of the above experimental observations, theoretical models have been developed to determine the effect of convection on the spacing of eutectic alloys. Baskaran and Wilcox [4] and Chandrasekhar et al. [5] developed a two-dimensional model to study the effect of convection on the microstructures of lamellar eutectics. Caram and Wilcox [7] developed a three dimensional numerical model for the influence of convection on rod-like eutectic microstructure.

Decantation experiments during the solidification of MnBi/Bi eutectic established that the MnBi fibers project ahead of the Bi matrix [6]. In all the prior numerical models developed to predict the effect of convection on eutectic microstructure it had been assumed that the interface is planar. In the present work a lamellar stepped structure was studied. This was selected rather than a rod structure for computational ease; the diffusional domain of a lamellar eutectic is two dimensional rather than three dimensional as in the case of a rod eutectic. The Jackson and Hunt treatment [8] was assumed to be valid, and we performed calculations similar to those of ref. [5]. The resulting conclusions are expected to hold for a rod structure in a semi-quantitative sense. Details are given elsewhere [9].

2. EQUATIONS

As the adjacent phases of a binary eutectic grow, atoms are rejected into the melt due to partitioning. This partitioning creates a lateral composition gradient, which generates lateral diffusion in order to redistribute the two components across the interface and to sustain growth. As a result, the eutectic phase transformation is influenced by mass transfer processes. In addition to diffusion, convective mass transfer generated by the flow along the solid liquid interface must be taken into account.

The general steady state mass transfer equation for a binary mixture can be written as:

$$D\nabla^2 C - \vec{U} \cdot \nabla C = 0 \tag{1}$$

where D is the diffusion coefficient, $\vec{U}$ is the velocity and C is the concentration of one of the components. To account for the influence of convection in eutectic growth, a well developed laminar shear flow was introduced in front of the solid-liquid interface, normal to both the growth direction of the lamellae and to the lamellae themselves. The velocity field generated by the flow of melt over the steps was computed numerically. The melt was assumed to possess constant material properties, including diffusivity D and kinematic viscosity ν. The two dimensional flow field was assumed to be periodic in the horizontal direction. The governing fluid flow equations were written in a reference frame that moves vertically upward at the growth velocity. A no-slip condition was used for the tangential component of the velocity at the interface. The boundary at the top of the domain was placed at such a distance from the interface that it did not influence either the flow field or the concentration field near the interface.

The fluid velocity components U_y in the y direction and U_x in the x direction were calculated using a software package called FLUENT. FLUENT is a computer code created by Creare Incorporated for simulating a wide range of fluid flow problems.

It uses a finite difference numerical procedure to solve the Navier-Stokes equation. The domain to be investigated is divided into a finite number of cells and the partial differential equation is discretized over these units to produce a sequence of algebraic relations. An iterative scheme is then employed to solve for the equations and yield the velocity components U_x and U_y at each point in the finite difference grid over the problem domain.

The velocities obtained as above were incorporated into the governing mass transfer equation, which was solved using finite difference techniques. The governing partial differential equation for mass transfer was simplified as:

$$\frac{\partial^2 C}{\partial x^2} + \frac{\partial^2 C}{\partial y^2} - \frac{U_y}{D}\ \frac{\partial C}{\partial y} - \frac{U_x}{D}\ \frac{\partial C}{\partial x} = 0 \tag{2}$$

The boundary conditions used for determining the solute concentration in the melt ahead of the solid liquid interface are as follows.

The composition remains at the eutectic far from the interface:

$$C = C_e \ at \ y = \infty \tag{3}$$

Due to conservation of matter at the interface, the flux of solute rejected at the freezing interface is equal to the solute diffusing into the melt away from the interface. This condition can be mathematically represented in the following form:

For α phase:

$$D\ (\frac{\partial C}{\partial y})_{y=0} = -V\ (C_l - C_s^{\alpha}) \tag{4}$$

For β phase, with a stepped interface:

$$D\ (\frac{\partial C}{\partial y})_{y=\kappa} = -V\ (C_l - C_s^{\beta}) \tag{5}$$

There is no side growth, i.e. along the side of the step there is no diffusion in the x direction:

$$(\frac{\partial C}{\partial x})_{y=0 \ to \ \kappa} = 0 \tag{6}$$

The concentration field is periodic owing to the periodicity of the lamellar structure:

$$C_{(x=0,y)} = C_{(x=\lambda,y)} = C_{(x=n\lambda,y)} \quad n = 1, 2, .. \tag{7}$$

The far field boundary condition, eq. 3, was tried for a stepped interface for increasing values of y until the solution was independent of the domain size. It was found in the initial computations that the computed average interface concentration with a far field condition at y=3λ/4 differed by less than 1% from that computed with y=λ/2. Hence in the subsequent computations we used C=C_e at y= 3λ/4.

The solid solubility was assumed to be negligible, so C^s_α=0 and C^s_β=1. The degree of non-planarity of the interface was altered by giving various values to κ, which is the height by which the alternate lamellae project into the melt. If we define κ = cλ, then c was chosen in the range 0 to 1, because Chandrasekhar [6] reported that the length-to-diameter ratio of the protruding MnBi rods averaged one.

