1170

BOUNDARY LAYER KINEMATICAL MODEL OF AUTOWAVE PATTERNS IN A TWO-COMPONENT REACTION-DIFFUSION SYSTEM

V.S. Zykov[1,2] and S.C. Müller[1]

[1]Max-Planck-Institut für molekulare Physiologie,
Rheinlanddamm 201, W-4600, Dortmund 1, Germany
zykov@mpi-dortmund.mpg.de

[2]Institute of Control Sciences, Moscow 117342

Abstract

A new approach is presented to describe spiral wave kinematics for many kinds of biological, chemical or ecological excitable media. In the framework of the approach a free boundary problem is formulated for both the front and the back of the excitation wave propagating in a two-component reaction-diffusion system. The boundary of excited region is considered as united continuous curve moving in a plane. In contrast to well known kinematical models it is assumed that the wave front is a boundary layer between excited and unexcited regions rather than thin line. It is shown that such approximation is necessary to reproduce important qualitative properties of spiral waves. This approach removes contradictions between some predictions of known free boundary formulations and the data of numerical and natural experiments.

Introduction

The spatio-temporal evolution of many kinds of biological, chemical or ecological systems is closely related to autowave phenomena (Zhabotinskii 1974, Winfree 1978, Svirezhev 1987). In particular, the rotating spiral autowave is a typical example of selfsustained activity in a two-dimensional excitable medium, such as heart muscle (Allesie *et al* 1973), chicken retina (Gorelova and Bures 1983) and Belousov-Zhabotinsky solution (Müller *et al* 1987).

There are two basic trends in the development of the modern theory of the spiral waves: the 'geometrical approach' and 'free boundary formulations'. Both of them are based on the classical works (Wiener and Rosenblueth 1946) and (Burton *at al* 1951) and consider the autowave front as a thin curve the position and the shape of which change with time.

The main purpose of the geometrical approach is to describe the evolution of the autowave front for stationary or non-stationary processes in excitable media (Zykov and Petrov 1977, Zykov and Morozova 1979, Zykov 1984, Davydov *et al* 1991). But it is impossible to study the structure of the spiral wave core with the aid of this method. On the other hand, the spiral wave structure is studied within the framework of the second approach, the free boundary formulation (Fife 1976, Tyson and Keener 1988, Meron and Pelce 1988, Karma 1991, Pelce and Sun 1991). But this approach is oriented only towards investigation of stationary processes such as rigid rotation of the spiral wave.

Now, one of the central problem in the spiral wave theory is to describe the processes within the spiral core under nonstationary circulation, especially related to the description of spiral wave meandering. To solve this problem, however, neither the geometrical approach nor free boundary formulations can be used.

The main ideas of a new approach described below is to consider the autowave front as a boundary layer rather than a thin curve. Hence, we shall assume that the triggering of the system from recovery to the excited state is not a steep jump, but a rather smooth process.

Reaction-diffusion model

The kinematical model can be used to simplify the study of autowave pattern formation in different types of reaction - diffusion models. As an example, let us consider a two-component reaction diffusion model with single diffusion and N-shaped function f in the equation for trigger variable:

$$\frac{\partial E}{\partial t} = D_E \Delta E + f(E) - g \,, \qquad (1)$$

$$\frac{\partial g}{\partial t} = \epsilon \, G(E,g) \,, \qquad (2)$$

where $f(E) = -Ek_1,\ E < \sigma,$

$= (E - a)k_f,\ \sigma \le E \le 1 - \sigma,$

$= (1 - E)k_2,\ 1 - \sigma < E$

with $k_1 = k_f(a - \sigma)/\sigma;\ \ k_2 = k_f(1 - \sigma - a)/\sigma;$

and $G(E,g) = k_g E - g,\ (k_g E - g) > 0$

$= k_\epsilon(k_g E - g),\ (k_g E - g) \le 0.$

We fix the following values of the parameters: $k_f = 1.7$, $k_g = 2$, $a = 0.1$, $\sigma = 0.01$, $k_\epsilon = 1.5$. In this case one can observe the formation of rigidly rotating spiral wave for any values of the small parameter ϵ within the interval $0 < \epsilon < 0.388$ (Zykov 1986).

