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INFLUENCE OF NATURAL CONVECTION ON STABILITY OF AN INCLINED FRONT PROPAGATION

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Abstract. This research work may be considered as a continuation of a series of investigations concerning the influence of natural convection on stability of reaction fronts propagation. We consider an inclined propagating polymerization front. The governing equations consist of the heat equation, the equation for the depth of conversion for one-step chemical reaction and of the Navier-Stokes equations under the Boussinesq approximation. We first perform a formal asymptotic analysis in the limit of a large activation energy to get an approximate interface problem. Then, we fulfill the linear stability analysis of the stationary solution and find the perturbation equations. A meshless collocation method based on multiquadric radial basis functions has been applied for numerical simulations. The conditions of convective instabilities obtained are in good agreement with some previous studies. This shows that the proposed approach is accurate and that it helps in describing the influence of the propagation direction on stability of polymerization fronts.

1. Introduction

Natural convection is a type of heat transport, in which the fluid motion is not generated by any external source but only by density differences in the fluid occurring due to temperature gradients if it is large enough. Natural convection attracts a great deal of attention from researchers because of its presence both in nature and engineering applications. One key issue concerning the heat transfer process in fluids, is how efficient it is, if it varies depending on some critical parameters. In this work, we consider the case when it is produced through a chemical reaction, that is frontal polymerization. This is a procedure that involves a localized reaction zone travelling through a monomer solution and converting this monomer into solid polymer, that is the product. An illustration of an ascending frontal polymerization is shown in Figure (1). In this case the monomer and the polymer are separated

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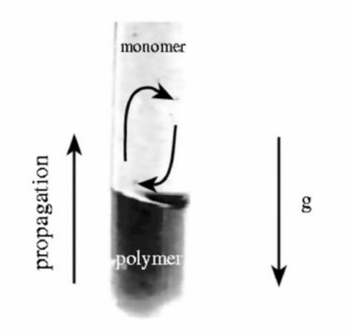

FIGURE 1. Ascending front propagation

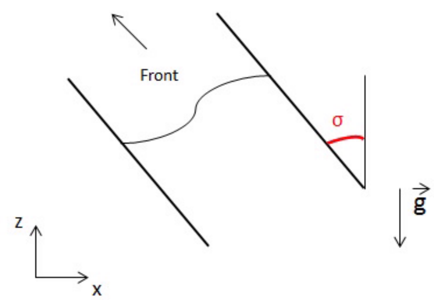

FIGURE 2. Inclined front propagation

by a narrow reaction zone, which is the front, that propagates if the reaction is exothermic and highly activated.
Most researches in this area, like [1, 2, 3, 5, 10], are concerned with the ascending and descending fronts. In the present case, we consider the case when the polymerization front is propagating toward an inclined enclosure.
The paper is organized as follows: The governing equations are presented in Section 2. The asymptotic analysis is performed in section 3. The linear stability analysis is carried out in section 4. Then, the numerical results based on the multiquadric radial basis function approach are presented in section 5.

2. Governing Equations

The system considered in this work consists of an inclined enclosure with an inclination angle σ as shown in figure (2). The governing equations consist of coupling two equations for the temperature and depth of conversion to the Navier-Stokes equations. The fluid is Newtonian and all the thermophysical properties are supposed to be constant, except for the density in the buoyancy term that can be adequately modelled by the Boussinesq approximation, and that compression effects and viscous dissipation are neglected. Under these assumptions, the problem is described in a three-dimensional space (x, y, z), $-\infty < x, y, z < +\infty$, by the following equations:

$$\frac{\partial T}{\partial t} + \mathbf{v}.\nabla T = \kappa \Delta T + qK(T)\phi(\alpha), \tag{1}$$

$$\frac{\partial \alpha}{\partial t} + \mathbf{v}.\nabla \alpha = \quad K(T)\phi(\alpha), \tag{2}$$

$$\frac{\partial \mathbf{v}}{\partial t} + \mathbf{v}.\nabla \mathbf{v} = -\frac{\nabla p}{\rho} + \nu \Delta \mathbf{v} + g\beta(T - T_0)\begin{pmatrix} -\sin\sigma \\ 0 \\ \cos\sigma \end{pmatrix}, \tag{3}$$

$$\nabla.\mathbf{v} = 0, \tag{4}$$

with the boundary conditions:

$$\begin{aligned} &T = T_i, \quad \alpha = 0 \text{ and } \mathbf{v} = 0 \quad \text{when } z \to +\infty, \\ &\frac{\partial T}{\partial z} = 0, \quad \alpha = 1 \text{ and } \mathbf{v} = 0 \quad \text{when } z \to -\infty. \end{aligned} \tag{5}$$

Here, T is the temperature, $\mathbf{v} = (v_x, v_y, v_z)$ the velocity, α the depth of conversion, p the pressure, κ the coefficient of thermal diffusivity, q is the adiabatic heat release, ρ is the density, ν the coefficient of kinematic viscosity, g the gravity acceleration, β the coefficient of thermal expansion, T_0 is the mean value of the temperature and T_i is an initial temperature while T_b is the temperature of the reacted mixture given by $T_b = T_i + q$.

