



Convection of Polymerization Front with Solid Product under Quasi-Periodic Gravitational Modulation

Karam Allali¹, Saadia Assiyad¹ and Mohamed Belhaq^{2*}

¹ *University Hassan II-Mohammedia, Department of Mathematics, Mohammadia, Morocco*

² *University Hassan II-Casablanca, Laboratory of Mechanics, Casablanca, Morocco*

Received: April 26, 2014; Revised: October 14, 2014

Abstract: The effect of quasi-periodic gravitational modulation on the convective instability of polymerization front with solid product is studied in this paper. The model we consider includes the heat equation, the concentration equation and the Navier-Stokes equations under the Boussinesq approximation. The linear stability analysis of the problem is carried out and the interface problem is established applying the narrow zone method and the matched asymptotic expansions. The convective instability threshold is determined using numerical simulation. It was shown that the frequencies ratio has a significant effect on the convective stability domain. In particular, the stability domain changes and undergoes a shift as the frequencies ratio of the quasi-periodic modulation varies.

Keywords: *convective instability; frontal polymerization; quasi-periodic modulation.*

Mathematics Subject Classification (2010): 35K57, 76D05, 76E15.

1 Introduction

Frontal polymerization phenomenon is the process of converting monomer to polymer via a narrow located zone, called reaction front [1]. The influence of periodic gravitational modulation on the convective instability of polymerization reaction front with solid product was studied in [2] and it was shown that the reaction front gains stability for increasing values of the modulation frequency. In this paper, we investigate the influence of quasi-periodic (QP) gravitational modulation on the convective instability of polymerization front with solid product. Such a QP modulation may result, for instance, from the existence of two simultaneous vibrations consisting of a basic vibration with

* Corresponding author: <mailto:mbelhaq@yahoo.fr>

a certain frequency and of an additional residual vibration having another frequency, such that the two involved frequencies are incommensurate. It is worth noticing that the influence of QP excitation on the dynamics of mechanical systems and the transition to chaos is studied in [3, 4].

To study the influence of QP gravitational modulation on the convective instability of polymerization front with solid product, we consider a system of reaction-diffusion equations coupled with incompressible Navier-Stokes equations. We notice that the case considering the influence of QP gravitational modulation on the reaction front in porous media has been examined in [5]. In this case [5], the system of reaction-diffusion equations is coupled with the equations of motion taking into account the Darcy law.

It is worthy to point out that only few works have been devoted to examine the effect of QP vibration on the convective instability. For instance, Boulal et al. [6] reported on the effect of a QP gravitational modulation on the convective instability of a heated fluid layer and it was shown that the frequencies ratio of QP vibration strongly influences the convective instability threshold. Moreover, the influence of QP gravitational modulation on convective instability in Hele-Shaw cell was analyzed in [7]. Similar study has been made to investigate the thermal instability in horizontal Newtonian magnetic liquid layer with non-magnetic rigid boundaries in the presence of a vertical magnetic field [8]. In [6, 7], the original problem was systematically reduced to a QP Mathieu equation using Galerkin method truncated to the first order. Since the Floquet theory cannot be applied in the case of QP modulation, the approach used to obtain the marginal stability curves was principally based on the harmonic balance method combined with Hill's determinants [9, 10].

Because one cannot truncate the problem under consideration to a QP Mathieu equation using Galerkin method and the Floquet theory as in [9, 10], the marginal stability curves are obtained by using the approximately narrow zone method (Frank-Kamenetskii method) and the matched asymptotic expansions. This approach leads to the interface problem which is solved by numerical simulation.

To introduce a QP gravitational modulation, we consider that the acceleration acting on the fluid is given by $g+b(t)$, where g is the gravity acceleration and $b(t) = \lambda_1 \sin(\mu_1 t) + \lambda_2 \sin(\mu_2 t)$ in which λ_1, λ_2 and μ_1, μ_2 are the amplitudes and the frequencies of the QP vibration, respectively.

This paper is organized as follows. In Section 2, the frontal polymerization model is introduced. The linear stability analysis is performed in Section 3, while the interface problem and the perturbation analysis are provided in Section 4. Results obtained by numerical simulations are given in Section 5 and the last section concludes the work.

2 Frontal Polymerization Model

The propagation of polymerization reaction front with solid product submitted to a QP gravitational modulation can be modeled by the system of equations

$$\frac{\partial T}{\partial t} + (v \cdot \nabla)T = \kappa \Delta T + qW, \quad (1)$$

$$\frac{\partial \alpha}{\partial t} + (v \cdot \nabla)\alpha = W, \quad (2)$$

$$\frac{\partial v}{\partial t} + (v \cdot \nabla)v = -\frac{1}{\rho} \nabla p + \nu \Delta v + g(1 + \lambda_1 \sin(\mu_1 t) + \lambda_2 \sin(\mu_2 t))\beta(T - T_0)\gamma, \quad (3)$$

$$\operatorname{div}(v) = 0, \tag{4}$$

with the following boundary conditions

$$z \rightarrow +\infty, \quad T = T_i, \quad \alpha = 0, \quad \text{and} \quad v = 0, \tag{5}$$

$$z \rightarrow -\infty, \quad T = T_b, \quad \alpha = 1, \quad \text{and} \quad v = 0, \tag{6}$$

where the gradient, divergence and Laplace operators are defined as

$$\nabla v = \left(\frac{\partial v}{\partial x}, \frac{\partial v}{\partial y}, \frac{\partial v}{\partial z} \right), \quad \operatorname{div} \vec{v} = \frac{\partial v_1}{\partial x} + \frac{\partial v_2}{\partial y} + \frac{\partial v_3}{\partial z}, \quad \Delta v = \frac{\partial^2 v}{\partial x^2} + \frac{\partial^2 v}{\partial y^2} + \frac{\partial^2 v}{\partial z^2}.$$

