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ON A FREE BOUNDARY PROBLEM ASSOCIATED WITH COMBUSTION AND SOLIDIFICATION (*)

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Abstract. — *It was recently shown that two free interface problems asociated with combustion and solidification allow a qualitatively identical quasi-local approximation of the interface dynamics expressed as a coordinate free relationship between the normal velocity of the surface and its local geometrical characteristics Based on the analyses of these models a simpler free boundary problem is proposed leading to the same interface dynamics which demonstrates development of a cellular pattern and self-chaotization Desirability of a rigorous mathematical study of the proposed model is discussed*

Résumé. — *On considère ici deux problèmes d'interfaces libres provenant de la combustion et de la solidification Il a été récemment prouvé qu'il produit une approximation quasi locale qualitative identique à la dynamique de l'interface exprimée comme un résultat intrinsèque entre la vitesse normale de la surface et ses caractéristiques géométriques. En se basant sur l'analyse de ces modeles on propose ici un problème à frontière libre plus simple qui conduit à la même dynamique d'interface produisant le développement d'un secteur cellulaire et d'un chaos Les problèmes mathématiques ouverts sont aussi discutés.*

I. INTRODUCTION.

The dynamics of chaos has become one of the foci of interest of both applied and pure mathematicians in recent years. A break of stability leading to chaotic behaviour is being discovered in a growing number of problems arising from various fields of applied mathematics and physics. In spite of serious mathematical difficulties some firm ground has been gained in understanding underlying mechanisms of the chaotic behaviour.

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However, many questions concerning the occurrence and development of turbulent solutions remain unanswered Unfortunately, complexity of the subject itself is somewhat amplified by the deficit of problems that allow a relatively simple formulation in terms, for instance of boundary value problems reasonably compact and preferably as close as possible (a least in appearance) to some well understood « classical » problem, yet demonstrating all the variety of qualitative features attributive of the physical systems from which they originate

In a recent study a coordinate free equation relating the normal propagation velocity of a flame front to its local geometrical characteristics such as the mean and Gaussian curvature was derived [1] The equation represents in fact a quasi-local approximation of the dynamics governed by transport of heat and reactants within the flame structure and is capable of developing a cellular pattern and self-chaotization It turns out that a qualitatively identical equation describes the interface dynamics in a free interface problem associated with solidification of an overcooled liquid of pure substance [2]

Based on the a posteriori analyses of the above models we propose a somewhat simplier free boundary problem that, as we show, yields the same boundary dynamics equation Thus, the proposed model will demonstrate a similar break of symmetry into a cellular pattern and self-turbulence On the other hand, we believe that the model proposed in the present note may be more suitable for both numerical and rigorous mathematical study due to its more compact and less « exotic » form from a point of view of an PDE expert as compared with the original combustion and solidification problems

In Section II we formulate briefly the free interface problem of the flame propagation, and describe the equation of interface dynamics Section III contains similar information concerning the solidification problem (The three-dimensional case with arbitrary attachement kinetics has not been published before) In Sections IV-VII we introduce and study the simplified model, and discuss the results in Section VIII

II. DIFFUSIONAL-THERMAL PROPAGATION OF FLAMES

The description of flame propagation in a combustible gaseous mixture requires equations of heat conduction and diffusion of the reacting species as well as equations of motion of the gas coupled through the thermal expansion of gas The diffusional-thermal mechanism of the flame dynamics is studied within the framework of the so-called constant density model that treats thermal expansion of the gas as qualitatively negligible and the chemical reaction as a surface δ-function type heat source for large activation energies. The gas flow cannot then be effected by the temperature distribution and the flame is fully described by the molecular transport of heat and a deficient chemical component taking place within a prescribed velocity field, which we assume to be zero for simplicity.

