Pergamon

Int. J. Heat Mass Transfer. Vol. 40, No. 9, pp. 2235–2240, 1997

0017–9310/97 $17.00+0.00

PII: S0017–9310(96)00144–5

Mathematical modelling of stability of non-adiabatic laminar premixed flame

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(*Received* 1 *August* 1994)

Abstract—A flat laminar non-adiabatic flame in premixed gas mixture is considered. Stability of gas mixture burning with instantaneous and periodic pertubations is theoretically studied. Zero-dimensional linearized models (dynamic systems of the second and third order) are studied analytically, the non-linear zero-dimensional and initial one-dimensional systems are solved numerically. Parameter regions with non-unique and auto-oscillatory combustion regimes are determined. The influence of lateral heat removal, radiation, burning temperature, reaction kinetics, injection rate, etc. on the non-unique and auto-oscillatory regime, character and number of critical conditions is studied. The performance of forced oscillations and the resonance phenomena are found. © 1997 Elsevier Science Ltd. All rights reserved.

1. INTRODUCTION

In refs [1, 2] critical phenomena in a one-dimensional flame were theoretically studied without consideration of the complex kinetic mechanism of chemical reactions, reagents expenses, lateral heat removal [2] and flame radiation [3].

In this paper the single and complex chemical reactions of heat removal by convection and radiation are considered. The stability to instantaneous and periodical perturbations and resonance phenomena in the flame are studied by a numerical solution of the non-linear problems and in an approximate-analytical way on the linearized zero-dimensional models. The critical conditions of ignition and extinction are established.

2. STEADY-STATE AND RESONANCE PHENOMENA

2.1. *Governing equation*

The problem is mathematically formulated by a system of equations for diffusion of the heat and reagents with chemical conversions:

$$\tau > 0: \quad 0 < S < 1$$

$$\frac{\partial C_1}{\partial \tau} + Pe\frac{\partial C_1}{\partial S} = Le_1\frac{\partial^2 C_1}{\partial S^2} - \omega_1 - \omega_p$$

$$\frac{\partial C_2}{\partial \tau} + Pe\frac{\partial C_2}{\partial S} = Le_2\frac{\partial^2 C_2}{\partial S^2} + 2\alpha_1\omega_1 - \omega_2 - \omega_t$$

$$\frac{\partial \theta}{\partial \tau} + Pe\frac{\partial \theta}{\partial S} = \frac{\partial^2 \theta}{\partial S^2} + \Sigma q_i\omega_i - \xi(\theta^5 - \beta\theta\theta_\infty^4) - \frac{Bi\,\theta^2}{\delta^2\,\theta_c^m}(\theta - \theta_\infty), \tag{1}$$

where

$$\frac{1}{\delta^2} = \frac{(\psi_h - \psi_c)^2}{\rho_c^2\theta_c^2 r_0^2}, \quad d\psi = \rho dx, \quad i = 1, 2, p, t.$$

The initial conditions are taken in the form

$$\tau = 0: \quad 0 \leqslant S \leqslant 1. \quad C_i = C_{i_H}, \quad \theta = \theta_H. \tag{2}$$

The Dankwerts boundary conditions are adapted at the burner

$$\tau > 0: \quad S = 0 \quad Le_1\frac{\partial C_1}{\partial S} = Pe(C_{1_c} - 1)$$

$$Le_2\frac{\partial C_2}{\partial S} = PeC_{2_c}, \quad \theta = \theta_c \tag{3}$$

and the smoothness condition—on the hot boundary of the flame

$$S = 1, \quad \frac{\partial C_1}{\partial S} = \frac{\partial C_2}{\partial S} = \frac{\partial \theta}{\partial S} = 0. \tag{4}$$

Two examples are considered. In the first case it is assumed that the reaction kinematic in the flame methane–oxygen–nitrogen may be approximated by a single reaction $A \to B$, when

$$C_2 = 0, \quad \omega_2 = \omega_p = \omega_t = 0,$$

$$Le_1 = 1, \quad \alpha_1 = 0, \quad \varepsilon = \frac{E}{RT_c} \quad \omega_1 = \Lambda C\exp(-\varepsilon/\theta),$$

$$q_i = q_1, \quad \theta = \frac{T}{T_c}, \quad m = 0. \tag{5}$$

NOMENCLATURE

A	oscillation amplitude
Bi	Biot number
C	concentration
E	activation energy
Le	Levis number
Pe	Peclet number
q	dimensionless heat of reaction
r	reactor radius
R	universal gas constant
S	dimensionless co-ordinate
T	absolute temperature
W	reactions rates
x	co-ordinate.