Here (x, y, z) are the spatial coordinates, such that $-\infty < x, y, z < +\infty$, T is the temperature, α is the depth of conversion, v is the velocity of the medium, p is the pressure, κ is the coefficient of thermal diffusivity, q is the adiabatic heat release, ρ is the density, ν is the coefficient of kinematic viscosity, γ is the unit vector in the z -direction (upward), β is the coefficient of thermal expansion, g is the gravitational acceleration, T_0 is a mean value of temperature, T_i is the initial temperature and $T_b = T_i + q$ is the temperature of the burned mixture. The reaction source term is given by

$$W = k(T)\phi(\alpha), \quad \phi(\alpha) = \begin{cases} 1, & \text{if } \alpha < 1, \\ 0, & \text{if } \alpha = 1, \end{cases}$$

in which the temperature dependence of the reaction rate is given by the Arrhenius Law $k(T) = k_0 \exp(-E/R_0T)$ [11], where k_0 is the pre-exponential factor, E is the activation energy assumed to be sufficiently large and R_0 is the universal gas constant. It is assumed that the liquid monomer and the solid polymer involved in the reaction are incompressible and the term of diffusivity in the concentration equation is neglected so that the diffusivity coefficient is very small comparing to the coefficient of thermal diffusivity.

We introduce the dimensionless spatial variables

$$\begin{aligned} x' &= \frac{xc_1}{\kappa}, & y' &= \frac{yc_1}{\kappa}, & z' &= \frac{zc_1}{\kappa}, \\ t' &= \frac{tc_1^2}{\kappa}, & p' &= \frac{p}{c_1^2\rho}, & c_1 &= \frac{c}{\sqrt{2}}, \\ v' &= \frac{v}{c_1}, & \theta &= \frac{T - T_b}{q}, & c^2 &= \frac{2k_0\kappa R_0 T_b^2}{qE} \exp\left(-\frac{E}{R_0 T_b}\right), \end{aligned}$$

where c denotes the stationary front velocity, which can be calculated asymptotically for large Zeldovich number [12]. For convenience, we drop the primes in variables, velocity and pressure, so that the system (1)–(6) takes the form

$$\frac{\partial \theta}{\partial t} + (v \cdot \nabla)\theta = \Delta \theta + Z \exp\left(\frac{\theta}{Z^{-1} + \delta\theta}\right) \phi(\alpha), \tag{7}$$

$$\frac{\partial \alpha}{\partial t} + (v \cdot \nabla)\alpha = Z \exp\left(\frac{\theta}{Z^{-1} + \delta\theta}\right) \phi(\alpha), \tag{8}$$

$$\frac{\partial v}{\partial t} + (v \cdot \nabla)v = -\nabla p + P\Delta v + PR(1 + \lambda_1 \sin(\sigma_1 t) + \lambda_2 \sin(\sigma_2 t))(\theta + \theta_0)\gamma, \tag{9}$$

$$\operatorname{div}(v) = 0, \quad (10)$$

with the boundary conditions

$$z \rightarrow +\infty, \quad \theta = -1, \quad \alpha = 0, \quad \text{and} \quad v = 0, \quad (11)$$

$$z \rightarrow -\infty, \quad \theta = 0, \quad \alpha = 1, \quad \text{and} \quad v = 0. \quad (12)$$

Here $P = \frac{\nu}{\kappa}$ is the Prandtl number, $R = g\beta q\kappa^2/(\nu c^3)$ is the Rayleigh number, $Z = qE/R_0T_b^2$ is the Zeldovich number, $\delta = R_0T_b/E$, $\theta_0 = (T_b - T_0)/q$, $\sigma_1 = 2\kappa\mu_1/c^2$ and $\sigma_2 = 2\kappa\mu_2/c^2$.

3 Linear Stability Analysis

To perform the linear stability analysis, it is convenient to reduce the original problem to a singular perturbation one assuming that the reaction zone is infinitely narrow and the reaction term is neglected outside the zone [13]. To implement a formal asymptotic analysis, it is convenient to choose $\epsilon = Z^{-1}$ as a small parameter ensuring the reaction occurrence in a narrow zone.