In order to determine the effect of convection on the lamellar spacing we minimized the average interfacial undercooling ΔT. The treatment is similar to that in Chandrasekhar and Wilcox [5]. To facilitate the numerical computations we non-dimensionalized equation (2) to the following form, with the symbols defined in the table of nomenclature:

$$\frac{\partial^2 C}{\partial X^2} + \frac{\partial^2 C}{\partial Y^2} + \Lambda \ \frac{\partial C}{\partial Y} - \Gamma \, Y \ \frac{\partial C}{\partial X} = 0 \tag{8}$$

Since compositional changes occur over distances on the order of λ, the dimensionless distances were defined by X=x/λ and Y=y/λ. Note that $\Lambda \equiv \lambda V/D$ is a lamellar spacing Peclet number and $\Gamma \equiv G_u\lambda^2/D$ is a convective Peclet number. Letting $S_\alpha + 2S_\beta = \delta$, the non-dimensional forms of the boundary conditions are:

$$at \ \ Y = 3/4 \qquad C = C_e \tag{9}$$

$$at \ \ Y = 0 \qquad 0 < X < S_\alpha/\lambda, \quad \delta/\lambda < X < 1, \quad \frac{\partial C}{\partial Y} = -\Lambda \, C_i \tag{10}$$

$$0 < Y < \kappa, \quad X = S_\alpha/\lambda \ \ or \ \ \delta/\lambda, \quad \frac{\partial C}{\partial X} = 0 \tag{11}$$

$$S_\alpha/\lambda < X < \delta/\lambda, \quad \frac{\partial C}{\partial Y} = -\Lambda\,(C_i - 1) \tag{12}$$

For typical growth conditions on earth Λ is on the order of 0.1 and Γ is of order 100.

3. Results and discussion

Figure 3 shows a typical result, the the iso-concentration contours for a eutectic of C_e=0.3 with a step height of $\lambda/8$ growing without the disturbing influence of convection. Convection distorts the contours as shown in figure 4 for a convective Peclet number $\Gamma = 40$. The computed concentration fields in the melt were converted to lamellar spacing by calculating the average interfacial composition $\bar{C}_i$ and minimizing the total interfacial undercooling ΔT. Following Chandrasekhar et al. [5] the deviation parameters are defined as follows:

$$\Delta_\alpha = (\bar{C}_{i_\alpha} - C_e)_o - (\bar{C}_{i_\alpha} - C_e) \tag{13}$$

$$\Delta_\beta = (\bar{C}_{i_\beta} - C_e)_o - (\bar{C}_{i_\beta} - C_e) \tag{14}$$

where Δ_α is the difference between the deviation from the eutectic composition without convection ($G_u = 0$) and that with convection ($G_u > 0$) averaged over the α phase. Here Δ_β is the difference between the deviation from the eutectic composition without convection ($G_u = 0$) and that with convection ($G_u > 0$) averaged over the β phase. The subscript o indicates the values without convection.

The deviation from eutectic composition without convection was found to be proportional to $\Lambda = \lambda$ V/D:

$$(\bar{C}_{i_\alpha} - C_e)_o = A_\alpha\,\Lambda \tag{15}$$

$$(\bar{C}_{i_\beta} - C_e)_o = A_\beta\,\Lambda \tag{16}$$

The analytical solution of Jackson and Hunt [8] gives the values of A_α and A_β for a planar interface and no convection. From Jackson and Hunt [8] A = 0.121 for C_e=0.3 and A = 0.135 for C_e=0.5. From our numerical results, A = 0.119 for C_e=0.3 and A = 0.136 for C_e= 0.5 for the planar interface. For a stepped interface with C_e =0.3

and $\kappa=\lambda/5$ we found A = 0.129. For C_e=0.3 and $\kappa=\lambda/4$, A = 0.134.

Following Baskaran and Wilcox [4] the spacing between the lamellae is given by:

$$\left(\frac{\lambda}{\lambda_o}\right)^2 = \left[1 - \frac{f}{A} - 2\,\frac{\Gamma}{A}\,\frac{df}{d\Gamma}\right]^{-1} \tag{17}$$

Differentiating f with respect to Γ we find df/dΓ and substitute this into eq. (17). Polynomial fits for λ/λ_o as a function of Γ_o are shown in figures 5 to 7.

