Investigation of combustion wave stability in the Zeldovich-Liñán model

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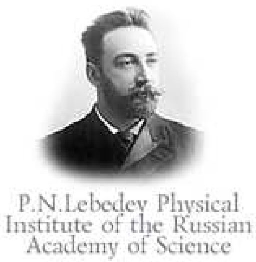

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Zeldovich-Liñán model

- Introduced by Y.B. Zeldovich in 1948, analyzed by A. Liñán in 1971 using the activation energy asymptotics (AEA).

  — Y.B. Zeldovich, Zh. Phys. Khim. 22, 27 (1948)

  — A. Liñán, Insituto Nacional de Technica Aerospacial "Esteban Terradas" (Madrid), USAFOSR Contract No. E00AR68-0031, Technical Report No. 1 (1971).

  Chain-branching: $A + B \to 2B \quad \mapsto Q = 0,\ E_a > 0$

  Chain-breaking: $B + B + M \to 2P + M \quad \mapsto Q > 0,\ E_a = 0$

- ZL model and H_2 - O_2 (air) combustion

  — Y.B. Zeldovich, Kinet. Katal. 2, 305-318 (1961)

  $$A + B \to 3B, \qquad \mapsto \qquad 3H_2 + O_2 = 2H + 2H_2O,$$
  $$B + B + M \to 2P + M \qquad \mapsto \qquad 2H + M = H_2 + M$$

  –A is the deficient component concentration, for example, O_2

  –B is the H atoms concentration which are the only radicals

  The rates of global reactions are governed by elementary steps:

  $H + O_2 \to OH + H$

  $H + H + M \to H_2 + M$ and $H + O_2 + M \to HO_2 + M$.

Model equations

— B.H. Chao, C.K. Law, Int. J. Heat Mass Transfer 37, 673 (1994).

- Governing PDEs

$$\rho c_p \frac{\partial T}{\partial t} = \lambda \Delta T + q_F W_A A_R \left(\frac{\rho Y_B}{W_B}\right)^2 \frac{\rho Y_M}{W_M},$$

$$\rho \frac{\partial Y_A}{\partial t} = \rho D_A \Delta Y_A - A_B \frac{\rho Y_A}{W_A} \frac{\rho Y_B}{W_B} e^{-E/RT},$$

$$\rho \frac{\partial Y_B}{\partial t} = \rho D_B \Delta Y_B + W_B \left(A_B \frac{\rho Y_A}{W_A} \frac{\rho Y_B}{W_B} e^{-E/RT} - 2 A_R \left(\frac{\rho Y_B}{W_B}\right)^2 \frac{\rho Y_M}{W_M} \right),$$

- Introducing the nondimensional variables

$$t' = \frac{\rho A_B}{\beta M^*} t, \quad x' = \sqrt{\frac{\rho^2 A_B c_p}{\lambda M^* \beta}} x, \quad u = \frac{T}{T^* \beta}, \quad v = \frac{Y_A}{Y_A^\infty}, \quad w = \frac{Y_B W_A}{Y_A^\infty W_B},$$

and dimensionless parameters

$$M^* = \frac{W_A}{Y_A^\infty}, \quad T^* = \frac{q_F Y_A^\infty}{2 c_p}, \quad \beta = \frac{E}{R T^*}, \quad L_i = \frac{\lambda}{D_i \rho c_p}, \quad r = \frac{2 \rho A_R Y_M}{A_B W_M}$$

Nondimensional equations

- Governing equations

$$
\begin{aligned}
u_t &= \Delta u + r w^2, \\
v_t &= {L_A}^{-1} \Delta v - \beta v w e^{\beta - 1/u}, \\
w_t &= {L_B}^{-1} \Delta w + \beta v w e^{\beta - 1/u} - r \beta w^2,
\end{aligned}
$$

where $\Delta = \dfrac{\partial^2}{\partial x^2} + \dfrac{\partial^2}{\partial y^2}$

- Boundary conditions

$$
\begin{array}{lllll}
u = u_a, & v = 1, & w = 0 & \text{for} & x \to +\infty, \\
u_x = 0, & v_x = 0, & w_x = 0 & \text{for} & x \to -\infty.
\end{array}
$$