The function $K(T)$ describes the reaction rate where the temperature dependence is given by the Arrhenius law $K(T) = k_0 \exp\left(-\frac{E}{R_0 T}\right)$, E is the activation energy supposed to be large in this problem, R_0 is the universal gas constant and k_0 is the pre-exponential factor.

$\phi(\alpha)$ is the kinetic function for which we consider the zero order reaction defined by

$$\phi(\alpha) = \begin{cases} 1 \text{ if } \alpha < 1 \\ 0 \text{ if } \alpha = 1 \end{cases} . \tag{6}$$

The coefficient of mass diffusion is supposed to be small comparatively to the thermal diffusivity coefficient, so that the diffusion term in the equation for the concentration is neglected.

In an inclined geometry, the differential operators Δ, ∇ and $\nabla.$ are expressed by:

$$\nabla = \begin{pmatrix} \cos\sigma \\ 0 \\ -\sin\sigma \end{pmatrix} \frac{\partial}{\partial x} + \begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \frac{\partial}{\partial y} + \begin{pmatrix} \sin\sigma \\ 0 \\ \cos\sigma \end{pmatrix} \frac{\partial}{\partial z} \quad , \quad \Delta = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

$$\text{and} \quad \nabla. = \left(\cos\sigma \frac{\partial}{\partial x} + \sin\sigma \frac{\partial}{\partial z}\right) + \frac{\partial}{\partial y} + \left(-\sin\sigma \frac{\partial}{\partial x} + \cos\sigma \frac{\partial}{\partial z}\right). \tag{7}$$

We now introduce the following spatial variables, with a view to obtain the dimensionless model:

$$x' = xc_1/\kappa, \;\; y' = yc_1/\kappa, \;\; z' = zc_1/\kappa, \;\; t' = tc_1^2/\kappa,$$

$$\mathbf{v}' = \mathbf{v}/c_1, \;\; p' = \frac{p}{c_1^2\rho} \;\text{ and }\; c_1 = c/\sqrt{2},$$

where c gives the stationary propagation front velocity, which can be calculated asymptotically for large Zeldovich number Z [5], where $Z = \dfrac{qE}{R_0T_b^2}$, we have:

$$c^2 = \frac{2k_0\kappa}{q}\frac{R_0T_b^2}{E}\exp\left(\frac{-E}{R_0T_b}\right).$$

Denoting the dimensionless temperature by $\theta = (T - T_b)/q$ and keeping for convenience the same notation for all the other variables, we may re-write system (1)-(4) as follows:

$$\frac{\partial\theta}{\partial t} + \mathbf{v}.\nabla\theta = \Delta\theta + W_Z(\theta)\phi(\alpha), \tag{8}$$

$$\frac{\partial\alpha}{\partial t} + \mathbf{v}.\nabla a = W_Z(\theta)\phi(\alpha), \tag{9}$$

$$\frac{\partial\mathbf{v}}{\partial t} + \mathbf{v}.\nabla\mathbf{v} = -\nabla p + P\Delta\mathbf{v} - PR(\theta + \theta_0)\begin{pmatrix} -\sin\sigma \\ 0 \\ \cos\sigma \end{pmatrix}, \tag{10}$$

$$\nabla.\mathbf{v} = 0, \tag{11}$$

with the boundary conditions

$$\begin{aligned} &\theta = -1, \;\; \alpha = 0 \;\;\text{ and } \mathbf{v} = 0 \quad \text{when } z \to +\infty, \\ &\frac{\partial\theta}{\partial z} = 0, \qquad\qquad\qquad\qquad \text{when } z \to -\infty. \end{aligned} \tag{12}$$

Here, $W_Z(\theta) = Z\exp\Big(\dfrac{\theta}{Z^{-1}+\delta\theta}\Big)$ and ϕ is the the kinetic function as defined in (6).
$P = \dfrac{\nu}{\kappa}$ is the Prandtl number, $R = \dfrac{g\beta q\kappa^2}{\nu c_1^3}$ the Rayleigh number, $Z = \dfrac{qE}{R_0T_b^2}$ the Zeldovich number, $\delta = R_0T_b/E$ and $\theta_0 = (T_b - T_0)/q$.

3. Asymptotic analysis

The asymptotic analysis of the problem is carried out based on the Zeldovich and Frank-Kamenetskii approach [13]. Indeed, most polymerization processes are exothermic. They are characterized by the fact that the basic chemical transformation takes place over a narrow temperature interval that is close to the maximum temperature. This has enabled Zeldovich and Frank-Kamenetskii to propose the infinitely narrow reaction zone method in which it is assumed that the reaction zone is concentrated at a point, and outside of this reaction zone, the non-linear source is set equal to zero. Then, the asymptotic solution can be sought, for large Zeldovich number Z, in the form of an expansion in a small parameter $\epsilon = 1/Z$ connected with the width of the reaction zone. This makes it possible, by using the asymptotic matching principle [9], to replace the non-linear differential equations by linear equations and algebraic matching conditions across the reaction zone.