For C_e=0.1 and a planar interface:

$$\lambda/\lambda_o = 1 + 0.0016\ \Gamma_o + 1.61\ \text{X}\ 10^{-5}\ \Gamma_o^2$$

For C_e = 0.1 and $\kappa=\lambda/8$:

$$\lambda/\lambda_o = 1 + 0.0019\ \Gamma_o + 2.28\ \text{X}\ 10^{-5}\ \Gamma_o^2$$

For C_e = 0.5 and a planar interface:

$$\lambda/\lambda_o = 1 + 0.0073\ \Gamma_o - 0.00015\ \Gamma_o^2$$

For C_e = 0.5 and $\kappa=\lambda/8$:

$$\lambda/\lambda_o = 1 + 0.0114\ \Gamma_o - 0.0003\ \Gamma_o^2$$

For C_e = 0.3 and a planar interface:

$$\lambda/\lambda_o = 1 + 0.00046\ \Gamma_o + 9.80\ \text{X}\ 10^{-5}\ \Gamma_o^2$$

For C_e = 0.3 and $\kappa=\lambda/5$:

$$\lambda/\lambda_o = 1 + 0.0076\ \Gamma_o - 0.0005\ \Gamma_o^2$$

4. Conclusions

Based upon the results obtained from the numerical analysis the following conclusions can be made:

1. Increasing the intensity of convection increases the spacing between the lamellae.

2. For the same convective Peclet number, the increase in lamellar spacing of a eutectic growing with a stepped interface is much higher than the increase in lamellar spacing observed for a eutectic growing with a planar interface. That is, the microstructure of stepped interface is more sensitive to convection than a planar interface.

3. The increase in lamellar spacing observed for the same value of convective Peclet number is more for the eutectic growing with a higher κ, i.e. more non-planar. That is, with increasing irregularity of the interface the eutectic experiences an increased change in the lamellar spacing due to convection.

4. The effect of convection is negligible if the flow velocity is very small in magnitude, i.e. Γ is small (<1).

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Nomenclature

A_α = constant in equation 15

A_β = constant in equation 16

C_e = Eutectic mass fraction

C_i = Interfacial melt composition

$\bar{C}_i$ = Average interfacial melt composition

C_s^α = Composition of the alpha phase (assumed 0 here)

C_s^β = Composition of the beta phase (assumed 1 here)

$f = \Delta/\Lambda$

G_u = Gradient of convective velocity in the y direction [s^{-1}]

S_α = Half width of α phase [m]

T = Temperature [K]

ΔT = Total interfacial undercooling [K]

U = Convective velocity [m/s]

V = Growth rate [m/s]

x = Distance along interface from beginning of α phase [m]

X = Dimensionless distance along interface (x/λ)

y = Distance into the melt from interface [m]

Y = Dimensionless distance into the melt from interface (y/λ)

α = The A-rich phase of the binary eutectic

β = The B-rich phase of the binary eutectic

$\delta = S_\alpha + 2S_\beta$

$\Delta = (\bar{C}_{i_\alpha} - C_e)_o - (\bar{C}_{i_\alpha} - C_e)$, the deviation parameter

$\Gamma = G_u\lambda^2/D$, Peclet number for convection

$\Gamma_o = G_u\lambda_o^2/D$

κ = The height of the step, as a fraction of λ

λ = Lamellar spacing [m]

$\Lambda = \lambda V/D$ Lamellar spacing based Peclet number

μ = Viscosity of the melt (4 X 10^{-3} kg/m.s used here)

ρ = Density of the melt (800 kg/m^3 used here)

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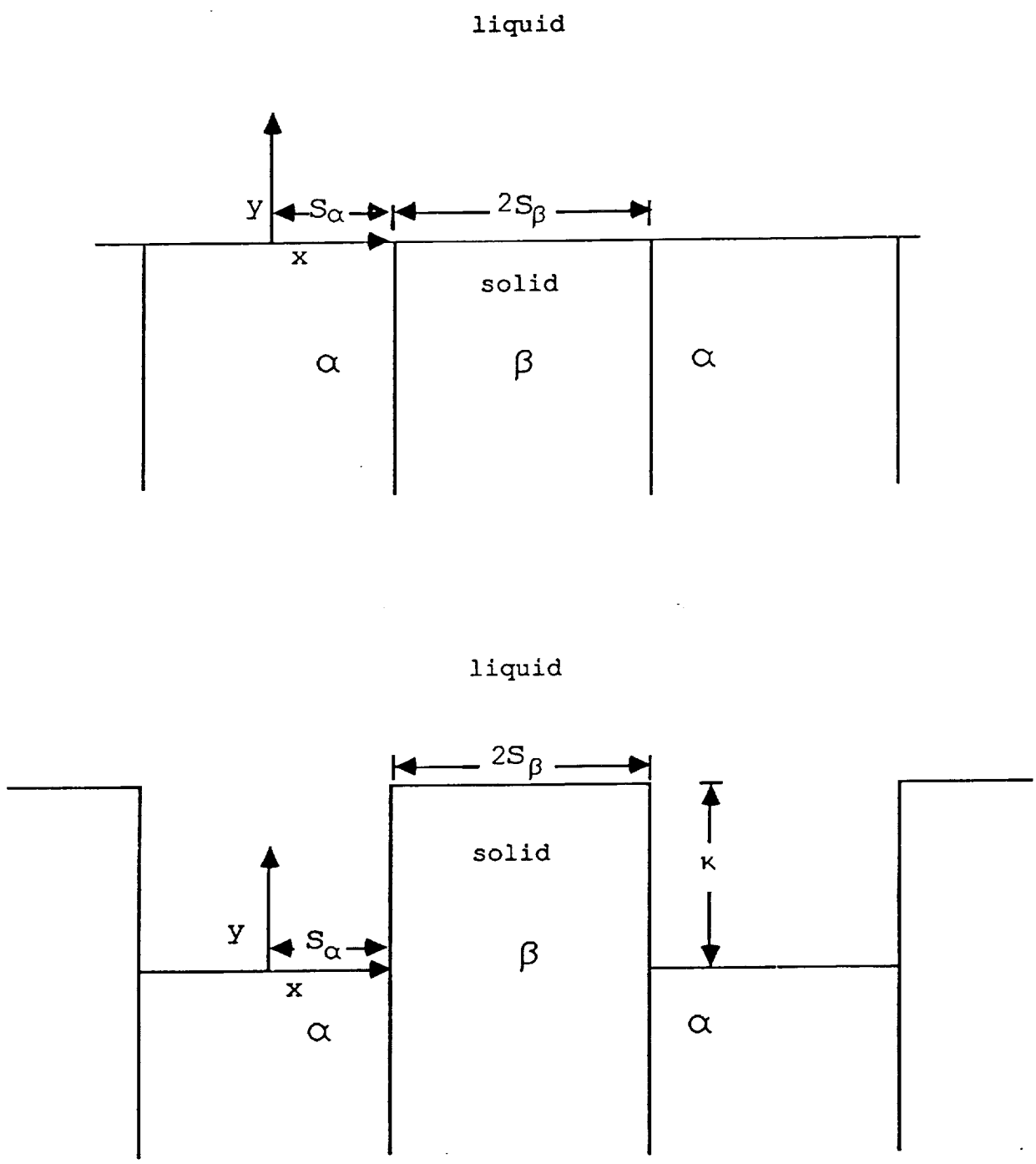