Moreover it was shown by direct integration of (1),(2) (Mikhailov and Zykov 1991), that the rotation period of the spiral wave is U-shaped function on the parameter ϵ. The first test for the boundary layer kinematical model is to reproduce this dependence.

Free boundary formulation

The boundary of any autowave (i.e. curve E=const) consists of two parts. These are the front (dE/dt>0) and the back (dE/dt<0) of the wave. For a broken autowave these two curves touch each other in the so-called 'phase change point' (dE/dt=0) (Gulko and Petrov 1972).

Denote the arc length of the boundary as s; s = 0 for phase change point; s > 0 for the front and s < 0 for the back. To specify the boundary we use the natural equation $K = K(s)$, where K is the curvature. Denote as $\theta(s)$ the normal velocity and as $V(s)$ the tangential velocity of a given boundary point. It was shown in (Zykov 1984) that these three functions obey the following system of differential equations

$$\frac{d\theta}{ds} = \omega - K V$$

$$\frac{dV}{ds} = K\theta \qquad (3)$$

with the initial conditions

$$\theta(0) = 0$$

$$V(0) = V_0$$

It is also well known that the normal wave front velocity depends on the curvature and on the value of the slow variable on the front. We present this dependence as a linear function:

$$\theta = \theta_0 + K - Ag \tag{4}$$

It is necessary to obtain the solution of eqs.(3),(4),(2) which satisfies the given boundary conditions. Particulary, in a boundless medium curvature K(s) should vanish if the absolute value of s goes to infinity. We emphasize here that the evolution of variable g in (4) obeys equation (2), for which the values of E are different in excited, recovery and boundary layer portions of the autowave.

For further more detailed explanation let us now consider the case of one spatial dimension.

One spatial dimension case

A rough scheme of a wave train profile is shown in fig.1a which is typical for the free boundary formulations. The variable E jumps from the unexcited state (E=0) to the excited one (E=1) and then the variations of the slow variable g occur obeying eq.(2). The value of the slow variable on the front is, in fact, the refractory tail of the previous impuls.

The situation is different in the framework of the boundary layer model (see fig.1b). Here the wave front is a boundary layer with a thickness H. Within this layer one has to take into account the variation of the slow variable. To simplify the calculations assume that inside the boundary layer the value of the variable E is equal to the mean value E_1.

$$E_1 = 1/H \int_0^H E \, d\xi$$

For the special case of linear growthof E we get $E_1 = 0.5$.Then we have the following system for describing the time evolution of the slow variable:

$$g_b = k_g - \exp(-D\epsilon)\ (k_g - g_f)$$

$$g_1 = g_b \exp(-(T - D - \tau_1) k_\epsilon \epsilon) \tag{5}$$

$$g_f = g_1 + \tau_1 \epsilon (k_g E_1 - g_1)$$

where g_b,g_1 and g_f are the values of g for the back, boundary layer and front respectively. T is the period of the wave train, D the duration of the impulses and τ_1 the duration of a jump of the system to the excited state:

$$\tau_1 = H/\theta \tag{6}$$

It is important that even for the case of solitary impuls the value g_f is not equal to zero, in contrast to the common model. Following eq.(5) g_f is in this case proportional to ϵ.

Substituting this value in (4) we obtain the dependence of propagation velocity θ on the small parameter ϵ.

$$\theta = \theta_0 - \epsilon\ H/\theta\ k_g A E_1 \tag{7}$$

One can compare this dependence derived in the framework of boundary layer model with the well known dependence related to the reaction - diffusion model

$$\theta = \theta_0 - \epsilon\,\theta_1 \qquad (8)$$

Obviously the dependence (8) can be reproduced in the boundary layer model by choosing the thickness of the boundary layer as

$$H = \theta_0\theta_1/(k_g E_1 A) \qquad (9)$$

Thus the thickness of the boundary layer is a well definedparameter, since there are analytical expressions for values of θ_0, θ_1 and A for a given reaction-diffusion model (e.g., in (Zykov 1984)). Particulary for the given model (1),(2) we have obtained the following values: $\theta_0 = 1.5$, $\theta_1 = 0.5$, $A = 2.0$. Hence one can calculate from (9) that the boundary layer thickness is $H = 0.375$.