We assume that the new independent variable is given by $z_1 = z - \zeta(x, y, t)$, where $\zeta(x, y, t)$ denotes the location of the reaction zone. Upon introducing the new functions $\theta_1, \alpha_1, v_1, p_1$ such that

$$\theta(x, y, z, t) = \theta_1(x, y, z_1, t), \quad \alpha(x, y, z, t) = \alpha_1(x, y, z_1, t),$$

$$v(x, y, z, t) = v_1(x, y, z_1, t), \quad p(x, y, z, t) = p_1(x, y, z_1, t),$$

the problem (7)-(12) can be rewritten in the following form (the index 1 in the new function is omitted)

$$\frac{\partial \theta}{\partial t} - \frac{\partial \theta}{\partial z_1} \frac{\partial \zeta}{\partial t} + (v \cdot \tilde{\nabla})\theta = \tilde{\Delta}\theta + Z \exp\left(\frac{\theta}{Z^{-1} + \delta\theta}\right)\phi(\alpha), \quad (13)$$

$$\frac{\partial \alpha}{\partial t} - \frac{\partial \alpha}{\partial z_1} \frac{\partial \zeta}{\partial t} + (v \cdot \tilde{\nabla})\alpha = Z \exp\left(\frac{\theta}{Z^{-1} + \delta\theta}\right)\phi(\alpha), \quad (14)$$

$$\frac{\partial v}{\partial t} - \frac{\partial v}{\partial z_1} \frac{\partial \zeta}{\partial t} + (v \cdot \tilde{\nabla})v = -\tilde{\nabla}p + P\tilde{\Delta}v + Q(1 + \lambda_1 \sin(\sigma_1 t) + \lambda_2 \sin(\sigma_2 t))(\theta + \theta_0)\gamma, \quad (15)$$

$$\frac{\partial v_x}{\partial x} - \frac{\partial v_x}{\partial z_1} \frac{\partial \zeta}{\partial x} + \frac{\partial v_y}{\partial y} - \frac{\partial v_y}{\partial z_1} \frac{\partial \zeta}{\partial y} + \frac{\partial v_z}{\partial z_1} = 0, \quad (16)$$

where

$$\tilde{\Delta} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z_1^2} - 2\frac{\partial^2}{\partial x \partial z_1} \frac{\partial \zeta}{\partial x} - 2\frac{\partial^2}{\partial y \partial z_1} \frac{\partial \zeta}{\partial y} +$$

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

$$\tilde{\nabla} = \left(\frac{\partial}{\partial x} - \frac{\partial}{\partial z_1} \frac{\partial \zeta}{\partial x}, \frac{\partial}{\partial y} - \frac{\partial}{\partial z_1} \frac{\partial \zeta}{\partial y}, \frac{\partial}{\partial z_1} \right), \quad Q = PR.$$

Using the matched asymptotic expansions, the outer solution of the problem (13)–(16) is sought in the form

$$\theta = \theta_0 + \epsilon\theta_1 + \dots, \quad \alpha = \alpha_0 + \epsilon\alpha_1 + \dots, \quad v = v_0 + \epsilon v_1 + \dots, \quad p = p_0 + \epsilon p_1 + \dots .$$

Moreover, to obtain the jump conditions toward the reaction zone, the inner problem is considered assuming the stretched coordinate as $\eta = z_1\epsilon^{-1}$. Then, the inner solution can be sought in the form

$$\theta = \epsilon\tilde{\theta}_1 + \dots, \quad \alpha = \tilde{\alpha}_0 + \epsilon\tilde{\alpha}_1 + \dots, \tag{17}$$

$$v = \tilde{v}_0 + \epsilon\tilde{v}_1 + \dots, \quad p = \tilde{p}_0 + \epsilon\tilde{p}_1 + \dots, \quad \zeta = \zeta_0 + \epsilon\zeta_1 + \dots . \tag{18}$$

Substituting these expansions into (13)–(16), we obtain to the leading-order the following inner problem

$$\left(1 + \left(\frac{\partial\zeta_0}{\partial x}\right)^2 + \left(\frac{\partial\zeta_0}{\partial y}\right)^2\right) \frac{\partial^2\tilde{\theta}_1}{\partial\eta^2} + \exp(\tilde{\theta}_1) \phi(\tilde{\alpha}_0) = 0, \tag{19}$$

$$-\frac{\partial\tilde{\alpha}_0}{\partial\eta} \frac{\partial\zeta_0}{\partial t} - \frac{\partial\tilde{\alpha}_0}{\partial\eta} \left(\tilde{v}_{0x} \frac{\partial\zeta_0}{\partial x} + \tilde{v}_{0y} \frac{\partial\zeta_0}{\partial y} - \tilde{v}_{0z}\right) = \exp(\tilde{\theta}_1) \phi(\tilde{\alpha}_0), \tag{20}$$

$$\left(1 + \left(\frac{\partial\zeta_0}{\partial x}\right)^2 + \left(\frac{\partial\zeta_0}{\partial y}\right)^2\right) \frac{\partial^2\tilde{v}_0}{\partial\eta^2} = 0, \tag{21}$$

$$-\frac{\partial\tilde{v}_{0x}}{\partial\eta} \frac{\partial\zeta_0}{\partial x} - \frac{\partial\tilde{v}_{0y}}{\partial\eta} \frac{\partial\zeta_0}{\partial y} + \frac{\partial\tilde{v}_{0z}}{\partial\eta} = 0. \tag{22}$$

The matching conditions as $\eta \rightarrow +\infty$ are given by

$$\tilde{v}_0 \sim v_0|_{z_1=+0},$$

$$\tilde{\theta}_1 \sim \theta_1|_{z_1=+0} + \left(\frac{\partial\theta_0}{\partial z_1}\Big|_{z_1=+0}\right)\eta, \quad \tilde{\alpha}_0 \rightarrow 0,$$

and as $\eta \rightarrow -\infty$, they read

$$\tilde{\theta}_1 \sim \theta_1|_{z_1=-0} \quad \tilde{\alpha}_0 \rightarrow 1 \quad \tilde{v}_0 \sim v_0|_{z_1=-0} .$$

From (21), we obtain

$$\frac{\partial^2\tilde{v}_0}{\partial\eta^2} = 0.$$

One concludes that $\tilde{v}_0(\eta)$ is a linear function of η and identically constant because the velocity is bounded. Thus, the first term in the expression of the velocity is continuous at the front.