Figure 1: Schematic of the planar and stepped interfaces

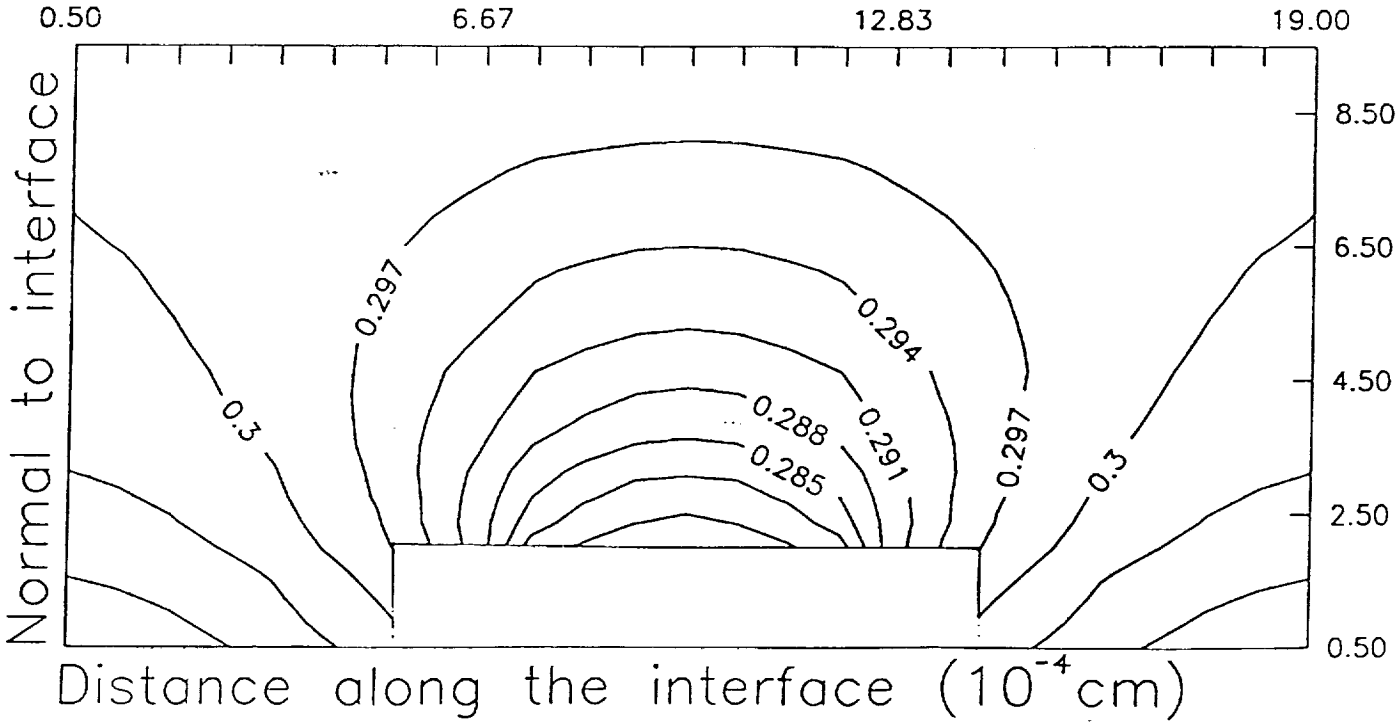

Figure 2: Isoconcentration profiles ahead of a stepped interface, no convection. (C_e=0.3, Λ=0.2, $\kappa=\lambda/8$)