3.1. **Inner and outer solutions.** Let the front be located at $z = \zeta(x, y, t)$ and propagate on the z axis moving direction.
We consider the new independent variable $z_1 = z - \zeta(x, y, t)$ and introduce new unknown functions θ_1, α_1, $\mathbf{v}_1$, p_1 as defined by:

$$\begin{aligned} &\theta(t,x,y,z) = \theta_1(t,x,y,z_1), \;\; \alpha(t,x,y,z) = \alpha_1(t,x,y,z_1), \\ &\mathbf{v}(t,x,y,z) = \mathbf{v}_1(t,x,y,z_1), \;\; p(t,x,y,z) = p_1(t,x,y,z_1). \end{aligned} \tag{13}$$

Thus, we may re-write the equations (8)-(11) in the form (the index 1 for the independent variables is omitted):

$$\frac{\partial\theta}{\partial t} - \frac{\partial\theta}{\partial z_1}\frac{\partial\zeta}{\partial t} + \mathbf{v}.\widetilde{\nabla}\theta = \widetilde{\Delta}\theta + W_Z(\theta)\phi(\alpha), \tag{14}$$

$$\frac{\partial\alpha}{\partial t} - \frac{\partial\alpha}{\partial z_1}\frac{\partial\zeta}{\partial t} + \mathbf{v}.\widetilde{\nabla}\alpha = W_Z(\theta)\phi(\alpha), \tag{15}$$

$$\frac{\partial\mathbf{v}}{\partial t} - \frac{\partial\mathbf{v}}{\partial z_1}\frac{\partial\zeta}{\partial t} + \mathbf{v}.\widetilde{\nabla}\mathbf{v} = -\widetilde{\nabla}p + P\widetilde{\Delta}\mathbf{v} - Q(\theta+\theta_0)\begin{pmatrix} -\sin\sigma \\ 0 \\ \cos\sigma \end{pmatrix}, \tag{16}$$

$$\left(\frac{\partial v_x}{\partial x}-\frac{\partial v_x}{\partial z_1}\frac{\partial \zeta}{\partial x}\right)\cos\sigma+\frac{\partial v_x}{\partial z_1}\sin\sigma+\frac{\partial v_y}{\partial y}-\frac{\partial v_y}{\partial z_1}\frac{\partial \zeta}{\partial y}-\left(\frac{\partial v_z}{\partial x}-\frac{\partial v_z}{\partial z_1}\frac{\partial \zeta}{\partial x}\right)\sin\sigma+\frac{\partial v_z}{\partial z_1}\cos\sigma=0. \tag{17}$$

Here, $Q = PR$ and

$$\widetilde{\Delta} = \frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z_1^2}-2\frac{\partial \zeta}{\partial x}\frac{\partial^2}{\partial x\partial z_1}-2\frac{\partial \zeta}{\partial y}\frac{\partial^2}{\partial y\partial z_1}+\left(\left(\frac{\partial \zeta}{\partial x}\right)^2+\left(\frac{\partial \zeta}{\partial y}\right)^2\right)\frac{\partial^2}{\partial z_1^2}-\left(\frac{\partial^2 \zeta}{\partial x^2}+\frac{\partial^2 \zeta}{\partial y^2}\right)\frac{\partial}{\partial z_1},$$

$$\widetilde{\nabla} = \begin{pmatrix}\cos\sigma\\ 0\\ -\sin\sigma\end{pmatrix}\left(\frac{\partial}{\partial x}-\frac{\partial \zeta}{\partial x}\frac{\partial}{\partial z_1}\right)+\begin{pmatrix}0\\ 1\\ 0\end{pmatrix}\left(\frac{\partial}{\partial y}-\frac{\partial \zeta}{\partial y}\frac{\partial}{\partial z_1}\right)+\begin{pmatrix}\sin\sigma\\ 0\\ \cos\sigma\end{pmatrix}\frac{\partial}{\partial z_1}.$$

We look for the outer solution of the problem (14)-(17) in the form of expansion

$$\begin{aligned}&\theta = \theta^0+\epsilon\theta^1+..., \quad \alpha=\alpha^0+\epsilon\alpha^1+...,\\ &\mathbf{v}=\mathbf{v}^0+\epsilon\mathbf{v}^1+..., \quad p=p^0+\epsilon p^1+....\end{aligned} \tag{18}$$

$(\theta^0, \alpha^0, \mathbf{v}^0)$ denotes the dimensionless form of the basic solution.

Then, in order to obtain the matching conditions across the reaction zone, we seek the inner solution using the stretched coordinate $\eta = z_1/\epsilon$ in the form of expansion:

$$\begin{aligned}&\theta = \epsilon\tilde{\theta}^1+..., \quad \alpha=\epsilon\tilde{\alpha}^1+...,\\ &\mathbf{v}=\tilde{\mathbf{v}}^0+\epsilon\tilde{\mathbf{v}}^1+..., \quad p=\tilde{p}^0+\epsilon\tilde{p}^1+..., \quad \zeta=\zeta^0+\epsilon\zeta^1+....\end{aligned} \tag{19}$$

Substituting these expansions into (14)-(17), we obtain the following first-order inner problem:

Order ϵ^{-2}

$$P\Big(1+\Big(\frac{\partial\zeta_0}{\partial x}\Big)^2+\Big(\frac{\partial\zeta_0}{\partial y}\Big)^2\Big)\frac{\partial^2\tilde{v}_0}{\partial\eta^2}=0. \tag{20}$$