Since the reaction is of order zero, one obtains $\phi(\tilde{\alpha}_0) \equiv 1$. Multiplying (19) by $\frac{\partial\tilde{\theta}_1}{\partial\eta}$ and integrating, we get

$$\left(\frac{\partial\tilde{\theta}_1}{\partial\eta}\right)^2\Big|_{+\infty} - \left(\frac{\partial\tilde{\theta}_1}{\partial\eta}\right)^2\Big|_{-\infty} = 2A^{-1}exp(\theta_1) \tag{23}$$

Subtracting (19) from (20) and integrating, we obtain

$$\frac{\partial \tilde{\theta}_1}{\partial \eta} \Big|_{+\infty} - \frac{\partial \tilde{\theta}_1}{\partial \eta} \Big|_{-\infty} = -A^{-1} \left(\frac{\partial \zeta_0}{\partial t} + s \right), \quad (24)$$

where

$$s = \tilde{v}_{0x} \frac{\partial \zeta_0}{\partial x} + \tilde{v}_{0y} \frac{\partial \zeta_0}{\partial y} - \tilde{v}_{0z}.$$

From the last equations (23)-(24), the temperature jump conditions across the reaction front can be calculated. Indeed, using the matching conditions above and truncating the expansion as

$$\theta \approx \theta_0, \quad \theta_1|_{z_1=-0} \approx Z\theta|_{z_1=+0}, \quad \zeta \approx \zeta_0, \quad v \approx v_0,$$

the jump conditions read

$$\begin{aligned} \left(\frac{\partial \theta}{\partial z_1} \right)^2 \Big|_{+0} - \left(\frac{\partial \theta}{\partial z_1} \right)^2 \Big|_{-0} &= 2Z \left(1 + \left(\frac{\partial \zeta}{\partial x} \right)^2 + \left(\frac{\partial \zeta}{\partial y} \right)^2 \right)^{-1} \exp(Z\theta|_0), \\ \frac{\partial \theta}{\partial z_1} \Big|_{z_1=+0} - \frac{\partial \theta}{\partial z_1} \Big|_{z_1=-0} &= - \left(1 + \left(\frac{\partial \zeta}{\partial x} \right)^2 + \left(\frac{\partial \zeta}{\partial y} \right)^2 \right)^{-1}. \end{aligned}$$

4 The Interface Problem and Perturbation

Next, we consider the case of the solid product where the velocity is zero behind the reaction zone, $v \equiv 0$ for $z < \zeta$. In this case, we obtain the interface problem:

In the liquid monomer ($z > \zeta$), we have the following system of equations

$$\frac{\partial \theta}{\partial t} + (v \cdot \nabla) \theta = \Delta \theta, \quad (25)$$

$$\alpha = 0, \quad (26)$$

$$\frac{\partial v}{\partial t} + (v \cdot \nabla) v = -\nabla p + P \Delta v + Q(1 + \lambda_1 \sin(\sigma_1 t) + \lambda_2 \sin(\sigma_2 t))(\theta + \theta_0) \gamma, \quad (27)$$

$$\operatorname{div}(v) = 0. \quad (28)$$

In the solid polymer ($z < \zeta$), the system of equations is given by

$$\frac{\partial \theta}{\partial t} + (v \cdot \nabla) \theta = \Delta \theta, \quad (29)$$

$$\alpha = 1, \quad (30)$$

$$v = 0. \quad (31)$$

While at the interface ($z = \zeta$), the system of equations reads

$$\theta|_{\zeta-0} = \theta|_{\zeta+0}, \quad (32)$$

$$\frac{\partial \theta}{\partial z} \Big|_{\zeta=-0} - \frac{\partial \theta}{\partial z} \Big|_{\zeta=+0} = \left(1 + \left(\frac{\partial \zeta}{\partial x} \right)^2 + \left(\frac{\partial \zeta}{\partial y} \right)^2 \right)^{-1} \left(\frac{\partial \zeta}{\partial t} \right), \quad (33)$$

$$\left(\frac{\partial\theta}{\partial z}\right)^2\Big|_{\zeta-0} - \left(\frac{\partial\theta}{\partial z}\right)^2\Big|_{\zeta+0} = -2Z \left(1 + \left(\frac{\partial\zeta}{\partial x}\right)^2 + \left(\frac{\partial\zeta}{\partial y}\right)^2\right)^{-1} \exp(Z\theta|_{\zeta}), \quad (34)$$

$$v_x = v_y = v_z = 0, \quad (35)$$

with the conditions at infinity

$$z = -\infty : \theta = 0, \quad v = 0; \quad z = +\infty : \theta = -1, \quad v = 0. \quad (36)$$