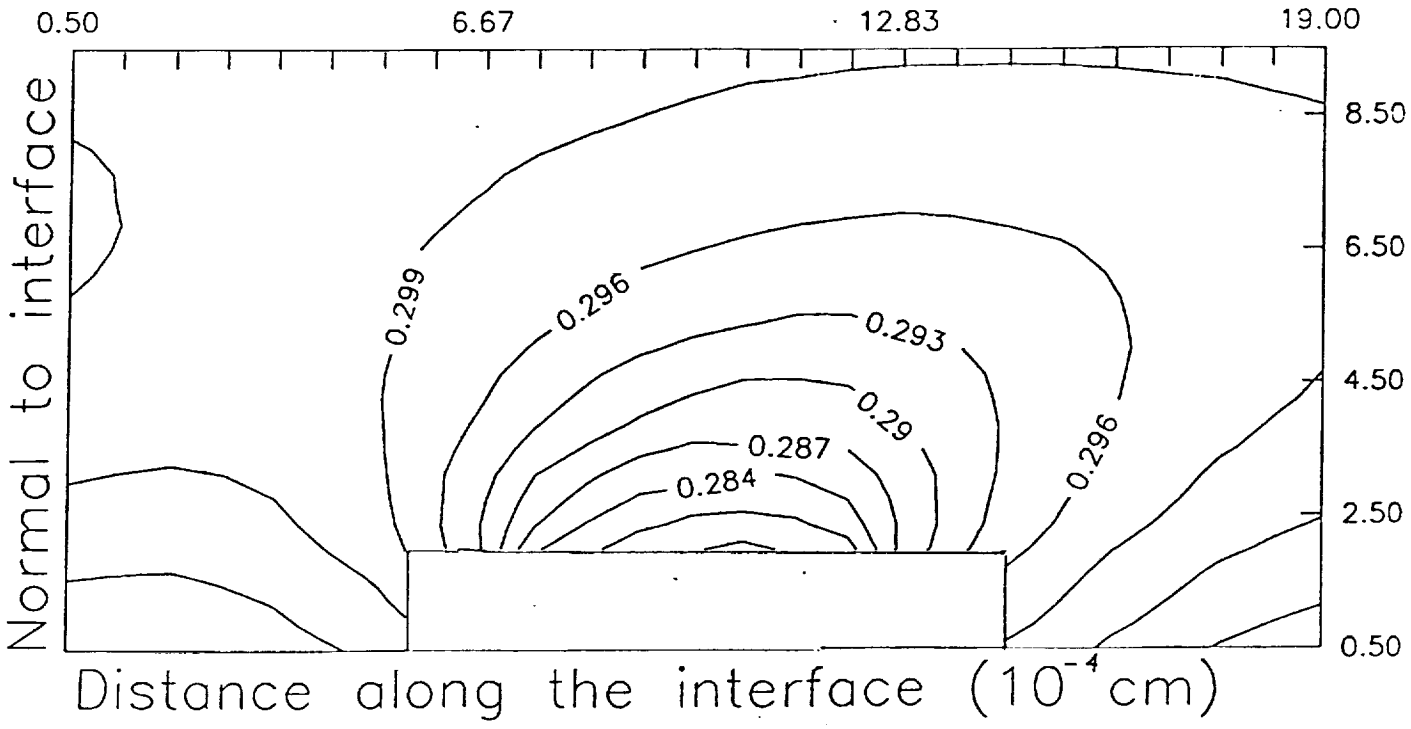

Figure 3: Isoconcentration profiles ahead of a stepped interface with convection. (C_e=0.3, Λ=0.2, Γ=40)