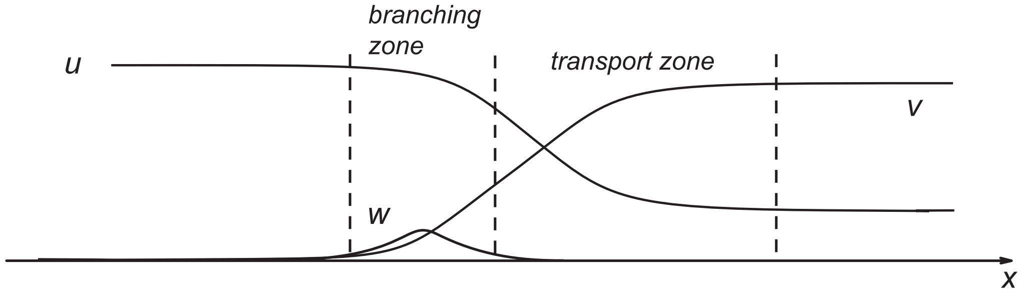
- Travelling wave solution, $\xi = x - ct$

$$
\begin{aligned}
& u_{\xi\xi} + c u_\xi + r w^2 = 0, \\
& {L_A}^{-1} v_{\xi\xi} + c v_\xi - \beta v w e^{\beta - 1/u} = 0, \\
& {L_B}^{-1} w_{\xi\xi} + c w_\xi + \beta v w e^{\beta - 1/u} - r \beta w^2 = 0
\end{aligned}
$$

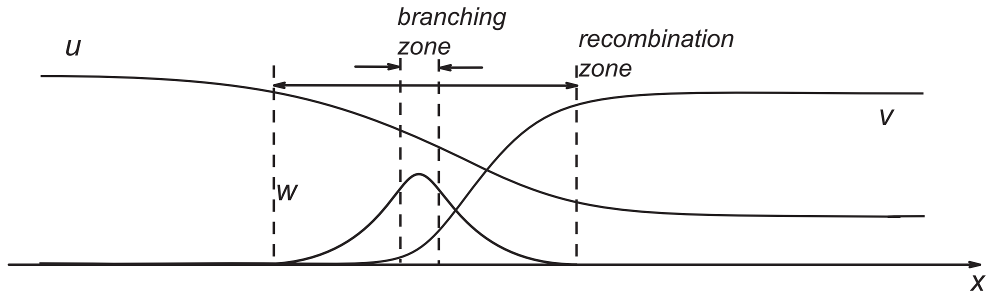
Liñán's analysis of flame structure

— A. Liñán, Insituto Nacional de Technica Aerospacial "Esteban Terradas" (Madrid), USAFOSR Contract No. E00AR68-0031, Technical Report No. 1 (1971).

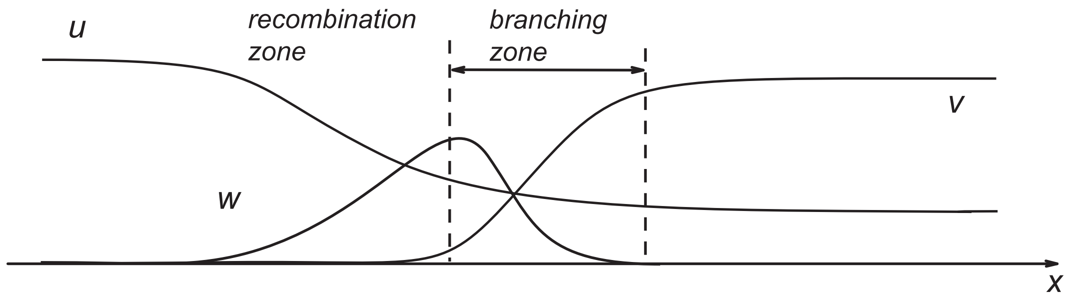
- Fast recombination $e^{-\beta} \ll r \rightarrow$ AEA 1-step: $c = L_A e^{-\beta}/\beta\sqrt{2r}$.