Let us assume that the burned matter occupies a domain Ω, and the flame front σ to be $\partial\Omega$. Then in appropriate nondimensional variables the constant density combustion is described as follows [3] :

$$\frac{\partial T}{\partial t} = \nabla^2 T , \quad \frac{\partial S}{\partial t} = \nabla^2 (S - \alpha T) , \quad \text{in } R^3 . \tag{2.1}$$

subject to the jump conditions

$$[\theta] = [S] = 0 , \quad \left[\frac{\partial \theta}{\partial \mathbf{n}} \right] = \left[\frac{\partial S}{\partial \mathbf{n}} \right] / \alpha = - \exp(S/2) , \quad \text{on } \sigma . \tag{2.2}$$

Additionally in the fresh mixture

$$\theta(\infty) = S(\infty) = 0 , \quad \text{and also} \quad \theta \equiv 1 , \quad S < \infty \quad \text{in } \Omega . \tag{2.3}$$

The unit normal $\mathbf{n}$ in (2.2) is chosen so that it points toward Ω. It can be shown [1] that dynamics of the flame front σ is approximately described by the following relationship :

$$v = P(\kappa, q) + G\Delta_\sigma \kappa . \tag{2.4}$$

Here

$$P(\kappa, q) = -1 + A\kappa + B\kappa^2 + Cq + D\kappa q + E\kappa^3 ,$$

with

$$A = 1 - \alpha , \quad B = -\alpha^2/2 - 1 , \quad C = 2\alpha^2 + 2 , \quad D = 20\alpha^2 + 8\alpha - 4 ,$$
$$E = \alpha^3/3 - 5\alpha^2 - 2\alpha , \quad G = -\alpha^2(\alpha + 3) .$$

In equation (2.4) κ is the sum of principal curvatures, q is the Gaussian curvature, and Δ_σ is the invariant Laplace-Beltrami operator :

$$\Delta_\sigma = g^{ij}(\partial_i \partial_j - \Gamma^k_{ij} \partial_k) , \quad (i, j, k = 1, 2) , \tag{2.5}$$

where g is the metric tensor and Γ is the connection :

$$ds^2 = g_{ij}\, dx^i\, dx^j , \quad \Gamma^k_{ij} = - \frac{\partial \vec{r}}{\partial x^j} \cdot \frac{\partial}{\partial x^i} \left(\frac{\partial \vec{r}}{\partial x^k} \right) \tag{2.6}$$

on the flame surface $\vec{r} = (x^1, x^2, f(x^1, x^2))$.

Near the stability threshold $\alpha = 1$, equation (2.4) is reduced to a remarkably compact form :

$$v = -1 + (1 - \alpha)\kappa - 4\Delta_\sigma \kappa , \tag{2.7}$$

which via an expansion of a small perturbation f of the plane steady solution of (2 1)-(2 3) can be further reduced to the Kuramoto-Sivashinsky equation [4]

$$f_t + (\nabla f)^2/2 + \nabla^2 f + 4\,\nabla^4 f = 0 \tag{2 8}$$

III NONOEQUILIBRIUM SOLIDIFICATION PROBLEM

Consider a motionless supercooled liquid of some pure substance with growing along the interface σ solid phase The heat released by the phase transition has to be diffused into surrounding medium which for simplicity we assume to have the same thermal conductivities on both sides of the interface The nondimensional free interface problem in this case is as follows

$$\frac{\partial \theta}{\partial t} = \nabla^2 \theta \quad \text{in } R^3 \tag{3 1}$$

$$\theta = 1 - \gamma\kappa + Q(v)\,, \quad \left[\frac{\partial \theta}{\partial \mathbf{n}}\right] = \delta v\,, \quad \text{on } \sigma\,,$$

$$\theta(\infty) = 0\,, \quad \theta(\Omega) < \infty$$

The interface attachement kinetics $Q(v)$ is assumed to be a monotone function $Q' > 0$