Steadily rotating spiral wave

In this section we assume that a spiral wave rotates with angular velocity ω around a fixed central point which can be considered as the origin of a polar coordinate system (see fig.2).There is a boundary layer with thickness H along the whole length of a wave front.

For any radius $r > r_q$ there is periodical picture of excitation along the polar angle β. The system of equations for the values of variable g for a given r is very similar to (5):

$$\begin{aligned} g_b &= k_g - \exp[-(\beta_f - \beta_b)\epsilon/\omega]\ (k_g - g_f) \\ g_1 &= g_b \exp[-(2\pi - \beta_f + \beta_b - \beta_1) k_\epsilon \epsilon] \qquad (10) \\ g_f &= k_g E_1 - (k_g E_1 - g_1)\ \exp(-\beta_1 \epsilon/\omega) \end{aligned}$$

wherethe angles β_f, β_b, β_1 determine the position of the front,the back and the boundary layer respectively and the angel β_1 is the effective thickness of the boundary layer expressed in polar coordinates.

The value of β_1 is found as a result of solving a pure geometrical problem which leads to the following equation:

$$(Kr - \sin\alpha)\cos\beta_1 - \cos\alpha\ \sin\beta_1 = Kr - \sin\alpha - (KH^2 - 2H)/(2r) \qquad (11)$$

where r is the radius and α is the angle between tangent and radial directions for given arc length.

With $\beta_1 \ll 1$ the equation (11) has the following solution

$$\beta_1 = \frac{\cos\alpha - [\cos^2\alpha + (Kr - \sin\alpha)(H^2 K - 2H)/r]^{1/2}}{Kr - \sin\alpha} \qquad (12)$$

It is very important to stress that in contrast to the one spatial dimension case the effective thickness of the boundary layer is not a constant but differs along the spiral wave front. Hence the value of the slow variable g on the front differs with arc length.

In oder to find the form of the spiral wave it is necessary to integrate the system (3),(4) taking into account (10) and (11). To simplify the calculations one can express the values of $\cos\alpha$ and $\sin\alpha$ in terms of the front velocities:

$$\cos\alpha = \theta/(\omega r) \qquad (13)$$

$$\sin\alpha = V/(\omega r) \qquad (14)$$

There are two unknown parameters in the system of eqs. (3),(4),(10),(11): the angular velocity ω and the tangential velocity V_0. Of course, the shape of the front and the back will depend onthese values. In particular, there is only one value of ω for which the front curvature K(s) vanishes when s goes to infinity.This is the natural boundary conditions for our problem, asalready pointed out in section 3. This way ω was fitted by direct integration of the equations. Similary one can fit a single value of V_0 to obtain the corresponding shape of the back curve.

In fig.3 the dependence of ω on ϵ is shown as obtained with the boundary layer kinimatical model and compared with to the data of direct integration of the system (1), (2). The results of computation with H = 0 are also shown. This limiting case of the boundary layer model is identical to the wave front interaction model considered in (Pelce and Sun 1991). It is obvious that the results of the boundary layer model is in a better agreement with the result of direct integration of the reaction-diffusion model.

In addition, we obtain new information about the spiral core.

In fig.4 the distribution of the slow variable g along the boundary is depicted. For the boundary layer model it is a smoothly decreasing function (fig.4a). At the wave tip (s = 0) there is same positive value of gwhich, of course, depends on ϵ.

By contrast, for the wave front interaction model (H=0) the value of g is equal to zero at the tip for any ϵ (fig.4b). Such distribution of g contradicts the data directly computed from different kinds of reaction-diffusion models.