Order ϵ^{-1}

$$\Big(1+\Big(\frac{\partial\zeta_0}{\partial x}\Big)^2+\Big(\frac{\partial\zeta_0}{\partial y}\Big)^2\Big)\frac{\partial^2\tilde{\theta}_1}{\partial\eta^2}+\exp\Big(\frac{\tilde{\theta}_1}{1+\delta\tilde{\theta}_1}\Big)\phi(\tilde{\alpha}_0)=0, \tag{21}$$

$$\begin{aligned}&-\frac{\partial\tilde{\alpha}_0}{\partial\eta}\frac{\partial\zeta_0}{\partial t}+\frac{\partial\tilde{\alpha}_0}{\partial\eta}\Big(\tilde{v_{0x}}\Big(\frac{\partial\zeta_0}{\partial x}\cos\sigma+\sin\sigma\Big)-\tilde{v_{0y}}\frac{\partial\zeta_0}{\partial y}\\&+\tilde{v_{0z}}\Big(\frac{\partial\zeta_0}{\partial x}\sin\sigma-\cos\sigma\Big)\Big)=\exp\Big(\frac{\tilde{\theta}_1}{1+\delta\tilde{\theta}_1}\Big)\phi(\tilde{\alpha}_0),\end{aligned} \tag{22}$$

$$-\frac{\partial\tilde{v_{0x}}}{\partial\eta}\Big(\frac{\partial\zeta_0}{\partial x}\cos\sigma-\sin\sigma\Big)-\frac{\partial\tilde{v_{0y}}}{\partial\eta}\frac{\partial\zeta_0}{\partial y}+\frac{\partial\tilde{v}_{0z}}{\partial\eta}\Big(\frac{\partial\zeta_0}{\partial x}\sin\sigma+\cos\sigma\Big)=0. \tag{23}$$

By using the asymptotic matching principle, we find the matching conditions:

$$\begin{aligned}&\eta\to+\infty:\quad \tilde{v}_0\sim v_0|_{z_1=+0},\ \ \tilde{\theta}_1\sim\theta_1|_{z_1=+0}+\Big(\frac{\partial\theta_0}{\partial z_1}\Big|_{z_1=+0}\Big)\eta,\ \ \tilde{\alpha_0}\to 0,\\&\eta\to-\infty:\quad \tilde{v}_0\sim v_0|_{z_1=-0},\ \ \tilde{\theta}_1\sim\theta_1|_{z_1=-0},\ \ \tilde{\alpha_0}\to 1.\end{aligned} \tag{24}$$

On account of the equation (20) and the boundedness of the solution, we conclude that $\tilde{v}_0$ does not depend on η. From this conclusion and the matching conditions, it follows that the first term of the outer expansion of the velocity v_0 is continuous at the front.

We denote

$$s=\tilde{v_{0x}}\Big(\frac{\partial\zeta_0}{\partial x}\cos\sigma-\sin\sigma\Big)+\tilde{v_{0y}}\frac{\partial\zeta_0}{\partial y}-\tilde{v_{0z}}\Big(\frac{\partial\zeta_0}{\partial x}\sin\sigma+\cos\sigma\Big). \tag{25}$$

From (22) it follows that the function s does not depend on η.
We derive next the jump conditions for the temperature from (21) in the same way as it is given in the references [5, 7].
Since we consider the zero order reaction $\phi(\tilde{\alpha_0})\equiv 1$.

From (21), we conclude that $\dfrac{\partial^2\tilde{\theta}^1}{\partial\eta^2}\leq 0$, so $\dfrac{\partial\tilde{\theta}^1}{\partial\eta}$ is decreasing from $\eta=-\infty$ to $\eta=+\infty$.

From (24) we have, $\dfrac{\partial\tilde{\theta}^1}{\partial\eta}\sim 0$ at $\eta=-\infty$, then $\dfrac{\partial\tilde{\theta}^1}{\partial\eta}\leq 0$ everywhere, this shows that $\tilde{\theta}^1$ is decreasing too.

Multiplying (21) by $\dfrac{\partial\tilde{\theta}_1}{\partial\eta}$ and integrating, we obtain:

$$\Big(\frac{\partial\tilde{\theta}^1}{\partial\eta}\Big)^2\Big|_{\eta=+\infty}-\Big(\frac{\partial\tilde{\theta}^1}{\partial\eta}\Big)^2\Big|_{\eta=-\infty}=\frac{2}{A}\int_{-\infty}^{\theta^1|_{z_1=0+}}\exp\Big(\frac{\tau}{1+\delta\tau}\Big)d\tau, \tag{26}$$

Subtracting (21) from (22) and integrating, we have

$$\frac{\partial\tilde{\theta}_1}{\partial\eta}\Big|_{\infty}-\frac{\partial\tilde{\theta}_1}{\partial\eta}\Big|_{-\infty}=-A^{-1}\Big(\frac{\partial\zeta_0}{\partial t}+s\Big). \tag{27}$$

where $A=1+\Big(\dfrac{\partial\tilde{\zeta}^0}{\partial x}\Big)^2+\Big(\dfrac{\partial\tilde{\zeta}^0}{\partial y}\Big)^2$.

Equations (26)-(27) represent the jump conditions for the temperature across the front.