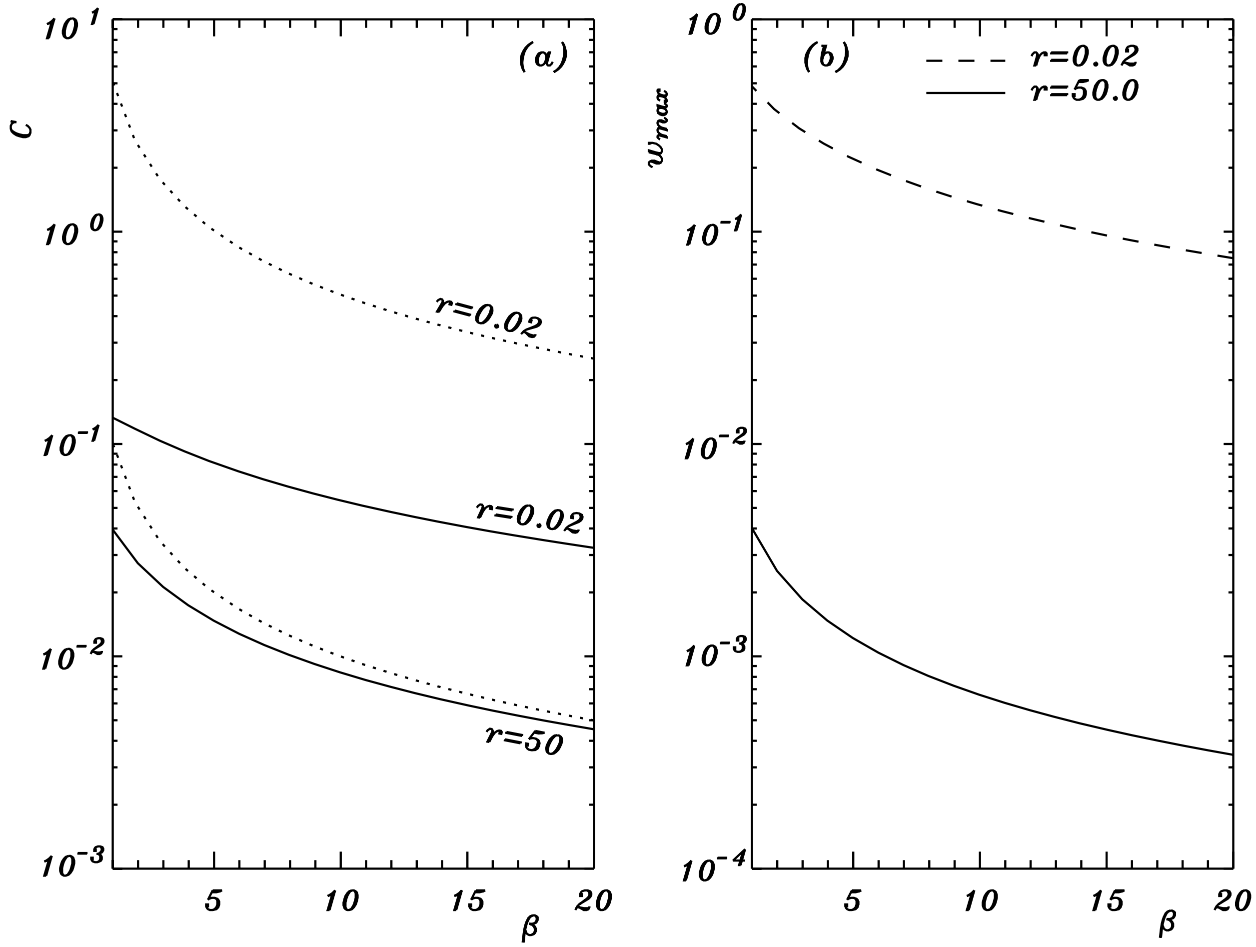
- Intermediate recombination $e^{-\beta} \sim r$