It can be shown [2] that dynamics of the interface in problem (3 1) is also described by equation (2 4) with

$$A = (\gamma - \delta)/Q'\,, \quad Q = -\,(\delta + Q'' A^2/2)/Q'\,, \quad C = 2\,\delta(2 - A)/Q'\,, \tag{3 2}$$

$$D = \left[\left(\frac{4}{Q'} - \frac{1}{\delta}\right) Q'' A^2 - \left(16 + 4\frac{Q''}{Q'}\right) A + 4\frac{\delta}{Q'} + 24\right]\frac{\delta}{Q'}\,,$$

$$E = \left[\left(1 - \frac{Q''}{\delta} A\right)(A/2 + B) - \frac{Q''' A^3}{6\,\delta} - 6\right]\frac{\delta}{Q'}\,,$$

$$G = -\,(A^2 - 4A + 3)\frac{\delta}{Q'}$$

Near the bifurcation point $\gamma = \delta$ the solid-liquid interface is described by the equation

$$v = -1 + A\kappa + G\Delta_\sigma \tag{3 3}$$

The latter is a spatially invariant form of the Kuramoto-Sivashinsky type equation obtained for the perturbation of planar solidification [5]

IV. A MODEL PROBLEM

Analyzing information obtained during derivation of the interface dynamic equations in the above problems one may notice that the interface conditions can also be approximately expressed in terms of local geometrical characteristics instead of the original « physical » form. Moreover, one may keep only the principal nontrivial terms in the « geometrical » corrections while preserving main qualitative features of the boundary dynamics. On the other hand, once the boundary values are expressed in local geometrical terms, all the information behind the interface (inside $\Omega(t)$) becomes unnecessary.

The above idea of reduction, however obvious, leads to noticeable simplifications. Let us therefore consider a boundary value problem :

$$\frac{\partial \theta}{\partial t} = \nabla^2 \theta \quad \text{in} \quad R^3 \backslash \Omega(t) , \tag{4.1}$$

$$\frac{\partial \theta}{\partial \mathbf{n}} = 1 + \alpha\kappa , \quad \theta = 1 + \beta\kappa \quad \text{on}\, \sigma , \quad \theta(\infty) = 0 , \tag{4.2}$$

where α and θ are some constants.

We shall be interested in describing boundary dynamics of the above problem in the case when it is weakly curved and $t \to \infty$, meaning by the latter that the initial condition « is forgotten » if the problem allows it. For that reason we note that problem (4.1)-(4.2) with condition at infinity appropriately understood supports a planar solution :

$$\theta_b = \exp(z + t) , \quad \sigma : \; z + t = 0 . \tag{4.3}$$

V. LINEAR STABILITY

In order to investigate stability of the planar solution we shift to a frame moving with the boundary : $\zeta = F(x, t) - z$ and employ the Laplace transform $(\zeta \to p)$

$$\theta_t = \left(F_{xx} - F_t + 2\, F_x \frac{\partial}{\partial x} \right) (p\theta - 1 - \beta\kappa) + \theta_{xx} + (1 + F_x^2) \times$$
$$\times \left(p^2 \theta - p - p\beta\kappa + \frac{1 + \alpha\kappa}{\sqrt{1 + F_x^2}} \right) . \tag{5.1}$$

Let $F = -t + f(x, t)$, $\theta_b = \dfrac{1}{(p + 1)}$, $\theta = \theta_b + U(x, p, t)$. Then for a small harmonic perturbation $f = A \exp(\omega t + ikx)$, $U = fu(p)$ linearization of (5.1) yields :

$$(p^2 + p - \omega - k^2)\, u = -\frac{\omega + k^2}{p+1} + \alpha k^2 - \beta k^2(1+p)\,. \qquad (5.2)$$

Demanding analyticity at $p_0 = -1/2 + \sqrt{1/4 + \omega + k^2}$, $\mathrm{Re}(p_0) > 0$ we obtain the following dispersion relationship

$$\alpha k^2 - (\omega + k^2)/(p^0 + 1) - \beta k^2 (p_0 + 1) = 0 \qquad (5.3)$$

which for $\alpha - \beta - 1 = \varepsilon \ll 1$, $\omega \sim \varepsilon^2$, $k^2 \sim \varepsilon$ is reduced (up to ε^2) to

$$\omega = \varepsilon k^2 + (1 - \beta)\, k^4\,. \qquad (5.4)$$

The last term in (5.4) will suppress short-wave disturbances if $\beta > 1$ so that only the long wave part of the spectrum is amplified for $\varepsilon > 0$.