Using the matching conditions (24) and truncating the expansion in the same way as that of the reference [7]:

$$\theta_0\approx\theta,\ \ \theta_1|_{z_1=-0}\approx Z\theta|_{z_1=+0},\ \ \zeta_0\approx\zeta\ \text{ and }\ v_0\approx v. \tag{28}$$

We may rewrite the jump conditions as follows :

$$\left(\frac{\partial\theta}{\partial z_1}\right)^2\Big|_{z_1=+0} - \left(\frac{\partial\theta}{\partial z_1}\right)^2\Big|_{z_1=-0} =$$
$$2Z\left(1+\left(\frac{\partial\zeta}{\partial x}\right)^2+\left(\frac{\partial\zeta}{\partial y}\right)^2\right)^{-1}\int_{-\infty}^{\theta_1|_{z_1=-0}} \exp\left(\frac{\tau}{1+\delta\tau}\right)d\tau, \tag{29}$$

$$\frac{\partial\theta}{\partial z_1}\Big|_{z_1=+0} - \frac{\partial\theta}{\partial z_1}\Big|_{z_1=-0} = -\left(1+\left(\frac{\partial\zeta}{\partial x}\right)^2+\left(\frac{\partial\zeta}{\partial y}\right)^2\right)^{-1}\times$$
$$\left(\frac{\partial\zeta}{\partial t}+\left(v_x\left(\frac{\partial\zeta}{\partial x}\cos\sigma-\sin\sigma\right)+v_y\frac{\partial\zeta}{\partial y}-v_z\left(\frac{\partial\zeta}{\partial x}\sin\sigma+\cos\sigma\right)\Big|_{z_1=+0}\right)\right). \tag{30}$$

3.2. **Interface problem.** We present the formulation of the interface problem which approximates the original system (8)-(11) as follows:

<u>$z > \zeta$</u> (in the unreacted medium):

$$\frac{\partial\theta}{\partial t} + \mathbf{v}.\nabla\theta = \Delta\theta, \tag{31}$$
$$\alpha = 0, \tag{32}$$
$$\frac{\partial\mathbf{v}}{\partial t} + (\mathbf{v}.\nabla)\mathbf{v} = -\nabla p + P\Delta\mathbf{v} + Q(\theta+\theta_0)\begin{pmatrix}-\sin\sigma\\ 0\\ \cos\sigma\end{pmatrix}, \tag{33}$$
$$\nabla.\mathbf{v} = 0. \tag{34}$$

<u>$z < \zeta$</u> (in the reacted medium):

$$\frac{\partial\theta}{\partial t} = \Delta\theta, \tag{35}$$
$$\alpha = 1, \tag{36}$$
$$\mathbf{v} = 0. \tag{37}$$

Where ∇ and Δ are defined by (7).

The jump conditions at the interface $\underline{z=\zeta}$ have the form:

$$\theta|_{\zeta-0} = \theta|_{\zeta+0}, \tag{38}$$

$$\frac{\partial\theta}{\partial z}\Big|_{\zeta-0} - \frac{\partial\theta}{\partial z}\Big|_{\zeta+0} = \Big(1+\Big(\frac{\partial\zeta}{\partial x}\Big)^2+\Big(\frac{\partial\zeta}{\partial y}\Big)^2\Big)^{-1}\frac{\partial\zeta}{\partial t}, \tag{39}$$

$$\Big(\frac{\partial\theta}{\partial z}\Big)^2\Big|_{\zeta-0} - \Big(\frac{\partial\theta}{\partial z}\Big)^2\Big|_{\zeta+0} = -2Z\Big(1+\Big(\frac{\partial\zeta}{\partial x}\Big)^2+\Big(\frac{\partial\zeta}{\partial y}\Big)^2\Big)^{-1}\int_{-\infty}^{\theta|_\zeta}\exp\Big(\frac{\tau}{1+\delta\tau}\Big)d\tau, \tag{40}$$

$$v_x = v_y = v_z = 0. \tag{41}$$

To complete the problem we should specify also the conditions at infinity :

$$\begin{aligned} z=-\infty: &\quad \theta=0,\ \ \mathbf{v}=0,\\ z=+\infty: &\quad \theta=-1,\ \ \mathbf{v}=0. \end{aligned} \tag{42}$$

4. Linear stability analysis

In this section, we perform the linear stability analysis of the steady-state solution for the interface problem. In the case of vertical propagation front, previous studies like [5, 12], have shown that the interface problem has a travelling wave solution. However, in the case of the inclined propagation, the explicit form of the stationary solution is unknown. We propose to find this solution numerically by using the multiquadric radial basis functions collocation (MQ-RBF) method.

4.1. **MQ-RBF method for finding the numerical stationary solution.**

Radial basis functions methods are generally means to approximate multivariable functions, which are too difficult to evaluate and only known at a finite number of points, called centers, by linear combinations of terms based on a single basis function.
The general principle is that we consider M collocation points $\mathbf{x_i},\ i=1,2,\dots,M$ on which we would like to interpolate a given function f. The method is applied in 2 dimensional Euclidean space which is fitted with the Euclidean norm $\|.\|_2$. There are N points in this space at which the function f is known, called centers

$\mathbf{x_i^c},\ i = 1, 2, \ldots, N$, where $\mathbf{x_i^c} = (x_i^c, y_i^c)$. These points are usually assumed to be all different from each other, otherwise the problem will become singular when interpolation is used.