This problem has a travelling wave solution in the form

$$\begin{aligned} (\theta(x, y, z, t), \alpha(x, y, z, t), v) &= (\theta_s(z - ut), \alpha_s(z - ut), 0) \\ (\theta_s(z - ut), \alpha_s(z - ut)) &= \begin{cases} (0, 1), & z_2 < 0, \\ (\exp(-uz_2) - 1, 0), & z_2 > 0, \end{cases} \end{aligned} \quad (37)$$

and

$$z_2 = z - ut,$$

where u is the speed of the stationary reaction front. This solution, referred to as a basic solution, is a stationary solution of (26), (28), (30)-(36) and

$$\frac{\partial\theta}{\partial t} + (v \cdot \nabla)\theta = \Delta\theta + u \frac{\partial\theta}{\partial z_2}, \quad (38)$$

$$\frac{\partial v}{\partial t} + (v \cdot \nabla)v = -\nabla p + P\Delta v + u \frac{\partial v}{\partial z_2} + Q(1 + \lambda_1 \sin(\sigma_1 t) + \lambda_2 \sin(\sigma_2 t))(\theta + \theta_0)\gamma, \quad (39)$$

for the liquid monomer, and

$$\frac{\partial\theta}{\partial t} = \Delta\theta + u \frac{\partial\theta}{\partial z_2}, \quad (40)$$

for the solid polymer.

To study the reaction front stability, we seek the solution of the problem in the form of a perturbed stationary solution as follows

$$\theta = \theta_s + \tilde{\theta}, \quad p = p_s + \tilde{p}, \quad v = v_s + \tilde{v}, \quad (41)$$

where $\tilde{\theta}$, \tilde{p} and \tilde{v} are, respectively, small perturbations of temperature, pressure and velocity.

Substituting (41) into (28), (38)–(40), we obtain to the first-order

for $z_2 > \xi$:

$$\frac{\partial\tilde{\theta}}{\partial t} = \Delta\tilde{\theta} + u \frac{\partial\tilde{\theta}}{\partial z_2} - \tilde{v}_z \theta'_s,$$

$$\frac{\partial\tilde{v}}{\partial t} = -\nabla\tilde{p} + P\Delta\tilde{v} + u \frac{\partial\tilde{v}}{\partial z_2} + Q(1 + \lambda_1 \sin(\sigma_1 t) + \lambda_2 \sin(\sigma_2 t))\tilde{\theta}\gamma,$$

$$\operatorname{div}(\tilde{v}) = 0,$$

for $z_2 < \xi$:

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

We note

$$(\tilde{\theta}, \tilde{v}_z) = \begin{cases} (\hat{\theta}_1, \hat{v}_{z_1}), & \text{for } z_2 > \xi, \\ (\hat{\theta}_2, \hat{v}_{z_2}), & \text{for } z_2 < \xi, \end{cases}$$

and we consider the perturbation in the form

$$\hat{\theta}_i = \theta_i(z_2, t) \exp(j(k_1x + k_2y)), \quad (42)$$

$$\hat{v}_{z_i} = v_{z_i}(z_2, t) \exp(j(k_1x + k_2y)), \quad (43)$$

$$\xi = \epsilon_1(t) \exp(j(k_1x + k_2y)), \quad (44)$$

where k_i , ($i = 1, 2$) and ϵ_1 are, respectively, the wave numbers (in x and y directions) and the amplitude of the perturbation and $j^2 = -1$. Linearizing the jump conditions by taking into account that

$$\theta|_{\xi=\pm 0} = \theta_s(\pm 0) + \xi \theta'_s(\pm 0) + \tilde{\theta}(\pm 0), \quad \left. \frac{\partial \theta}{\partial z_2} \right|_{\xi=\pm 0} = \theta'_s(\pm 0) + \xi \theta''_s(\pm 0) + \left. \frac{\partial \tilde{\theta}}{\partial z_2} \right|_{\xi=\pm 0},$$

we obtain up to the higher-order

$$\hat{\theta}_2|_{z_2=0} - \hat{\theta}_1|_{z_2=0} = u\xi, \quad \left. \frac{\partial \hat{\theta}_2}{\partial z_2} \right|_{z_2=0} - \left. \frac{\partial \hat{\theta}_1}{\partial z_2} \right|_{z_2=0} = -u^2\xi - \frac{\partial \xi}{\partial t},$$

$$u^2\xi + \left. \frac{\partial \hat{\theta}_2}{\partial z_2} \right|_{z_2=0} = -\frac{Z}{u} \hat{\theta}_1|_{z_2=0},$$

$$\hat{v}_{2z}|_{z_2=0} = \hat{v}_{1z}|_{z_2=0} = 0, \quad \left. \frac{\partial \hat{v}_{2z}}{\partial z_2} \right|_{z_2=0} = \left. \frac{\partial \hat{v}_{1z}}{\partial z_2} \right|_{z_2=0} = 0.$$

By applying twice the operator curl to the Navier-Stokes equations, the pressure can be eliminated. Considering only the z component in velocity in (38)–(40), one obtains the following system of equations

$$\frac{\partial \tilde{\theta}}{\partial t} = \Delta \tilde{\theta} + u \frac{\partial \tilde{\theta}}{\partial z_2} - \tilde{v}_z \theta'_s, \quad (45)$$

$$\frac{\partial \Delta \tilde{v}_z}{\partial t} = P \Delta \Delta \tilde{v}_z + u \frac{\partial \tilde{v}_z}{\partial z_2} + Q \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} \right) (1 + \lambda_1 \sin(\sigma_1 t) + \lambda_2 \sin(\sigma_2 t)) \tilde{\theta} \gamma, \quad (46)$$