Greek symbols

β	ratio of absorptivity to emissivity
δ	dimensionless radius of reactor
θ	dimensionless temperature
Λ	dimensionless frequency factor
ξ	dimensionless radiation coefficient
ρ	density
τ	dimensionless time
ω_1	action frequency
ω_{1_c}	mass fraction.

Subscripts

c	burner
h	hot boundary of the flame
H	initial conditions
∞	surroundings.

Example 2 concerns heat and mass transfer in a flat flame of a compressible liquid with multistage reactions: oxidation, branching (two stages) and chain termination. System (1)–(4) is solved under conditions

$$Le_1 = 1, \quad \xi = 0, \quad \omega_1 = \frac{\Lambda_1 C_1 C_2 C_3}{\theta} \exp(-1/\theta)$$

$$\omega_2 = \frac{\Lambda_2 C_2^2 C_3}{\theta^2},$$

$$\omega_j = \frac{\Lambda, C_1 C_2 C_3}{\theta^2} \exp(1/\varepsilon_j \theta)$$

$$j = p, t, \quad \theta = \frac{RT}{E}, \quad \varepsilon_j = \frac{E_j}{E_1}, \quad m = 2. \qquad (6)$$

It should be noted that the rate of oxidation reaction increases with temperature, while that of branching reactions decreases exponentially. The rate of chain termination reaction changes with the temperature in a much weaker manner.

In the particular case of the set of kinetic constants as in example 2, expression (6) describes either the four-stage or the two-stage reaction mechanism (by $\Lambda_p = \Lambda_t = 0$) in a hydrogen–oxygen–nitrogen rich flame [4].

The influence of injection rate, radiation factor, lateral heat removal (Bi/δ^2, Bi = Biot number, δ = reactor radius), and surrounding temperature, kinetic mechanism, etc. on the combustion regime is studied. Values of fixed parameters are listed in the Appendices. Values of variable parameters are given in captions.

At the first stage of designing numerical experiments using model (1)–(4) the spatial one-dimensional system of partial derivative equations (1) is brought into correspondence with the lumped model [3]:

$$\frac{dC_i}{d\tau} = n_{1_i}(C_{i_c} - C_i) - \Sigma\omega_i \equiv \mathscr{P}_i(C_i, \theta)$$

$$\frac{d\theta}{d\tau} = n_2(\theta_c - \theta) + \Sigma q_i w_i - \xi(\theta^5 - \beta\theta\theta_\infty^4)$$

$$- \frac{\beta i}{\delta^2} \frac{\theta^2}{\theta_c^m}(\theta - \theta_\infty) \equiv Q(C_i, \theta) \qquad (7)$$

where $n_{1_i} = Pe(4Le_i + Pe)/(2Le_i + Pe)$, $n_2 = 4 + Pe$. The coefficients n_{1_i}, n_2 depend on boundary conditions (3), (4) of system (1) and the method of averaging the spatial differential operations.

2.2. *The steady states*

The steady states are determined from the equations

$$\mathscr{P}_i(C_{i_S}, \theta_S) = Q(C_{i_S}, \theta_S) = 0. \qquad (8)$$

The equations system (8) is reduced to

$$F(\theta_S, \mathbf{p}, p^*) = 0, \qquad (8')$$

where $\mathbf{p}$ is a vector of process parameters, p^* is a bifurcation parameter, and index S will be omitted.