- Slow recombination $e^{-\beta} \gg r$

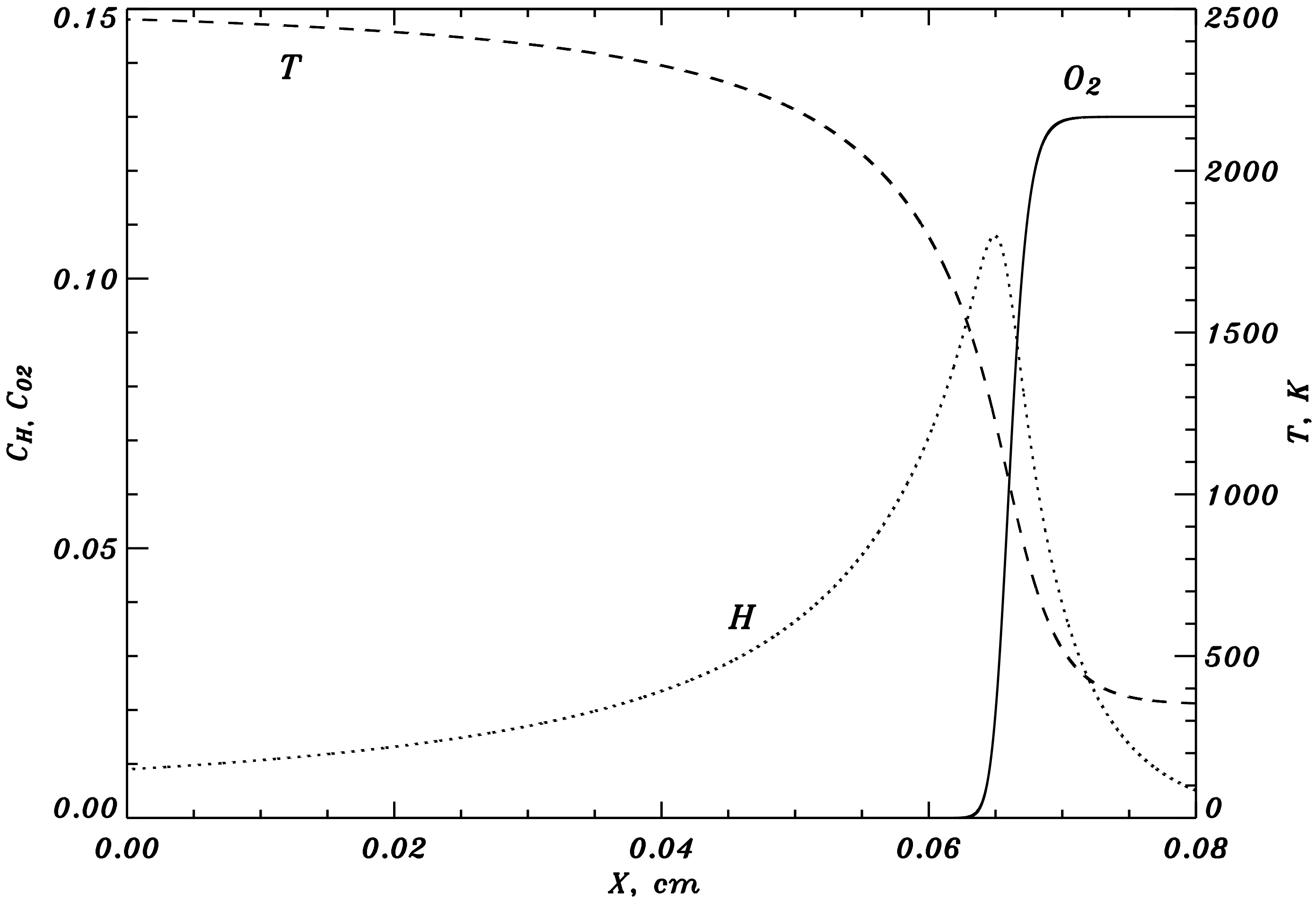


Flame speed



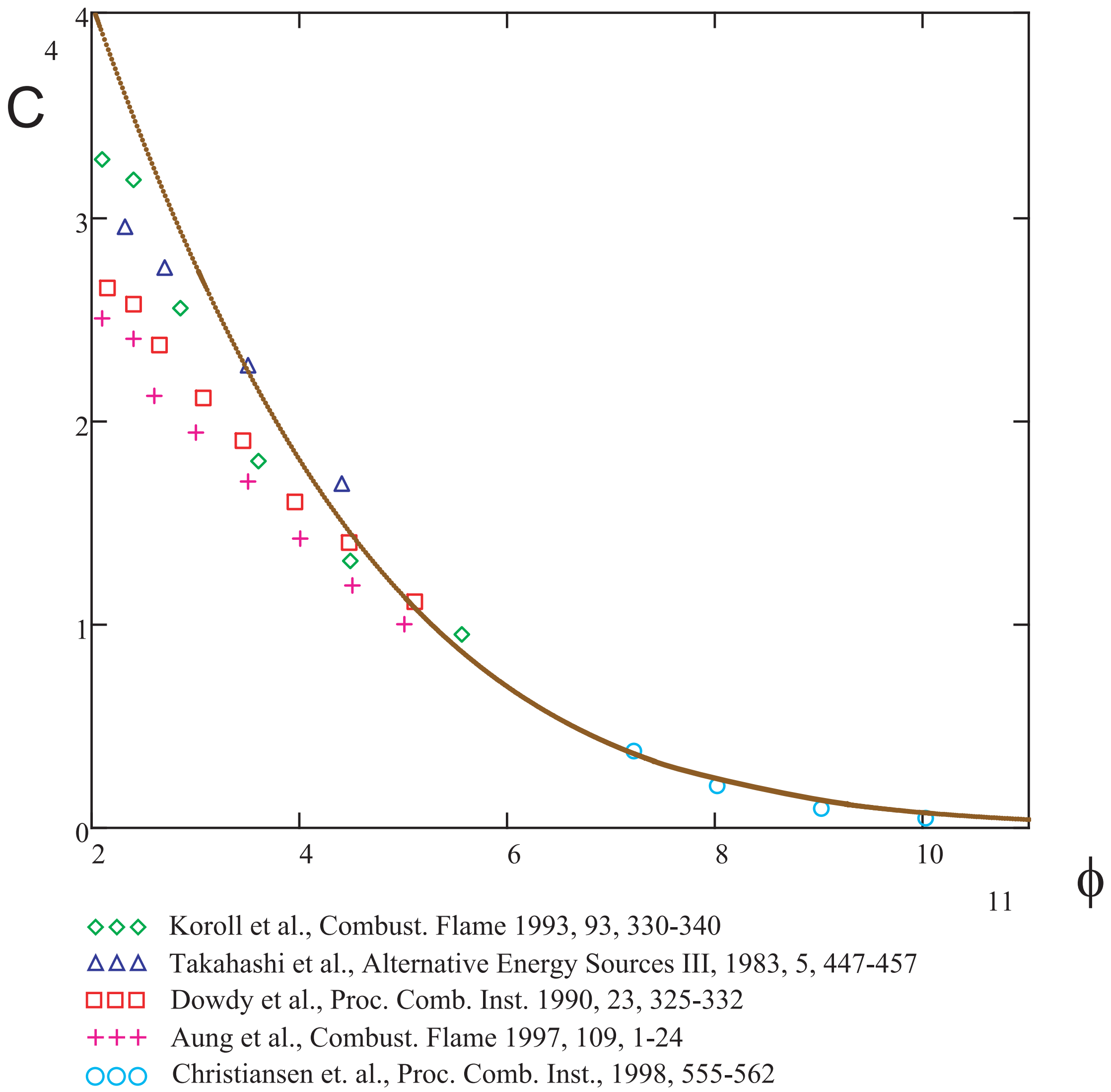
Dependence of (a) flame speed, c, and (b) maximal concentration of radicals, w_{max}, on the activation energy, β, for two values of the recombination parameter $r = 0.02$, $r = 50$ and $L_A = L_B = 1$.

Flame structure in the H_2-O_2 mixture



Concentration of H and O2 (left axis) and temperature (right axis) pofiles for combustion wave in 26/13/61 H2/O2/Ar mixture at $p = 1$ atm and $T_a = 370$K. Parameters of the model: $\beta \approx 3.9$, $r \approx 0.002$, $L_A \approx 2$, and $L_B \approx 0.3$. The flame speed, $c \approx 4$ m/s, whereas the numerical calculations using the detailed kinetic scheme yields 3.37 m/s according to O. Korobeinichev, T. Bolshova, Combust. Explos. Shock Waves 45 (2009) 507-510

Flame speed for H_2-air mixture



Dependence of the flame speed, c, on equivalence ratio, ϕ, at normal conditions.

Stability analysis

- We seek the solution of the form

$$\begin{aligned} u(\mathbf{r},t) &= U(\xi) + \epsilon\phi(\xi)\exp(\lambda t + iky), \\ v(\mathbf{r},t) &= V(\xi) + \epsilon\psi(\xi)\exp(\lambda t + iky), \\ w(\mathbf{r},t) &= W(\xi) + \epsilon\chi(\xi)\exp(\lambda t + iky), \end{aligned}$$

  where $U(\xi)$, $V(\xi)$, $W(\xi)$ is the travelling combustion wave, $\xi = x - ct$ is a coordinate in the moving frame.