Substituting the perturbation forms (42)–(43) in the two last equations (45)–(46), we obtain

$$\begin{aligned} \frac{\partial}{\partial t} (v'' - k^2 v) - u(v''' - k^2 v') - P \left((v^{(4)} - k^2 v'') - k^2 (v'' - k^2 v) \right) = \\ -Qk^2 (1 + \lambda_1 \sin(\sigma_1 t) + \lambda_2 \sin(\sigma_2 t)) \theta, \end{aligned} \quad (47)$$

$$\frac{\partial \theta}{\partial t} - \theta'' - u\theta' + k^2 \theta = u \exp(-uz_2) v, \quad (48)$$

where $k = \sqrt{k_1^2 + k_2^2}$, and the boundary conditions

$$v'(0, t) = v(0, t) = 0, \quad (49)$$

$$\theta'(0, t) = -u\theta(0, t) = 0. \quad (50)$$

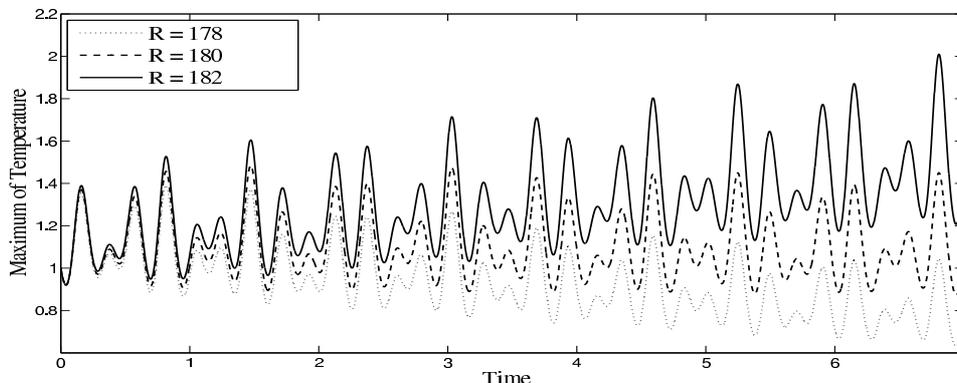


Figure 1: The evolution of the maximum of temperature versus time for $\lambda_1 = 1$, $\lambda_2 = 2$, $P = 10$, $\sigma_1 = 20$, $\frac{\sigma_2}{\sigma_1} = \sqrt{2}$ and different values of R .

5 Main Results

Introducing the vorticity $w = v'' - k^2v$, the system of equations (47)–(50) becomes

$$\frac{\partial w}{\partial t} - uw' - P(w'' - k^2w) = -Qk^2(1 + \lambda_1 \sin(\sigma_1 t) + \lambda_2 \sin(\sigma_2 t))\theta, \tag{51}$$

$$w = v'' - k^2v, \tag{52}$$

$$\frac{\partial \theta}{\partial t} - \theta'' - u\theta' + k^2\theta = u \exp(-uz)v \tag{53}$$

with the following conditions

$$z = 0 : \theta' = -u\theta, v' = v = 0, \tag{54}$$

$$z = L : \theta = v = w = 0. \tag{55}$$

In order to determine the stability threshold, we solve numerically the problem (51)–(55) using the finite-difference approximation with implicit scheme. The onset of stability is determined by evaluating the evolution of maximum of temperature versus time for different values of the Rayleigh number R . The jump between bounded and unbounded values of maximum of temperature leads precisely to the convective instability onset.

Figure 1 shows the maximum of temperature as function of time for different values of the Rayleigh number R . It can be observed that the evolution of the maximum of temperature becomes unbounded when the Rayleigh number exceeds a certain critical value.

The critical Rayleigh number as a function of the amplitude of vibration λ_2 is shown in Figure 2 for $P = 10$, $k = 1.5$, $\lambda_1 = 5$, $\sigma_1 = 5$ and for different frequencies ratio. It can be clearly seen that an increase of the frequencies ratio leads to an increase of the stability region, especially in certain interval of the amplitude λ_2 (approximately between 7 and 20). In contrast, a decrease of the frequencies ratio produces instability in the whole range of the amplitude λ_2 . This result indicates that for appropriate values of parameters, a decrease in the frequencies ratio has a destabilizing effect on the reaction front.

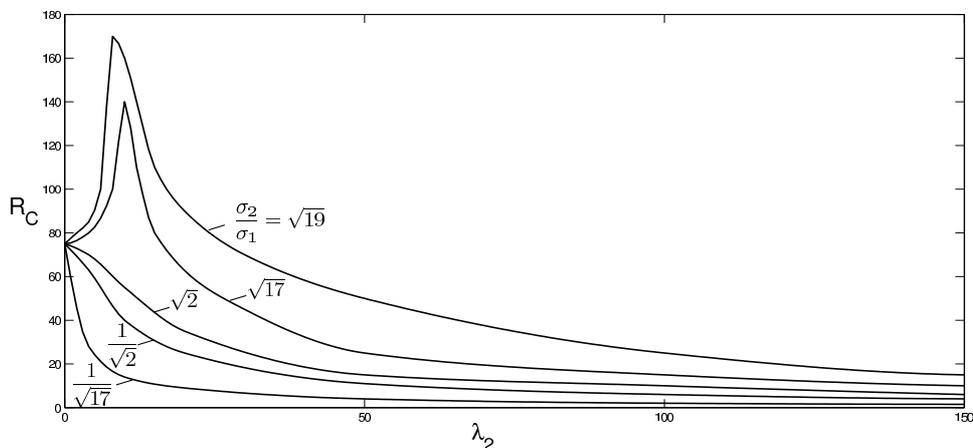


Figure 2: The critical Rayleigh number versus the amplitude of vibration λ_2 for $\lambda_1 = 5$, $P = 10$, $\sigma_1 = 5$, $k = 1.5$ and for different frequencies ratio.