Given this information, we create the sought approximant by a sum

$$s(\mathbf{x_i}) = \sum_{j=1}^{N} \alpha_j \varphi(\|\mathbf{x_i} - \mathbf{x_j^c}\|), \tag{43}$$

where $s(\mathbf{x_i})$ is the interpolant of f at the collocation point $\mathbf{x_i} = (x_i, y_i)$, the φ is a univariate, normally continuous function $\varphi : R_+ \longrightarrow R$, namely the radial basis function.

The expansion coefficients $\alpha_j,\ j = 1, 2, \ldots, N$ are chosen in such a way as to enforce the following interpolation conditions at all the centers;

$$s(\mathbf{x_j^c}) = f(\mathbf{x_j^c}). \tag{44}$$

In this work, the multiquadric radial basis function (MQ-RBF) is used due to its popularity in many applications and its good approximation properties [11]. The multiquadric is representive of the class of RBFs that are global, infinitely diffetentiable, and that contain a shape parameter $\varepsilon \neq 0$ which plays an important role for the accuracy of the method. The MQ-RBF is radially symmetric about its center, $\mathbf{x} \in \mathbb{R}^2$, and its argument $r = \|\mathbf{x}\|_2$ is dependent on the node location.

The MQ-RBF is defined by

$$\varphi(r, \varepsilon) = \sqrt{r^2 + \varepsilon^2}. \tag{45}$$

So, for each collocation point $\mathbf{x} = (x, y) \in \mathbb{R}^2$, the MQ-RBF can be described by

$$\varphi(\|\mathbf{x} - \mathbf{x_j^c}\|, \varepsilon) = \sqrt{(x - x_j^c)^2 + (y - y_j^c)^2 + \varepsilon^2}, \tag{46}$$

and therefore, the MQ-RBF interpolant takes the form

$$s(\mathbf{x_i}) = \sum_{j=1}^{N} \alpha_j \varphi(\|\mathbf{x_i} - \mathbf{x_j^c}\|, \varepsilon). \tag{47}$$

Enforcing the interpolation conditions (44) at the N centers results in a $N \times N$ linear system

$$\mathbf{B}\boldsymbol{\alpha} = \mathbf{F}, \tag{48}$$

to be solved for the expansion coefficients $\alpha = [\alpha_1, \alpha_2, \ldots, \alpha_N]^T$.

The matrix B is called the *interpolation matrix* and its entries are given by the formula

$$\mathbf{B}_{ij} = \varphi(\|\mathbf{x_i^c} - \mathbf{x_j^c}\|, \varepsilon) = \sqrt{(x_i^c - x_j^c)^2 + (y_i^c - y_j^c)^2 + \varepsilon^2}, \quad i, j = 1, \ldots, N. \tag{49}$$

The system (48) is equivalent to a matrix equation of the form

$$\begin{pmatrix} \varphi_{11} & \varphi_{12} & \cdots & \cdots & \varphi_{1N} \\ \varphi_{21} & \varphi_{22} & \cdots & \cdots & \varphi_{2N} \\ \vdots & \vdots & \ddots & & \vdots \\ \vdots & \vdots & & \ddots & \vdots \\ \varphi_{N1} & \varphi_{N2} & \cdots & \cdots & \varphi_{NN} \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \\ \vdots \\ \vdots \\ \alpha_N \end{pmatrix} = \begin{pmatrix} f_1 \\ f_2 \\ \vdots \\ \vdots \\ f_N \end{pmatrix}. \tag{50}$$

If $\varphi(\mathbf{x})$ is a strictly positive definite function on a linear space, then the eigenvalues of $\mathbf{B}$ are positive and its determinant is positive. Therefore we can use a linear combination translation of $\varphi(\mathbf{x})$ for interpolation [4]. The multiquadric is a strictly positive definite function, this means that for any set of distinct collocation points, the matrix $\mathbf{B}_{ij} = \varphi(\|\mathbf{x_i^c} - \mathbf{x_j^c}\|, \varepsilon)$ is strictly positive definite, non-singular and invertible [8].

The multiquadric expansion coefficient α is given by

$$\alpha = \mathbf{B^{-1}F}. \tag{51}$$

To evaluate the interpolant at M points $\mathbf{x_i}$ using (47), the $M \times N$ evaluation matrix is constructed with the elements

$$\Phi_{ij} = \varphi(\|\mathbf{x_i} - \mathbf{x_j^c}\|_2, \varepsilon), \quad i = 1, \ldots, M \text{ and } j = 1, \ldots, N. \tag{52}$$

Then, the interpolant is evaluated at the M points by the matrix multiplication

$$\mathbf{S} = \mathbf{\Phi} \times \boldsymbol{\alpha}. \tag{53}$$

To deal with the diffusion part of the interface problem we consider the implicit scheme for the time derivative, and assume that the stationary solution (θ^n, α^n, $\mathbf{v}^n$) is known at a given time $t = n\Delta t$ so that it can be approximated in this way:

$$\begin{aligned} {\theta_s}^n &\simeq \sum_{j=1}^{N} \alpha_j^n \varphi(\|\mathbf{x_i} - \mathbf{x_j}^c\|_2, \varepsilon), \qquad {\alpha_s}^n \simeq \textstyle\sum_{j=1}^{N} \beta_j^n \varphi(\|\mathbf{x_i} - \mathbf{x_j}^c\|_2, \varepsilon), \\ {\mathbf{v}_s}^n &\simeq \sum_{j=1}^{N} \gamma_j^n \varphi(\|\mathbf{x_i} - \mathbf{x_j}^c\|_2, \varepsilon). \end{aligned}$$

If we substitute these expressions in (31)-(37), we can find numerically the stationary solution.