VI. WEAKLY NONLINEAR DYNAMICS OF PERTURBATION

Equation (5.4) reflects separation of scales that can be used for a description of nonlinear dynmamics of the perturbations of planar solution of the model problem near bifurcation $\alpha - \beta = 1$. Following [4] we introduce scaled variables

$$\xi = \sqrt{\varepsilon}\,, \quad \tau = \varepsilon^2 t\,, \quad \phi = f/\varepsilon\,, \quad U = \varepsilon^2 w(\xi, p, \tau) \qquad (6.1)$$

and seek a solution of equation (5.1) as an asymptotic expansion in powers of ε : $\phi(\xi, \tau) = \phi_0 + \varepsilon\phi_1 + \cdots$, $w = w_0 + \varepsilon w_1 + \cdots$. Equation (5.1) in scaled variables becomes up to ε^3

$$pw + \phi_{\xi\xi}\frac{p(\beta p + 2\beta - \alpha)}{(p+1)^2} + \varepsilon\left[\frac{w_{\xi\xi} - \phi_\xi^2/2}{\mathrm{p}+1} + \frac{\phi_{\xi\xi} + \phi_\tau + \phi_\xi^2}{(p+1)^2}\right] = 0\,. \qquad (6.2)$$

In the zero order we get

$$w_0 = \phi_{0_{\xi\xi}}(\beta p + 2\beta - \alpha)/(p+1)^2\,. \qquad (6.3)$$

In the first order equation (6.2) yields at $p = 0$:

$$w_{0_{\xi\xi}} + \phi_{0_{\xi\xi}} + \phi_{0_\xi}^2/2 + \phi_{0_\tau} = 0 \qquad (6.4)$$

from where upon substitution from (6.3) we obtain a Kuramoto-Sivashinsky equation :

$$\phi_{0_\tau} + \phi_{0_\xi}^2/2 + \phi_{0_{\xi\xi}} + (\beta - 1)\,\phi_{0_{\xi\xi\xi\xi}} = 0\,. \tag{6.5}$$

VII. INVARIANT STRONGLY NONLINEAR EQUATION

The weakly nonlinear analysis conducted in the previous section is based on the separation of scales existing near bifurcation point, and leads to equation (6.5) associated with a certain coordinate system. In this section we exercize a different approach that results in the invariant strongly nonlinear equation (2.4).

Let us assume that the boundary is only slightly curved $\kappa \sim \varepsilon \ll 1$. It is natural to expect then that the solution is close locally to the planar solution propagating with unit velocity in the direction normal to the boundary. In other words, the solution is quasi-planar and quasi-steady. We come, therefore, to the following idea of rescaling :

$$\xi = \varepsilon x\,, \quad \tau = \varepsilon t\,, \quad \Phi = \varepsilon F\,. \tag{7.1}$$

Note that the small parameter ε in (7.1) is not associated with closeness to the bifurcation point. Equation (5.1) in scaled variables (7.1) becomes up to ε^3 :

$$\varepsilon \frac{\partial \theta}{\partial \tau} = \left(\varepsilon \Phi_{\xi\xi} - \Phi_\tau + 2\,\varepsilon \Phi_\xi \frac{\partial}{\partial \xi}\right)(p\theta - \theta_\sigma) + \varepsilon^2\,\theta_{\xi\xi} + s_\xi^2 (p^2\,\theta - p\theta_\sigma - j)\,, \tag{7.2}$$

where s is the arc-length : $s_\xi = \sqrt{1 + \Phi_\xi^2}$,

$$\theta_\sigma = 1 + \varepsilon\beta K\,, \quad j = -\,s_\xi(1 + \varepsilon\alpha K)\,, \quad K = \Phi_{\xi\xi}/(s_\xi)^3\,.$$