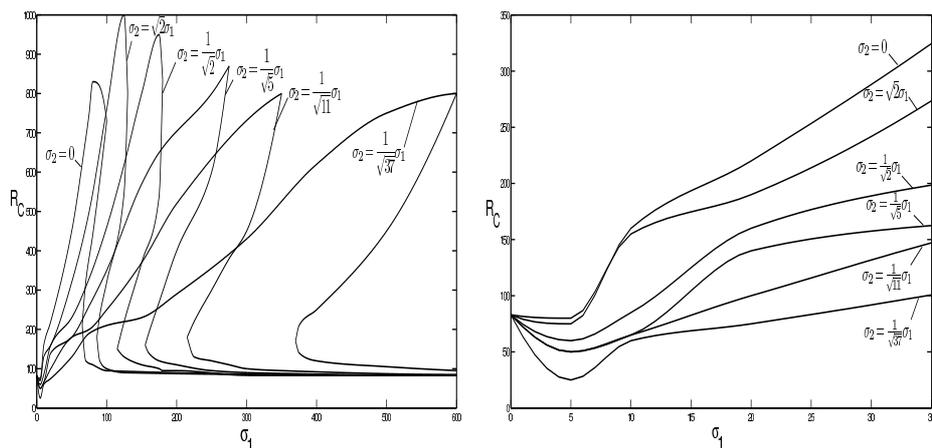


Figure 3: The critical Rayleigh number versus the frequency σ_1 for $\lambda_1 = \lambda_2 = 5$, $P = 10$, $k = 1.5$ and for different frequencies ratio (left); zoomed region (right).

The critical Rayleigh number versus the frequency σ_1 is shown in Figure 3 for the given values $P = 10$, $k = 1.5$, $\lambda_1 = \lambda_2 = 5$ and for different frequencies ratio. It can be observed from this figure that in the absence of modulation, the modulated critical value of the Rayleigh number $R_C \simeq 83$ is found [2]. In the presence of QP vibration, the convective instability boundaries are illustrated in the figure showing that as the frequencies ratio decreases, the stability domain becomes larger and shifts toward higher values of the frequency σ_1 . It can be concluded that the location of the stability domain can be controlled by tuning the frequencies ratio. It is worthy to notice that this phenomenon has not been depicted in the case where the reaction front propagates in porous media [5]. It is interesting to notice that for large values of the frequency σ_1 , the critical Rayleigh number tends to the unmodulated critical value R_C which means that

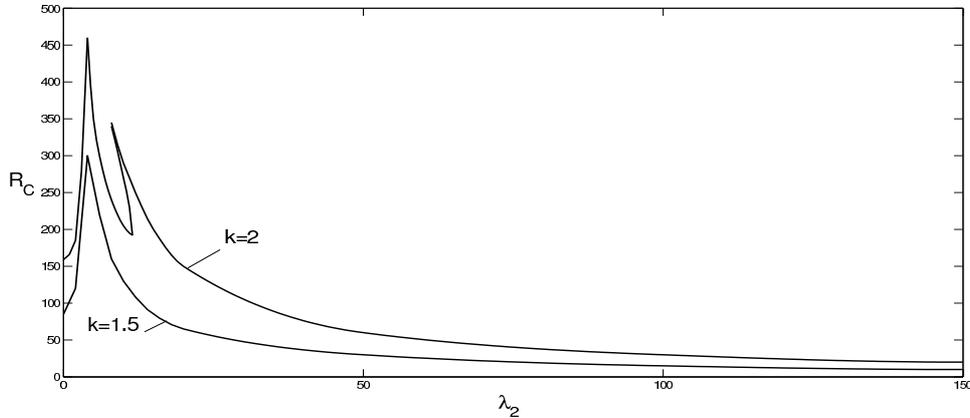


Figure 4: The critical Rayleigh number versus the amplitude of vibration λ_2 for different wave number and for $P = 10$, $\lambda_1 = 1$, $\sigma_1 = 20$, $\frac{\sigma_2}{\sigma_1} = \sqrt{2}$.

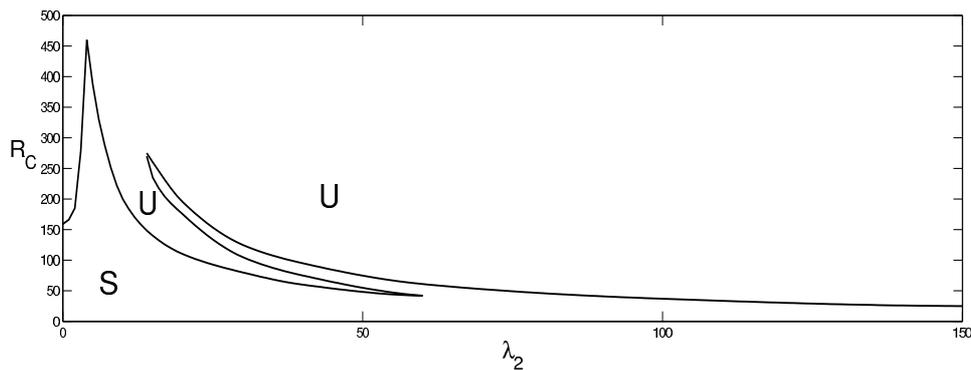


Figure 5: The critical Rayleigh number versus the amplitude of vibration λ_2 for $P = 10$, $\lambda_1 = 1$ and $\frac{\sigma_2}{\sigma_1} = \sqrt{3}$ (compare with the case $\frac{\sigma_2}{\sigma_1} = \sqrt{2}$ in Figure 4); *S*: stable, *U*: unstable.