Conclusions

Some new approach to investigate autowaves kinematics is suggested. It is based on both the geometrical approach and the free boundary formulation. In contrast to these two approaches the whole medium is separated into three regions. The boundary layer is placed between the two common regions (excited and recovery). This new step of approximation essentially improves both qualitative and quantitative description of the spiral wave motion, particulary, the description of the spiral wave core.

This new approach can be considered as a modification of the geometrical approach to the description of autowave patterns and can be applied to different types of excitable media.

References

Allesie, M.A., Bonke, F.I.M. and Schopman, F.J.G. 1973. Circus movement in rabbit atrial as a mechanism of tachicardia. *Circ. Res.* 33, 54-62.

Burton, W.K., Cabrera, N. and Frank, F.C. 1951. The growth of crystals and the equilibrium structure of their surfaces, *Phil. Trans. Roy. Soc. (London)* 243, 299-358.

Davydov, V.A., Zykov, V.S. and Mikhailov A.S. 1991. *Sov. Phys. Usp.* 34, 665.

Gorelova, N.A. and Bures, J. 1983. Spiral waves of spreading depression in the isolated chicken retina. *J. Neurobiology* 14, 353-363.

Gulko, F.B. and Petrov, A.A. 1972. Formation of closed conduction paths in excitable medium. *Biofizika* 17, 261-264.

Fife, P.C. 1976. Singular perturbation and wave front techniques in reaction-diffusion problems. *SIAM-AMS Proc.* 10, 23-50.

Karma, A. 1991. Universal limit of spiral wave propagation in excitable media. *Phys. Rev. Lett.* 66, 2274-2277.

Meron, E. and Pelce, P. 1988. Model for spiral wave formation in excitable media. *Phys. Rev. Lett.* 60, 1880-1883.

Mikhailov, A.S. and Zykov V.S. 1991. Kinematical theory of spiral waves in excitable media: comparison with numerical simulations. *Physica D* 52, 379-397.

Müller, S.C., Plesser, T. and Hess, B. 1987. Two-dimensional spectrophtometry and spiral wave propagation in the Belousov-Zhabotinsky reaction. *Physica D* 24, 71-86.

Pelce, P. and Sun, J. 1991. Wavefront interactions in steadily rotating spirals *Physica D* 48, 353-366.

Svirezhev, Yu.M. 1987. Nonlinear Waves, Dissipative Structures and Catastrophes in Ecology. Nauka, Moscow.

Tyson, J.J. and Keener, J.P. 1988. Singular perturbation theory of traveling waves in excitable media. *Physica D* 32, 327-361.

Wiener, N. and Rosenblueth, A. 1946. The mathematical formulation of the problem of conduction of impulses in a network of connected excitable elements, specifically in cardiac muscle. *Arch. Inst. Cardiol. Mexico* 16, 205-265.

Winfree, A.T. 1987. When Time Breaks Down. Princeton Univ. Press.

Zhabotinskii, A.M. 1974. Concentration Autooscillations. Nauka, Moscow.

Zykov, V.S. 1984. Simulation of Wave Processes in Excitable Media. Nauka, Moscow (Engl. Transl., Manch. Univ. Press, 1988)

Zykov, V.S. 1986. Cycloidal circulation of spiral waves in excitable media. *Biophizika*, 31, 862-865.

Zykov, V.S. and Morozova, O.L. 1979. Rate of excitation propagation in a two-dimensional excitable medium. *Biofizika* 24, 717-720.

Zykov, V.S. and Petrov, A.A. 1977. On the role of inhomogeneity of an excitable medium in mechanism of self-sustained activity.*Biofizika* 22, 300-303.