When Bi/δ^2 is bifurcation parameter then the bifurcation diagram is determined in the first example from the equation:

$$\frac{Bi}{\delta^2} = \frac{n_2(1-\theta) - \xi(\theta^5 - \beta\theta\theta_\infty^4) + (\Lambda q_1 n_1)/[\Lambda + \mathrm{n}\exp(\varepsilon/\theta)]}{\theta^2(\theta - \theta_\infty)}$$

and in the second example from

$$\frac{Bi}{\delta^2} = \frac{\theta_c^2}{\theta^2(\theta - \theta_\infty)} \left[-n_2(\theta - \theta_c) + \Lambda_1 q_1 \frac{C_1 C_2}{\theta} \exp(-1/\theta) \right.$$

$$+(\Lambda_p q_p+\Lambda_t q_t)\frac{C_1C_2}{\theta^2}\exp(1/\varepsilon\theta)+\Lambda_2 q_2\frac{C_2^2}{\theta^2}\Big]$$

where

$$C_1=\frac{f_1 n_{1_1}\theta^2-\tilde{\Lambda}_2 n_{1_1}}{2f_1f_2}\left(1\pm\sqrt{1+\frac{4n_{1_1}\tilde{\Lambda}_2 f_1 f_2}{(f_1 n_{1_2}\theta^2-\lambda_2 n_{1_1})^2}}\right)$$

$$C_2=\frac{(n_{1_2}\theta^2+(2\alpha_1\Lambda_p+\Lambda_t)C_1\exp(1/\varepsilon\theta)}{2\tilde{\Lambda}_2}\times\left(\sqrt{1+\frac{8n_{1_1}\theta^2\alpha_1(1-C_1)\tilde{\Lambda}_2}{[n_{1_2}\theta^2+2(\alpha_1\Lambda_p+\Lambda_t)}}-1\right)\times C_1\exp(1/\varepsilon\theta)]^2$$

$$f_1=\frac{\Lambda_1}{\theta}\exp(-1/\theta)+\frac{\Lambda_p}{\theta^2}\exp(1/\varepsilon\theta)$$

$$f_2=2\alpha_1\Lambda_1\theta\exp(-1/\theta)-\Lambda_t\exp(1/\varepsilon\theta)\quad\tilde{\Lambda}_2=\Lambda_2\frac{1}{\tilde{\omega}_1 c}.$$

It can be seen that under different values of heat exchange in the flame there are from one to three steady states in the one-stage (Fig. 1(a)) and two-stage (line 1, Fig. 1(b)) reactions. In the four-stage reaction their number increases from, three to five (line 2, Fig. 1(b)) lines 1–4, Fig. 1(c)). For analysing values of the frequency factors one of five steady states falls to physically unreal values of the reagent concentration.

There exist critical conditions for ignition (I) and extinction (E), which depend on the radiation coefficient (Fig. 1(a)), injection rate, burning temperature, etc. At smaller values of radiation coefficient (Fig. 1(a)) the difference between critical values of heat removal coefficient (reactor radius) for ignition and extinction is rather greater and regions of multiple regimes increase. At particular value of Bi/δ^2 lateral heat removal and radiation do not affect the steady-state temperature (Fig. 1(a)).

It is evident from Fig. 1(c) that there are two critical values of heat removal coefficient (radius of reactor) for ignition and one for extinction at small values of burner temperature and rate injection ($Pe < 1$, line 2). Increase of the two last parameters (at Peclet number $Pe \geqslant 1$) leads to two critical conditions for extinction and one for ignition (lines 1, 3, 4), and next the flame propagation becomes crisis free (line 5).

Packing of diameter $d_{cr} = 4.8$ mm for methane–oxygen–nitrogen flame is received from the extinction-condition (Fig. 1(a), line 2 by $Bi/\delta^2 = 1$) and correlates with the literature data—$d_{cr} = 4.1$ mm [5].

From the bifurcation diagram equation (8′), together with extremum condition parametrical equations, is determined for the boundary of the multiple combustion regimes.

It is established from the multiplicity boundary, on the 'radiation coefficient-lateral heat removal parameter' plane, that increase of surrounding temperature leads to increase of critical values $(Bi/\delta^2)_I$ and $(Bi/\delta^2)_E$. The critical values of radiation coefficient and lateral heat removal parameter of ignition and extinction are increased with growth of the activation energy and decrease of the rate injection.