the case of QP modulation with high frequency σ_1 is similar to the unmodulated case.

In Figure 4, we show the variation of R_c versus λ_2 for different values of the wave number. It can be observed that an increase of the wave number has a stabilizing effect and gives rise to a new domain of stability.

The influence of the frequency ratio on the convective instability boundary is shown in Figure 5 indicating that increasing the frequencies ratio increases significantly the new domain of stability.

6 Conclusion

In this work, we have studied the influence of the QP gravitational modulation on the convective instability of polymerization front with liquid reactant and solid product. The model we have considered includes the heat equation, the concentration equation and the Navier-Stokes equations under Boussinesq approximation. The Zeldovich Frank-Kamenetskii method has been applied assuming that the reaction occurs in a narrow zone.

A linear stability analysis was performed to determine the interface problem assuming that the solution is chosen as a perturbed stationary solution. To find the convective instability threshold, the reduced system of equations has been discretized using the finite difference method with implicit scheme. The obtained numerical results have shown that for fixed value of the amplitude λ_1 , an increase of the frequencies ratio stabilizes the reaction front, especially for moderate values of the amplitude of vibration λ_2 . Instead, a decrease of the frequencies ratio destabilizes the reaction front in the whole range of the amplitude λ_2 . More interestingly, it was observed that decreasing the frequencies ratio shifts the stability domain toward higher values of the frequency σ_1 . The influence of the wave number on the convective instability of the reaction front was also examined showing that, as in the periodic modulation case [2], an increase of the wave number has a stabilizing effect and gives rise to a new stability domain.

References

- [1] Goldfeder, P.M., Volpert, V.A., Ilyashenko, V.M., Khan, A.M., Pojman, J.A. and Solovyov, S.E. Mathematical modeling of free-radical polymerization fronts. *J. Phys. Chem. B* **101** (1997) 3474–3482.
- [2] Allali, K., Pojman, J. and Volpert, V. Influence of vibrations on convective instability of polymerization fronts. *J. Engrg. Math.* **41** (2001) 13–31.
- [3] Mikhlin, Yu.V., Avramov, K.V. and Rudnyeva, G.V. Analytical Methods for Analysis of Transitions to Chaotic Vibrations in Mechanical Systems. *Nonlinear Dynamics and Systems Theory* **9** (2009) 375–406.
- [4] Belhaq, M. and Houssni, M. Quasi-periodic oscillations, chaos and suppression of chaos in a nonlinear oscillator driven by parametric and external excitations. *Nonlinear Dynamics* **18** (1999) 1–24.
- [5] Allali, K., Belhaq, M. and El Karouni, K. Influence of quasi-periodic gravitational modulation on convective instability of reaction fronts in porous media. *Commun. Nonlinear Sci. Numer. Simul.* **17** (2012) 1588–1596.
- [6] Boulal, T., Aniss, S., Belhaq, M. and Rand, R.H. Effect of quasiperiodic gravitational modulation on the stability of a heated fluid layer. *Phys. Rev. E* **76** (2007) 56320.
- [7] Boulal, T., Aniss, S., Belhaq, M. and Azouani, A. Effect of quasi-periodic gravitational modulation on the convective instability in Hele-Shaw cell. *Int. J. Non Linear Mech.* **43** (2008) 852–857.
- [8] Boulal, T., Aniss, S. and Belhaq, M. Quasiperiodic gravitational modulation of convection in magnetic fluid, Thermal non-equilibrium. In: *Lecture notes of the 8th international meeting of thermodiffusion* (Wiegand S., Khler W. and Dhont J.K.G., eds). 9-13 June, 2008, Bonn, Germany; 2008, ISBN: 978-3-89336-523-4.
- [9] Rand, R.H., Guennoun, K. and Belhaq, M. 2:2:1 Resonance in the quasi-periodic Mathieu equation. *Nonlinear Dynamics* **31** (2003) 367–374.
- [10] Sah, S.M., Recktenwald, G., Rand, R.H. and Belhaq, M. Autoparametric quasiperiodic excitation. *Int. J. Non-linear Mech.* **43** (2008) 320–327.
- [11] Menzinger, M. and Wolfgang, R. The meaning and use of the Arrhenius activation energy. *Angewandte Chemie International Edition in English* **8** (1969) 438–444.
- [12] Novozhilov, B.V. The rate of propagation of the front of an exothermic reaction in a condensed phase. *J. Dokl. Phys. Chem.* **141** (1961) 836–838.
- [13] Zeldovich, Y.B. and Frank-Kamenetskii, D.A. A theory of thermal propagation of flame. *Acta Physicochim. USSR* **9** (1938) 341–350.