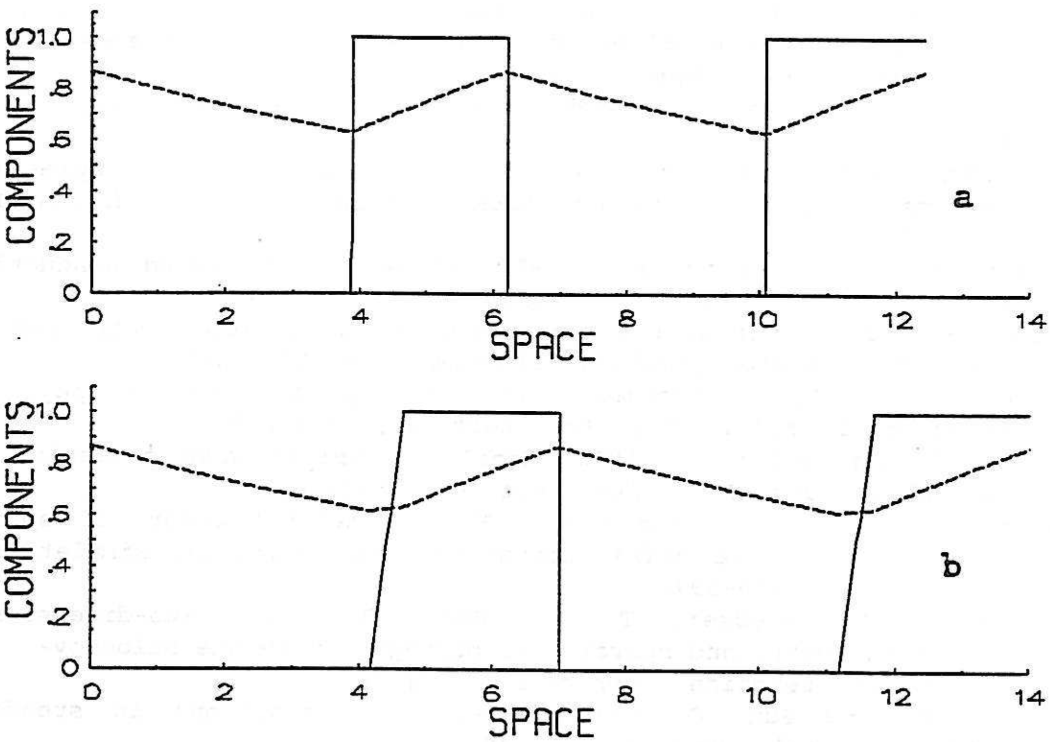

Fig.1 . Variations of the components E (solid) and g (dashed) in a wave train for common model (a) and for boundary layer model (b).

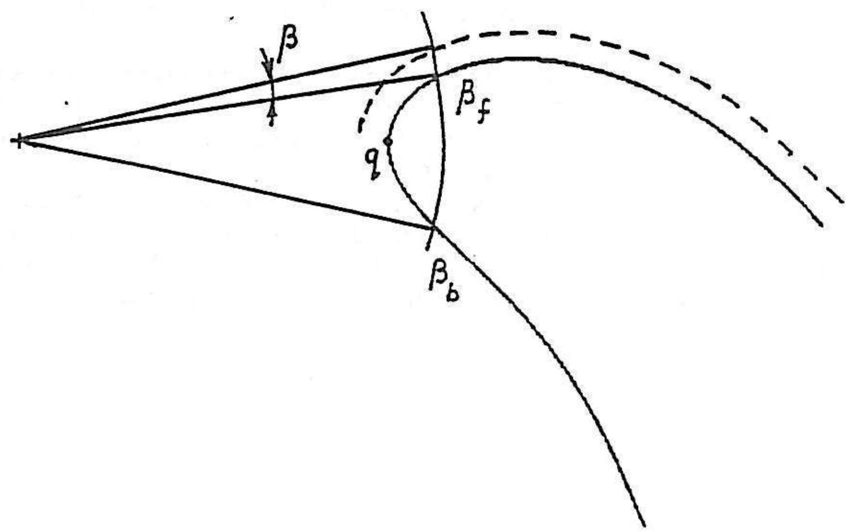

Fig.2. The shape of the steadily rotating spiral wave (solid) and the position of the boundary layer (dashed). Point q is the phase change point.