- Substituting this expansion into govening PDEs

$$\mathbf{v}_\xi = \hat{A}(\xi, \lambda, k)\mathbf{v},$$

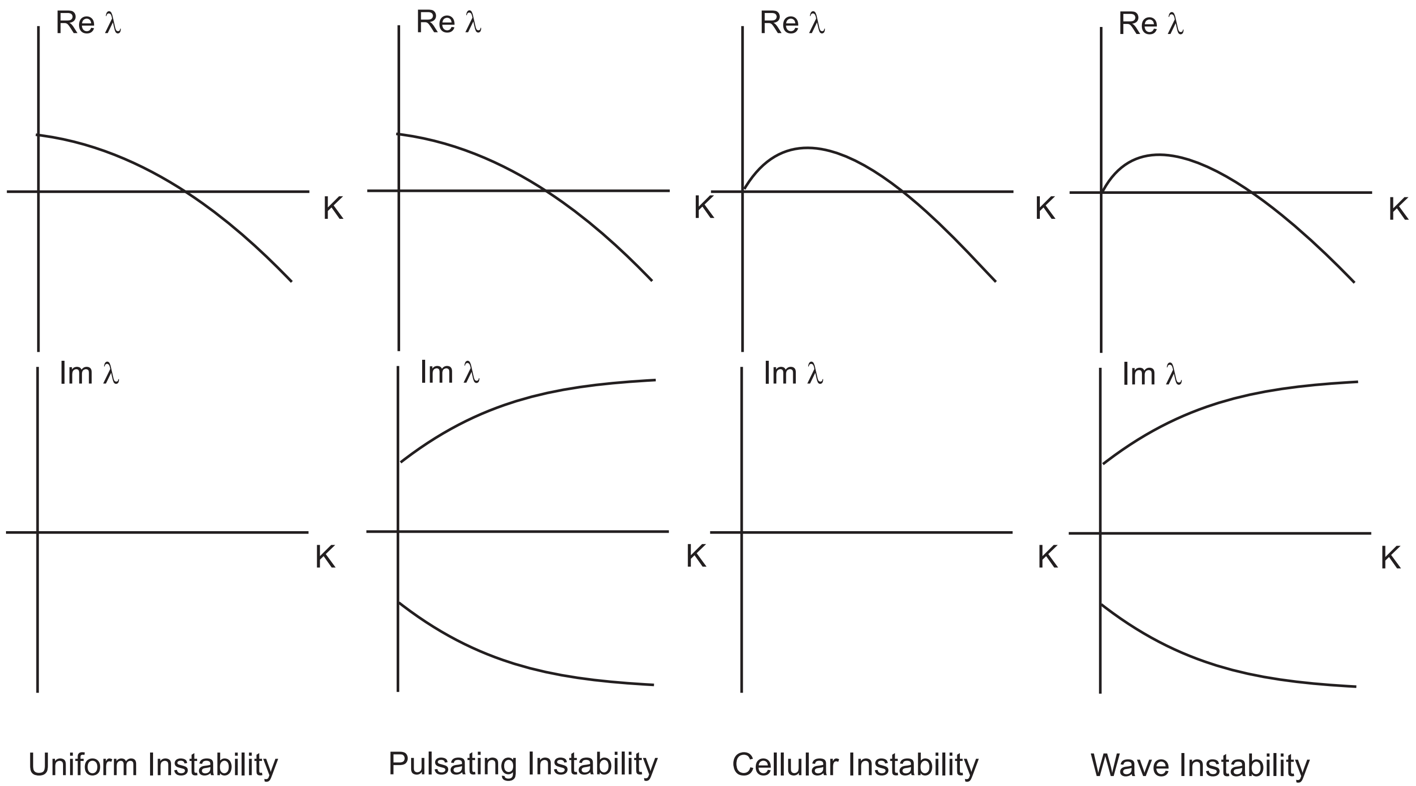
  where $\mathbf{v}(\xi) = [\phi,\ \psi,\ \chi,\ \phi_\xi,\ \psi_\xi,\ \chi_\xi]^T$ and $\hat{A}(\xi,\lambda,k)$ is 6×6 matrix those elements are functions of $U(\xi)$, $V(\xi)$, $W(\xi)$

- We seek λ and $k : \exists\ \mathbf{v}(\xi)$ bounded for both $\xi \to \pm\infty$. If for some $k\ \exists\lambda$: $Re\lambda > 0$ then the travelling wave is linearly unstable, otherwise, if $\forall k\ Re\lambda \leq 0$, then the travelling wave solution is linearly stable.