Figure 2 shows the boundaries of multiple steady-state regions on the 'reaction heat–burner temperature' plane. The number of steady states is given by numerals. It can be seen that with the increase of lateral heat removal the regions of multiple regimes increase and displace to higher burner temperatures if reactor walls are cold and to lower burner temperatures if they are hot (Fig. 2(a,b)). There are 'zero'

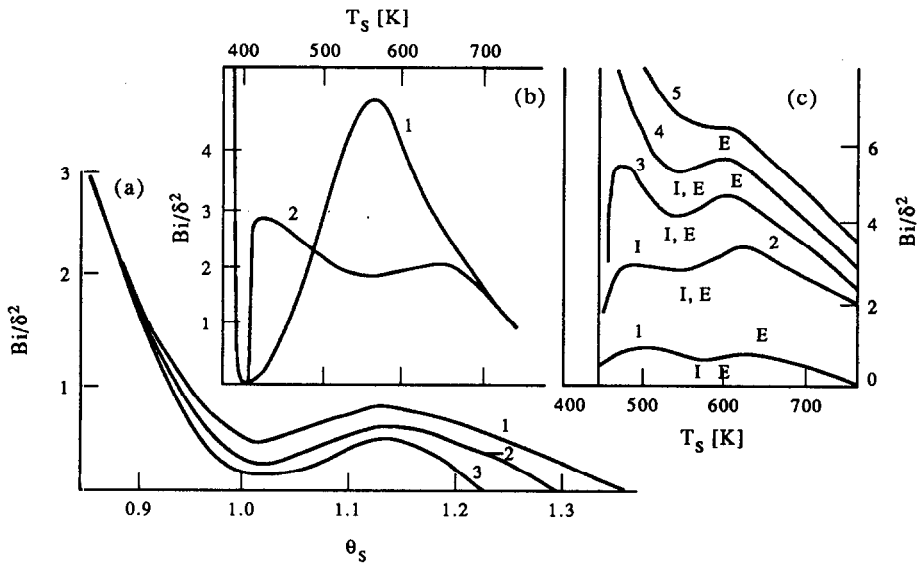

Fig. 1. Steady states: (a) $Pe = 0.3$—$\xi = 0$ (1), 0.08 (2), 0.15 (3); (b) $q_1 = 0.25$, $Pe = 0.4$, $T_c = 380$K—two-stage mechanism (1), four-stage mechanism (2); (c) $q_1 = 0.25$—$Pe = 0.4$, $T_c = 340$ K (1), $Pe = 1$, $T_c = 340$ K (2), 350 K (3), 400 K (4), 420 K (5).

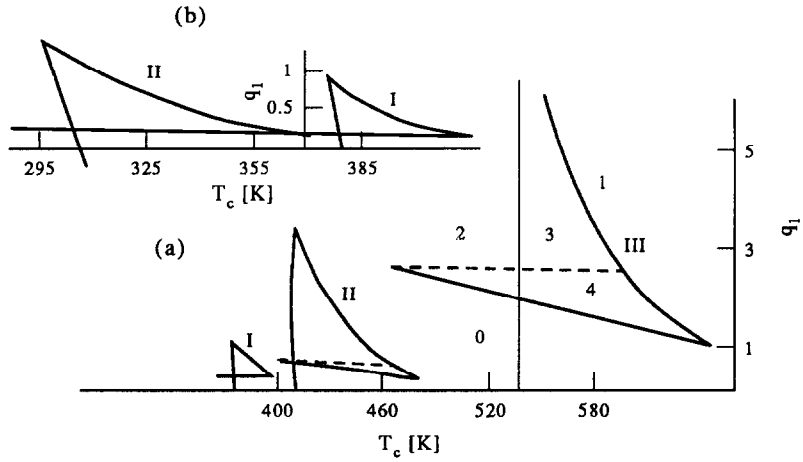

Fig. 2. Multiplicity boundaries; $Pe = 0.4Bi/\delta^2 = 0$(I), 1(II), 2(III); $T_c = 300$ K (a), $T_c = 600$ K (b).

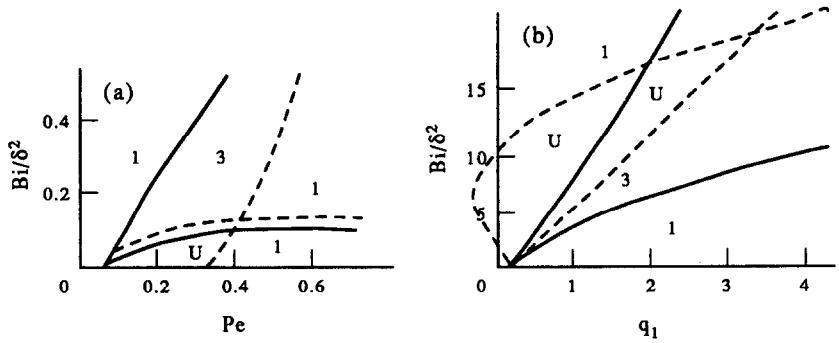

Fig. 3. Stability of steady states: (a) example 1; (b) example 2; $Pe = 0.4$, $T_c = 436$ K.

regions, where steady-state flame propagation is distinguished.