4.2. **Perturbation equations.** We now consider the moving coordinate frame $z_2 = z - ut$ and introduce small perturbations $(\tilde{\theta}, \tilde{p}, \tilde{v})$ to the stationary solution in the form of

$$\theta = \theta_s + \tilde{\theta}, \quad p = p_s + \tilde{p}, \quad \mathbf{v} = v_s + \tilde{v}, \tag{54}$$

where

$$\begin{aligned}
&\tilde{\theta}(t,x,y,z_2) = \theta_i(z_2)e^{\omega t + j(k_1 x + k_2 y)}, \quad i = 1,2 \\
&\tilde{v}_z(t,x,y,z_2) = v_{zi}(z_2)e^{\omega t + j(k_1 x + k_2 y)}, \quad i = 1,2 \\
&z_2 = y - \zeta(t,x) = y - ut - \xi(t,x), \\
&\text{with } \ \xi(t,x) = \epsilon_1 e^{\omega t + j(k_1 x + k_2 y)}.
\end{aligned} \tag{55}$$

Here, the number u stands for the stationary front velocity that can be easily found from the jump conditions at the interface. $j^2 = -1$, $i = 1$ corresponds to $z_2 < \xi$ and $i = 2$ to $z_2 > \xi$, ω is the frequency, k_i, $i = 1,2$ are the wave numbers and ϵ_1 the perturbation amplitude.

Substituting (54) in (31)-(37), we obtain for the first-order terms:

$\underline{z_2 > \xi}$:

$$\frac{\partial \tilde{\theta}}{\partial t} = \Delta\tilde{\theta} + u\frac{\partial \tilde{\theta}}{\partial z_2} - \cos(\sigma)\tilde{v}_z\theta_s', \tag{56}$$

$$\frac{\partial \tilde{v}}{\partial t} = -\nabla\tilde{p} + P\Delta\tilde{v} + u\frac{\partial \tilde{v}}{\partial z_2} + Q\tilde{\theta}\begin{pmatrix} -\sin\sigma \\ 0 \\ \cos\sigma \end{pmatrix}, \tag{57}$$

$$\nabla.\tilde{v} = 0. \tag{58}$$

$\underline{z_2 < \xi}$:

$$\frac{\partial \tilde{\theta}}{\partial t} = \Delta\tilde{\theta} + u\frac{\partial \tilde{\theta}}{\partial z_2}. \tag{59}$$

We linearize system (56)-(59) about the stationary solution and apply the *rot rot* transformation to equation (57). This allows us to eliminate the pressure and to consider only the velocity component v_z.

Next, we replace $\tilde{\theta}$ and $\tilde{v}_z$ with its expressions as in (55), we find the perturbation equations for $z > 0$:

$$\begin{aligned}
\omega(v'' - k^2 v) - u(v''' - k^2 v') &= P(v'''' - 2k^2 v'' + k^4 v) \\
&- Q\left[(k_1^2\cos(2\sigma) + k_2^2)\cos(\sigma)\theta - \sin(2\sigma)\sin(\sigma)\theta''\right],
\end{aligned} \tag{60}$$

$$Q\,k_1(1 - 4\cos^2(\sigma))\sin(\sigma)\theta' = 0, \tag{61}$$

$$\omega\theta - u\theta' + \cos(\sigma)v\theta_s' = \theta'' - k^2\theta, \tag{62}$$

with $k^2 = k_1^2 + k_2^2$.

In order to linearize the jump conditions (38)-(41), we use the *Taylor* formula at the position of the reaction zone $z = z_2$:

$$\theta|_{\xi=\pm 0} = \theta_s(\pm 0) + \xi\theta_s^{'}(\pm 0) + \widetilde{\theta}(\pm 0),$$

$$\left.\frac{\partial \theta}{\partial z}\right|_{\xi=\pm 0} = \theta_s^{'}(\pm 0) + \xi\theta_s^{''}(\pm 0) + \left.\frac{\partial \widetilde{\theta}}{\partial z}\right|_{\xi=\pm 0}.$$

For the highest order the jump conditions become:

$$[\theta] = u\xi, \tag{63}$$

$$[\theta\,'] = -u^2\xi - \xi\,', \tag{64}$$

$$-\,u(u^2\xi + \theta_2'(0)) = Z\theta_1(0), \tag{65}$$

$$\tilde{v}_z = 0, \quad \cos(\sigma)\frac{\partial \tilde{v}_z}{\partial z} = 0, \tag{66}$$

with

$$[\theta] = \theta_2(0) - \theta_1(0), \quad [\theta\,'] = \theta_2'(0) - \theta_1'(0), \quad \theta_i'(0) = \left.\frac{\partial \theta_i}{\partial z_2}\right|_{z_2=0} \text{ and } \quad \xi\,' = \frac{d\xi}{dt}.$$

The problem (60)-(62) subject to the jump conditions (63)-(66) is an eigenvalue problem with time-dependent coefficients. Again, we solve it numerically by using the multiquadric radial basis functions approximation with an implicit scheme to determine the stability boundaries.