We seek the solution of equation (7.2) as an asymptotic expansion in powers of ε. A detailed description of the method of computations can be found in [1]. As a result we obtain the following expressions for the expansion terms of normal boundary velocity :

$$v_0 = -\,1\,, \quad v_1 = AK_0\,, \quad v_2 = AK_1 + BK_0^2\,, \tag{7.3}$$
$$v_3 = AK_2 + 2\,BK_0\,K_1 + EK_0^3 + GK_{0_{ss}}\,,$$

where

$$A = 1 + \beta - \alpha\,, \; B = (\beta + 1)A\,, \; E = 1(\beta^2 - A + 2\,\beta) + 3\,\beta + 5\,,$$
$$G = (A - 1)(A + \beta + 1)\,. \tag{7.4}$$

Using expressions (7 3) one can « synthesize » the boundary dynamics equation modulo ε^3

$$v = v_0 + \varepsilon v_1 + \varepsilon^2 v_2 + \varepsilon^3 v_3 =$$
$$= -1 + \varepsilon A(K_0 + \varepsilon K_1 + \varepsilon^2 K_2) + \varepsilon^2 B(K_0^2 + 2K_0 K_1) + \varepsilon^3 EK_0^3 + \varepsilon^3 GK_{0_{ss}}$$
$$= -1 + A\varepsilon K + B\varepsilon^2 K^2 + E\varepsilon^3 K^3 + G\varepsilon^3 K_{ss} ,$$

or, in the original non-scaled variables

$$v = -1 + A\kappa + B\kappa^2 + E\kappa^3 + G\kappa_{ss} , \tag{7 5}$$

that is the two-dimensional form of equation (2 4) Near the bifurcation point $A \ll 1$ equation (7 5) can be reduced to the following

$$v = -1 + A\kappa - (\beta - 1)\kappa_{ss} \tag{7 6}$$

VIII. DISCUSSION

Our main goal in the present note was to introduce the simplified model of « exothemal phase transition » (4 1)-(4 2), that is capable of developing cellular and turbulent boundary As it is shown above problem (4 1)-(4 2) allows a quasi-local approximation of the boundary dynamics based on the quasi-planar quasi-steady behaviour of its solution near a weakly curved boundary The latter is due to existence of the plane wave (4 3) which is a « built-in » feature in our model It is worth mentioning that similar analyses of the solidification problem (3 1) is made possible only via introduction of the interface kinetics term $Q(v)$, without which it becomes, in our view, essentially non-local

The curvature dependent boundary conditions (4 2) can be prescribed a physical interpretation in both combustion or solidification context However, problem (4 1)-(4 2) is not claimed to describe correctly either process, but only simulate certain qualitative features in their dynamics while gaining in simplicity in comparison to them For instance, (4 1)-(4 2) is the simpliest problem known to the author that leads to the Kuramoto-Sivashinsky equation

The above remarks reflect author's opinion that the free boundary problem (4 1)-(4 2) is more suitable and « promising » for rigorous mathematical study Another goal of the present communication is to attract attention of the pure mathematicians to the model introduced here as well as to the surface propagation of (2 4), (2 5) type both represent in our view interesting and challenging mathematical objects For that reason we would like to complete this note by formulating several questions, however naive in view of complexity of the subject

1 In what sense can be an initial value problem for (4 1)-(4 2) well posed ? Is there a global existence ? For instance, will initially connected Ω with smooth boundary remains such for any t ?

2 Will the intrinsic chaos in the proposed model remain bounded in some suitable norm ? What is the dynamics of fractal dimension for a turbulent solution of (4 1)-(4 2) ?

Similar questions concerning global existence and complexity (e g estimates similar to the ones obtained in [6] for Kuramoto-Sivashinsky equation) with respect to the boundary dynamics equation (2 4) should be asked Additionally, can the steadily propagating solutions of (2 4) be classified similar to [7] including a purely spatial chaos ? And, finally, can the invariant equation (2 4) be rigorously shown to approximate the exact boundary dynamics of the model free boundary problem (4 1)-(4 2) ?

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