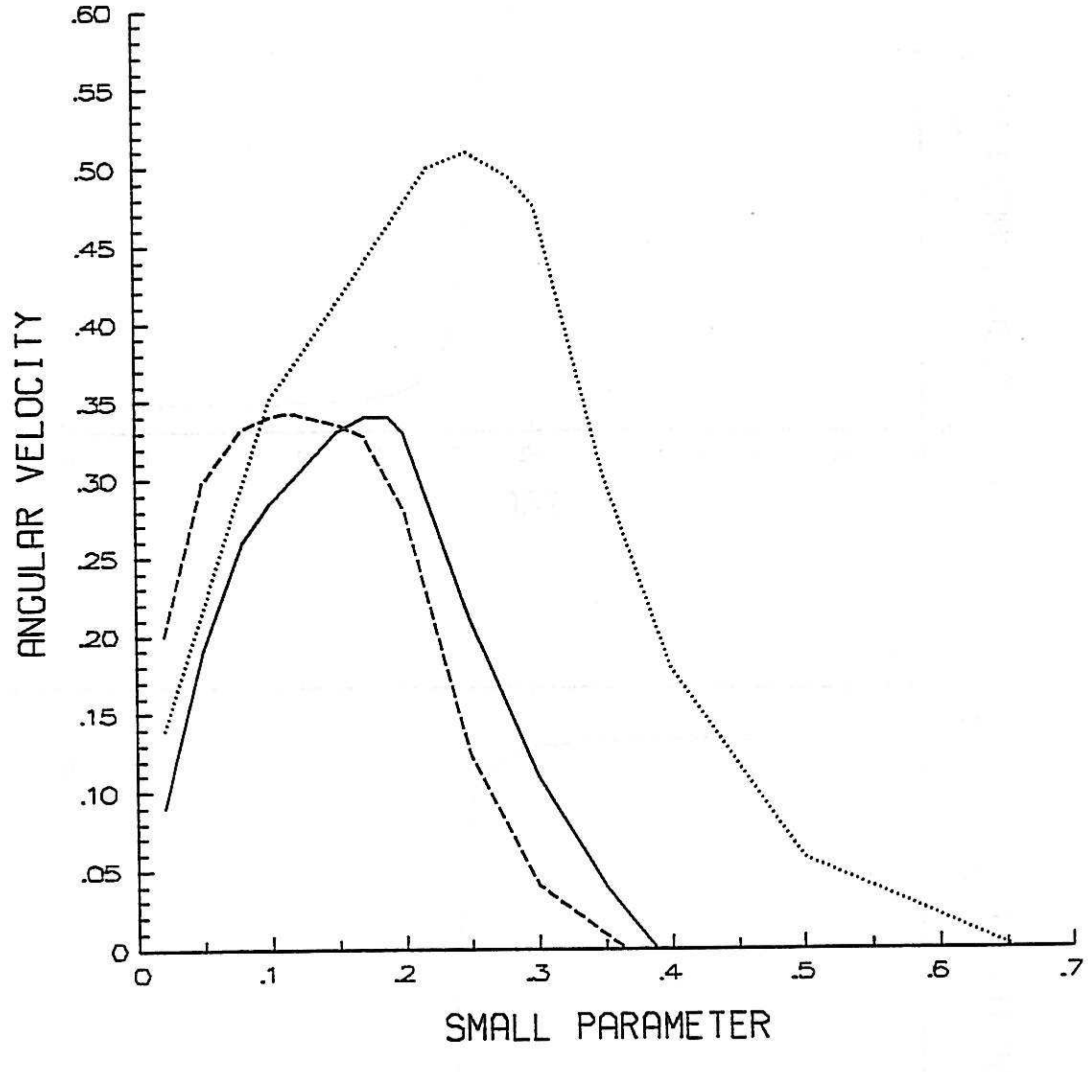

Fig.3. The dependence of angular velocity ω on small parameter ϵ obtained for reaction - diffusion model (solid), boundary layer model (dashed) and wave front interaction model (dotted).