5. Numerical results

In this section, we present the stability boundaries of the propagating polymerization front. There are basically two types of instabilities: the oscillatory instability and the cellular instability. In the first case a pair of complex conjugate eigenvalues cross the imaginary axis resulting in a Hopf bifurcation. In the second case, which we consider here, an eigenvalue crosses the imaginary axis through zero. This corresponds to the case where the frequency ω is assumed equal to zero.
For propagating fronts, the exothermic chemical reaction heats the liquid reactants from below. Then, under some conditions a convective motion of the liquid can appear. These critical conditions can be expressed in the form $R > Ra_c(P, u, \sigma, k)$, this means that the frontal Rayleigh number should exceed a critical value which depends on the Prandtl number, on the front velocity, on the inclination angle and on the wave number. Figure (3) shows the stable and the unstable critical areas which are found by drawing the critical Rayleigh number Ra_c as a function of the wave number k for different values of the Prandtl number P and the front velocity u. In this case, the reaction front is propagating upward, this means that the inclination angle σ is assumed equal to zero. We remark that when we increase the Prandtl number and the front velocity, the stationary front loses its stability. These results are in good agreement with the results which were obtained in [5]. Likewise, the curves in Figure (4) separates the stable and the unstable regions but

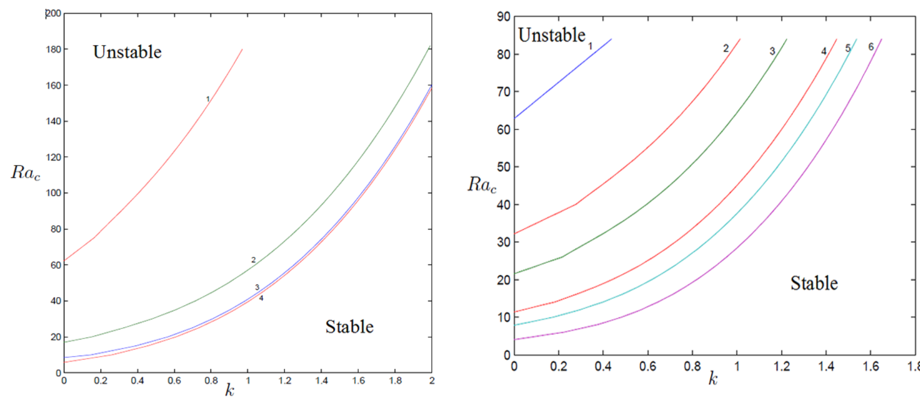

FIGURE 3. Stability boundaries for the upward propagating front. Left: $u = \sqrt{2}$, $P = 0.1$ (1), $P = 0.5$ (2), $P = 2$ (3), $P = 30$ (4). Right : $P = 0.99$, $u = 1$ (1), $u = 1.25$ (2), $u = \sqrt{2}$ (3), $u = 1.75$ (4), $u = 2$ (5), $u = 2.5$ (6).

now, in the case of the inclined propagating front. These show that, for fixed values of the front velocity and the Prandtl number, the stability conditions depend on the angle of inclination. If its value is greater, the front becomes more stable.

6. Conclusion

Natural convection can have an essential influence on the thermal instability of reaction fronts in the case where the product of the reaction is solid. In this work, a polymerization front problem is studied in situations where the fluid enclosure inclination is changing. The Prandtl number, the front velocity and the inclination angle are considered to be the critical parameters. In the case of an inclined medium, the instability grows extensively by decreasing the value of the inclination angle. Then, natural convection makes inclined propagating front more stable than without inclination and ascending fronts less stable.

It would be interesting to study the oscillatory instability which corresponds to the case where the frequency is a complex value. From the linear stability analysis of the stationary solution, we obtain complex valued perturbation equations that are very complicated and should be solved numerically. The next step is to study polymerization fronts problems in inclined porous media using the same approach. In this case, the mathematical formulation consists of a nonlinear reaction-diffusion equation coupled to Darcy's law.

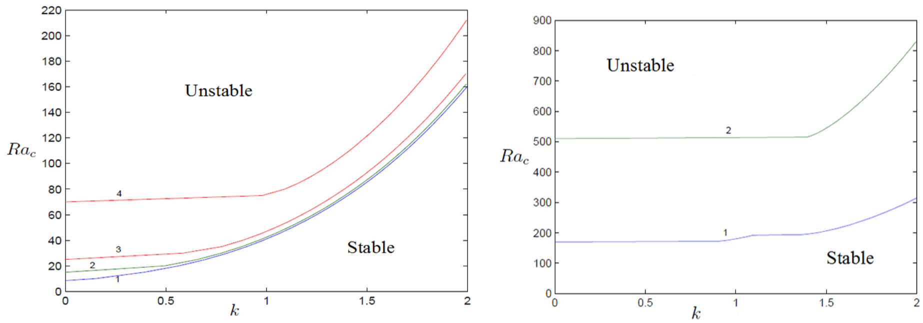

FIGURE 4. Stability boundaries for the inclined propagating front for $u = \sqrt{2}$ and $P = 2.1$. Left: $\sigma = 0.2$ (1), $\sigma = 5.3$ (2), $\sigma = 10.4$ (3), $\sigma = 20$ (4). Right: $\sigma = 30$ (1), $\sigma = 45$ (2).

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