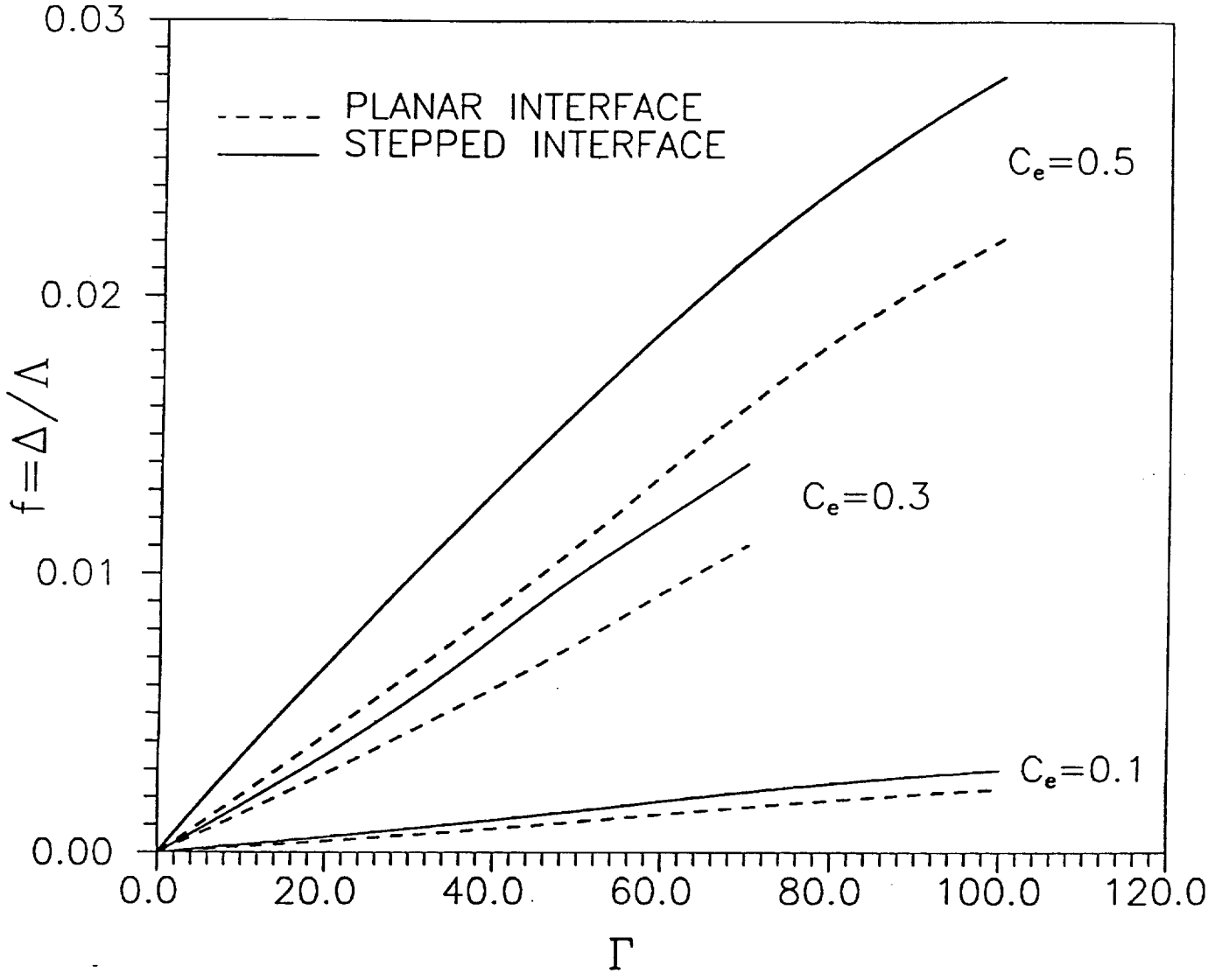

Figure 4: $\Delta/\Lambda = f$ versus Γ from numerical results. ($\Lambda = 0.2$)