2.3. *Linear stability analysis*

The stability of steady states for the multiparametric systems is determine by the first Lyapunov's method on separate planes of two parameters while the values of other parameters are taken in the form

$$\dot{\xi} = M\xi$$

where ξ- is vector of small deviations of the function from the steady state values, and M is the linear transformation matrix of equation (7).

The boundary of multiple steady state coincides with the boundary

$$\tilde{\theta} = \det M = 0.$$

The neutral stability boundary can be determined for the first example from equation

$$\sigma = SpM = 0$$

and for the second example

$$\Delta = \sum_{i=1}^{i=n-1} \sum_{j=n-1}^{j=n} a_{ii}a_{jj} - a_{ij}a_{ji}$$

where n is the order of the dynamic system.

Figure 3 shows the patterns of the division of 'lateral heat removal–rate injection' plane (a) and 'lateral heat removal–heat of oxidation reaction' plane (b) into regions of unique stable (1), auto-oscillatory (U) and multiple (3) steady-state regimes. It can be seen that the auto-oscillations are possible in the unique cases and multiple steady-state regimes (Fig. 3(b)) under Peclet number $Pe < 1$ (a, b). This result was obtained for the adiabatic flame, H_2–O_2–N_2 [3]. It is shown that by four-stage reactions the oscillation is possible only in the flame with lateral heat removal.

The linear theory also makes it possible to study the influence of periodical actions on combustion and resonance phenomena in the flame in an approximate analytical way. So, forced oscillations of the reagent concentration in the flame with pulsating burner temperature:

$$T_c = T_{c_1}[1 + A_1 \cos(\omega_1 \tau)] \tag{9}$$

are described by the equation

$$\ddot{\xi}_1 + \sigma\dot{\xi}_1 + \Delta\xi_1 = A_1 \cdot f \cdot \cos(\omega_1 \tau) \tag{10}$$

where $\xi = C - C_S$ is a small deviation of the concentration from steady state value, C_S.

Solving this equation with initial conditions, one can easily find the frequency of the undamped natural

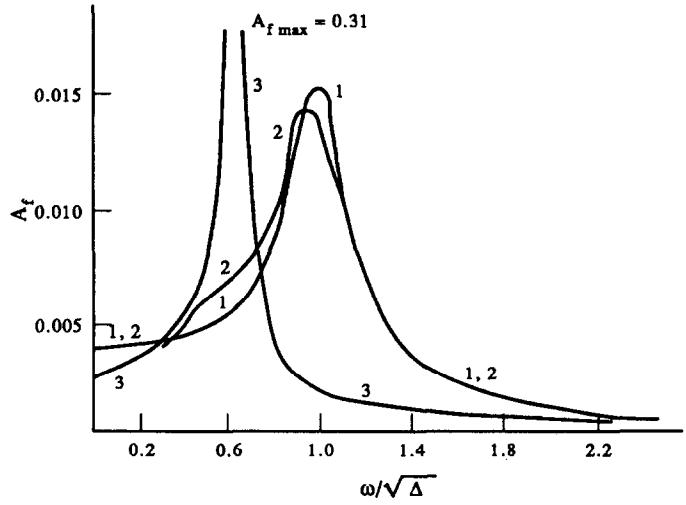

Fig. 4. Amplitude–frequency characteristics at $A = 0.01$. Example 2: $Bi/\delta^2 = 0$, $\xi = 0.08$, $Pe = 0.3$.