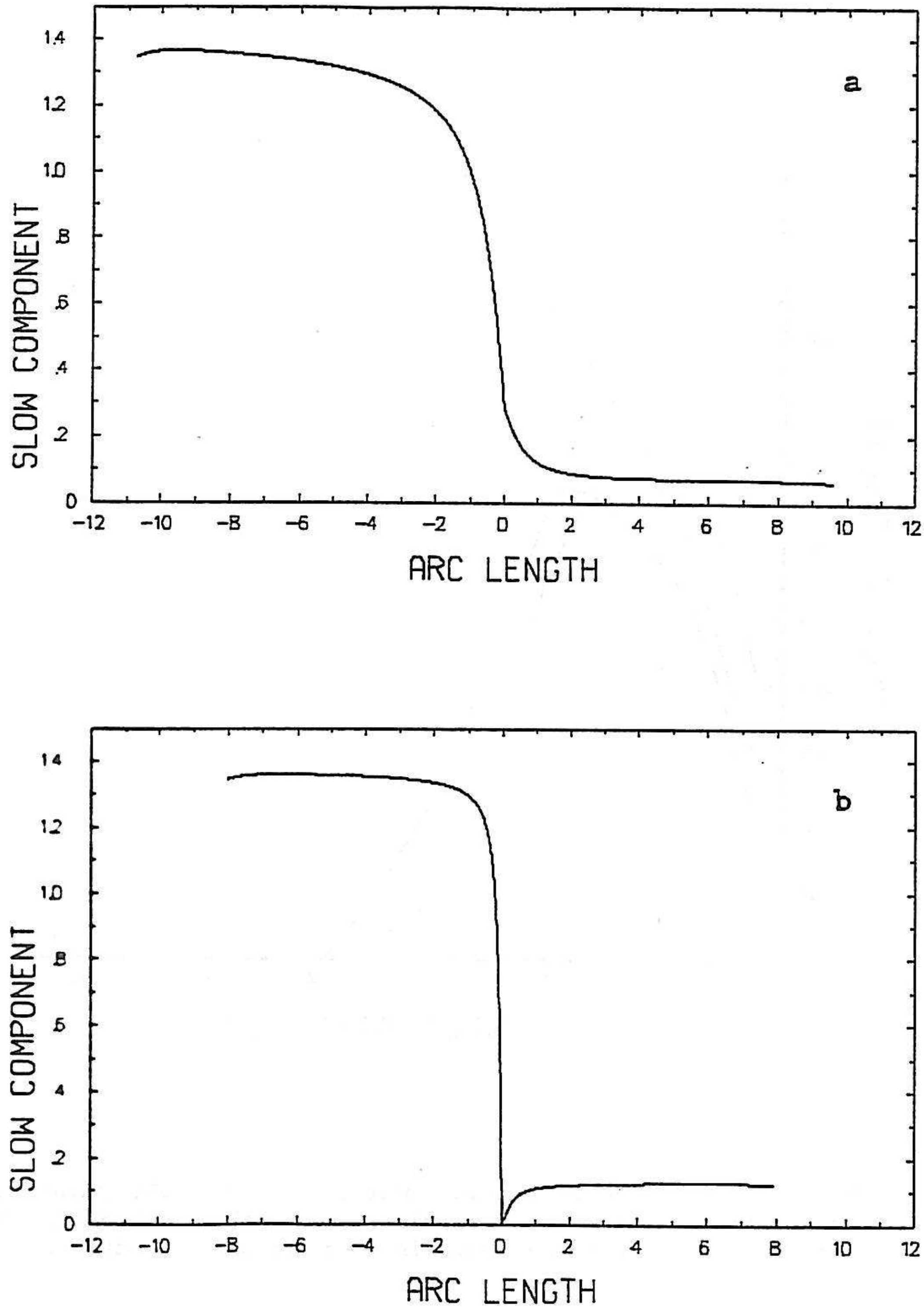

Fig.4. The distribution of the slow variable g along the wave boundary computed (a) for boundary layer model and (b) for wave front interaction model.