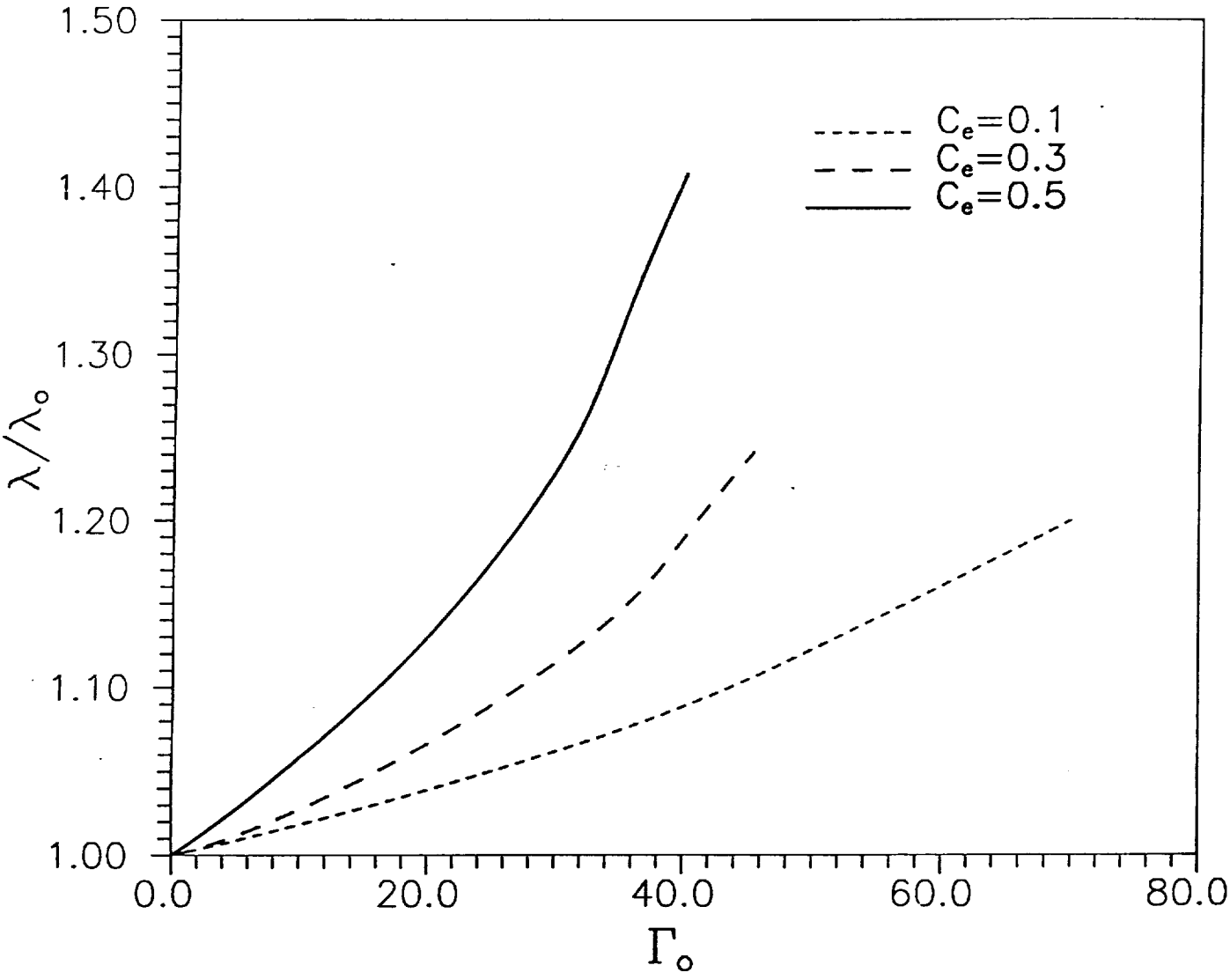

Figure 5: λ/λ_o versus Γ_o for planar interface from fig. 5 using eq.(17).