oscillations, the damping coefficient and quality factor, frequency of the natural damped oscillations,

$$\omega_0 = \sqrt{\Delta}, \quad \omega_\alpha = \omega_0\sqrt{1-\gamma^2}, \qquad \gamma = \frac{\sigma}{2\sqrt{\Delta}}, \quad Q = \frac{\sqrt{1-\gamma^2}}{2\gamma} \tag{11}$$

the amplification factor, amplitude and phase angle of the forced oscillations

$$\beta = 1\Big/\left\{\left[1-\left(\frac{\omega_1}{\sqrt{\Delta}}\right)^2\right]^2 + 4\gamma^2\left(\frac{\omega_1}{\sqrt{\Delta}}\right)^2\right\}$$

$$A_1 = \frac{A_1 f\beta}{\Delta},$$

$$\varphi = \operatorname{arctg}\left\{\left(2\gamma\frac{\omega_1}{\sqrt{\Delta}}\right)\Big/\left[\left(1-\left(\frac{\omega_1}{\sqrt{\Delta}}\right)^2\right]\right\}. \tag{12}$$

It is established from the solution that the system is very sensitive to the damping coefficient in the resonance vicinity. In systems with small damping, the amplification has maximum value at a frequency close to the resonance frequency. At action frequencies very different from the natural frequency the damping effect can be neglected.

2.4. *Results of numerical solutions of non-linear problems*

The system (7) is solved by the Runge–Kutta–Feldberg method. Equations (1)–(4) under conditions (5) or (6) are solved by the explicit finite-difference scheme: the time step automatically decreases with the increase in reaction rates. Implicit finite-difference calculations were made at a fixed time step with iterations both in temperature and concentration (example 1). The two solutions for auto-oscillatory regimes in the one-dimensional system good agree in temperature values, but are slightly shifted in phase. In both cases oscillations occur in the vicinity of the solution of problem (8). The numerical solutions agree with those of the zero-dimensional model in the regime character, oscillation frequency and steady-state values of temperature and concentration. Thus, for example, frequency of damped oscillations determined from the system (1)–(6) is $w_\alpha = 6.28$ and agrees with the value calculated by formula (11), $w_\alpha = 6.76$ and from the system (7), $w_\alpha = 6.36$. Temperature and concentration profiles for the high-temperature regime in a H_2–O_2–N_2–flame is good agreement with experimental data [3, 7].

The resonance phenomena in the non-linear system of a high-quality factor were studies numerically for the adiabatic flame H_2–O_2–N_2 and for combustion without flow reactor [3]. The resonance phenomena in the combustion systems of a low quality factor are described approximately analytically in the linear approximation [8].

Figure 4 illustrates the result of action (9) on the regime of damped oscillations in a radiating flame with lateral heat removal. For the numerical solutions $A_f = (C_{max} - C_{min})/2$. It can be seen that solution (12) of linear problem (10) predicts the resonance at the natural frequency that agrees at $\omega_1 = 0.3$ and $\omega_1 = 1.1$ with solution of non-linear zero-dimensional problem (7) (line 2). At $\omega_1(0.3, 1.1)$ these solutions are close (lines 1 and 2), but in non-linear problems a non-linear effect of resonance shifting can be observed toward frequencies lower than the natural one, and at the $\omega_1 \sim 0.5$ the resonance is in formation (line 2). Numerical solution of problems (1)–(5) for output concentration of reactor (line 3) confirms this resonance. Under action (9) on the non-unique regimes the resonance is observed at frequencies closer to zero.

3. CONCLUSION

Stability for immediate and oscillating disturbances and resonance phenomena in non-adiabatic flame have been theoretically investigated. Parametric

regions of non-unique and self-oscillatory combustion processes and critical conditions are determined. Formulae are derived connecting the amplitude of contrained oscillations and the phase angle with the combustion parameters to contrained oscillations. Numerical solutions of non-linear problems are in good agreement with approximately analytical ones.

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APPENDIX

The fixed parameter values for the first example are:

$$\Lambda = 5.01 \times 10^9; \quad q = 2.788; \quad \theta_\infty = 0.6; \quad \beta = 1, \quad \varepsilon = 25.$$

The fixed parameter values for the second example are:

$$\Lambda_1 = 2.85 \times 10^8; \quad \Lambda_2 = 3.45 \times 10^3; \quad \Lambda_p = 79.8;$$

$$\Lambda_t = 0.0097; \quad q_1 = 1.29; \quad q_2 = 1.29;$$

$$q_p = 8.97 \times 10^{-2}; \quad \varepsilon_p = \varepsilon_t = 11;$$

$$\omega_{1_c} = 0.063; \quad Le_1 = 1; \quad Le_2 = 5.654.$$