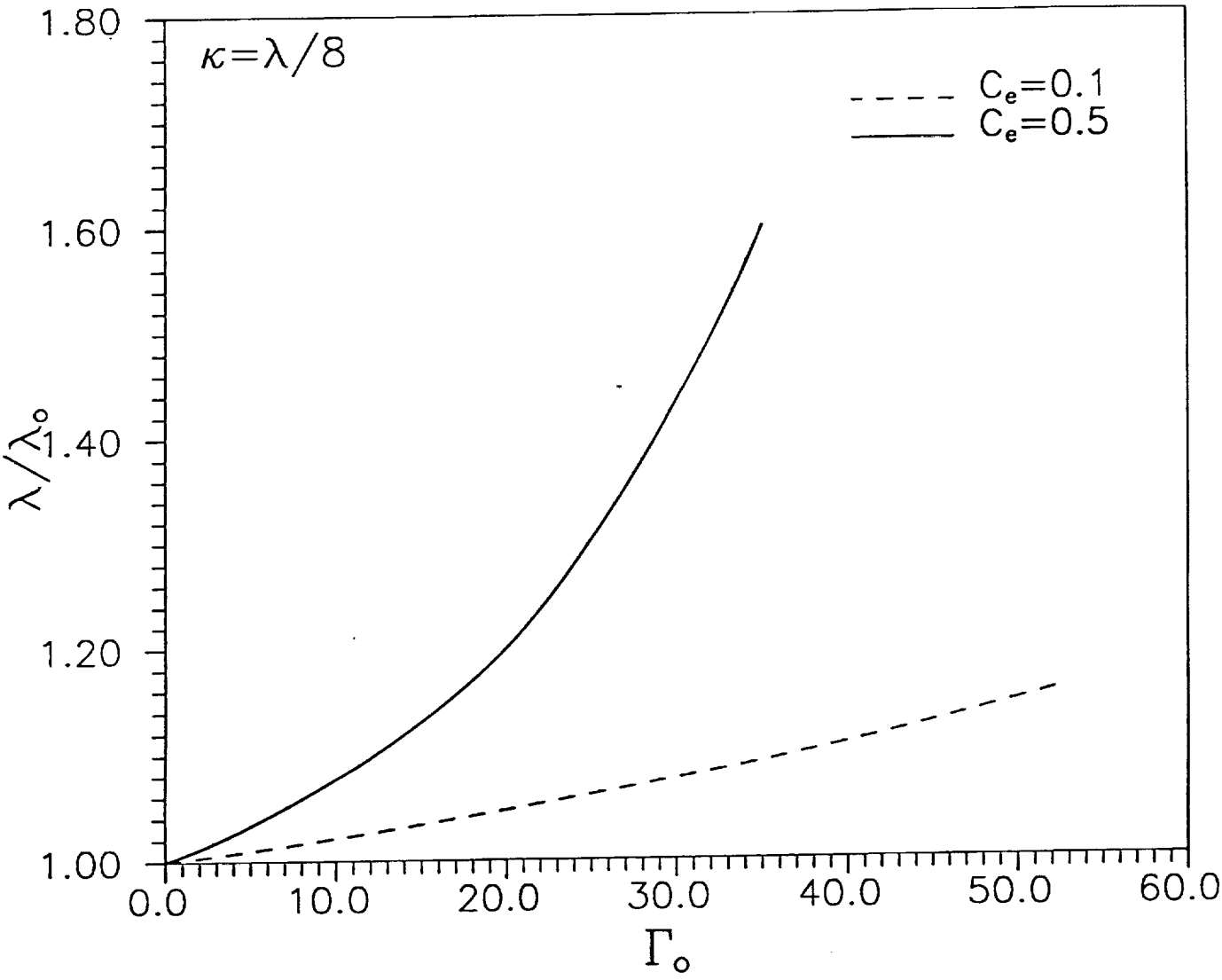

Figure 6: λ/λ_o versus Γ_o for stepped interface from fig. 5 using eq.(17), $\kappa=\lambda/8$

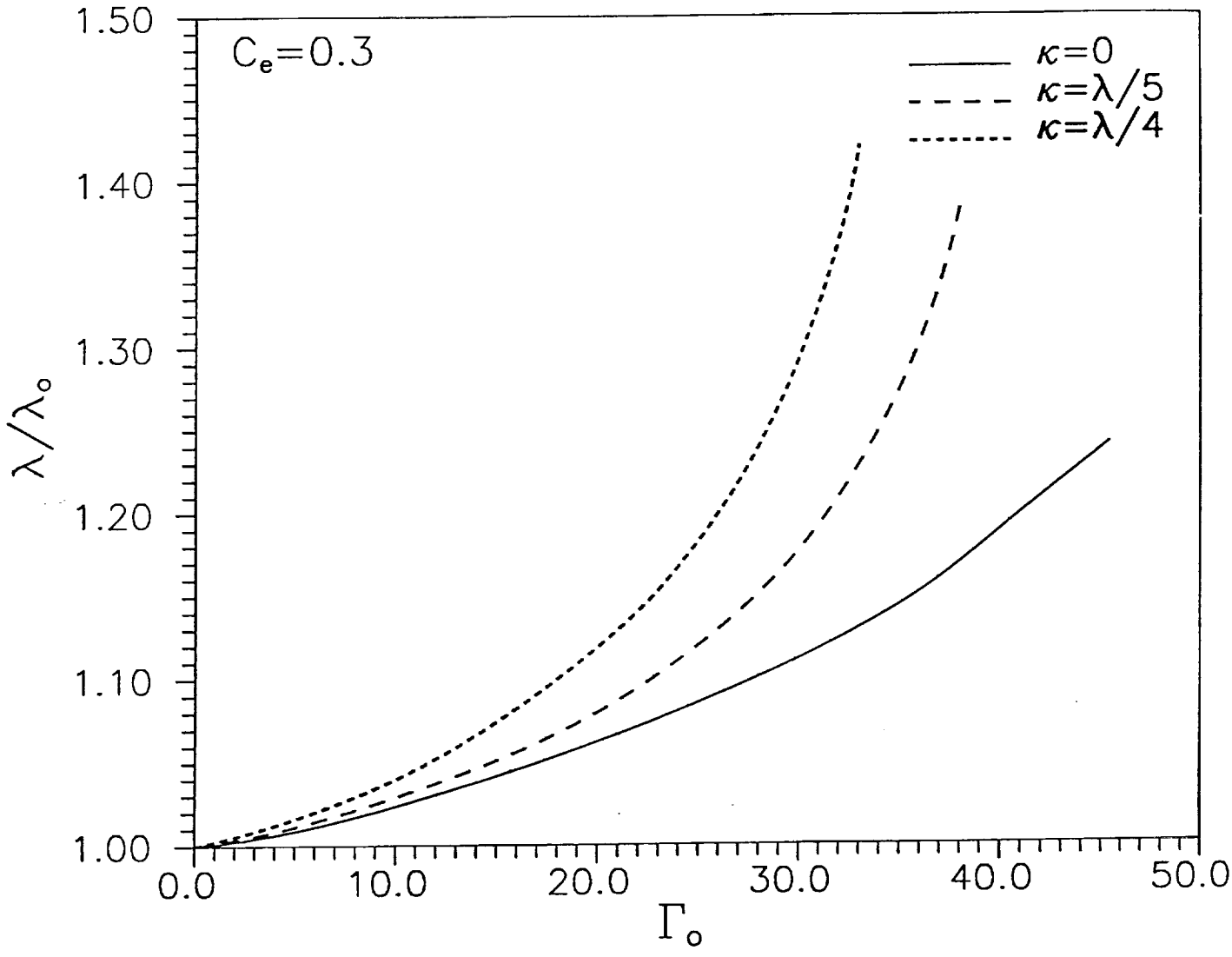

Figure 7: λ/λ_o versus Γ_o from fig. 5 using eq.(17) for C_e=0.3.