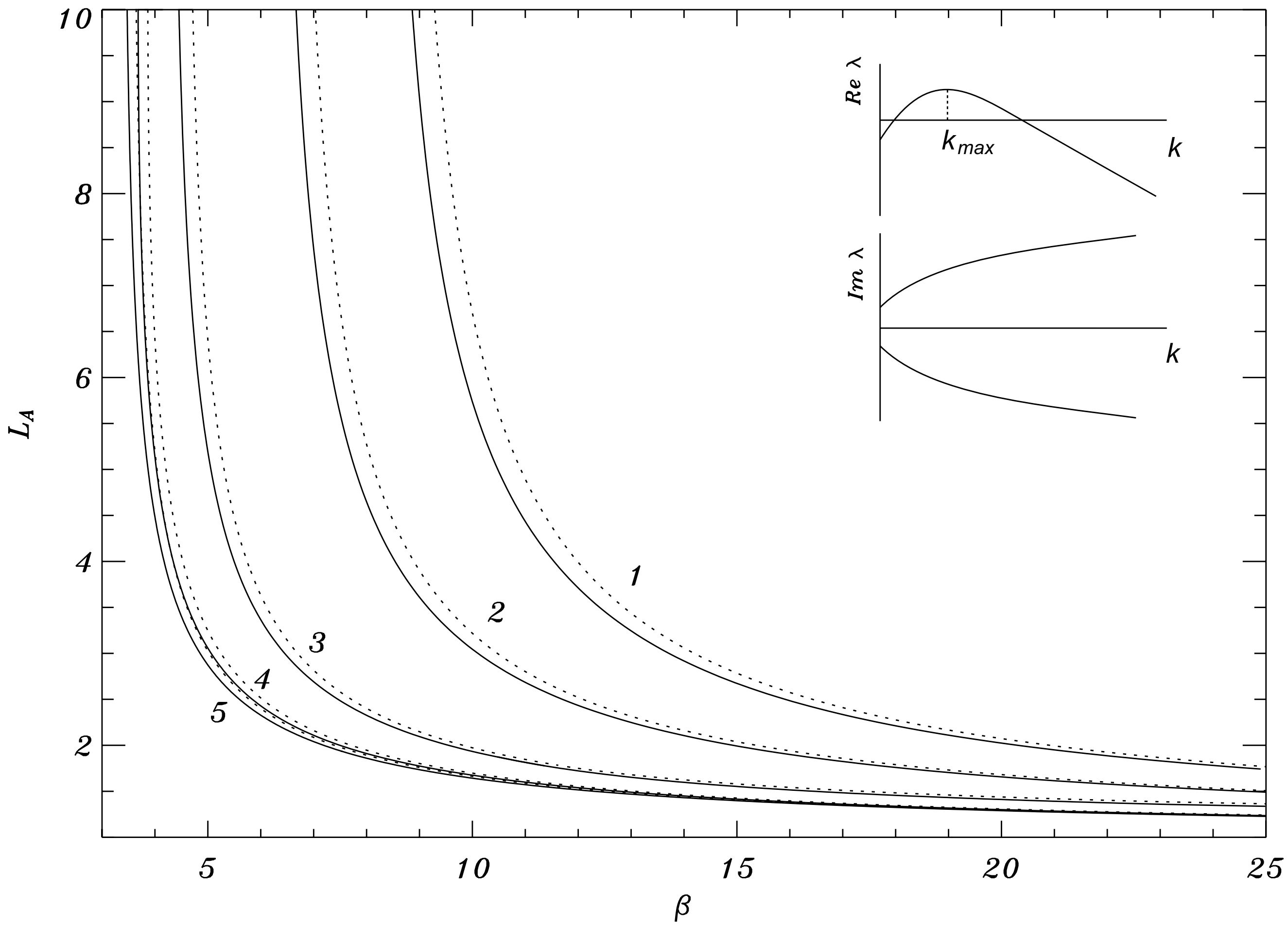
- Evans function $D(\lambda, k)$: for dispersion relation $\lambda(k)$ $\to D(\lambda, k) = 0$

- Nonlinear analisys - FDE

Instabilities in 2D

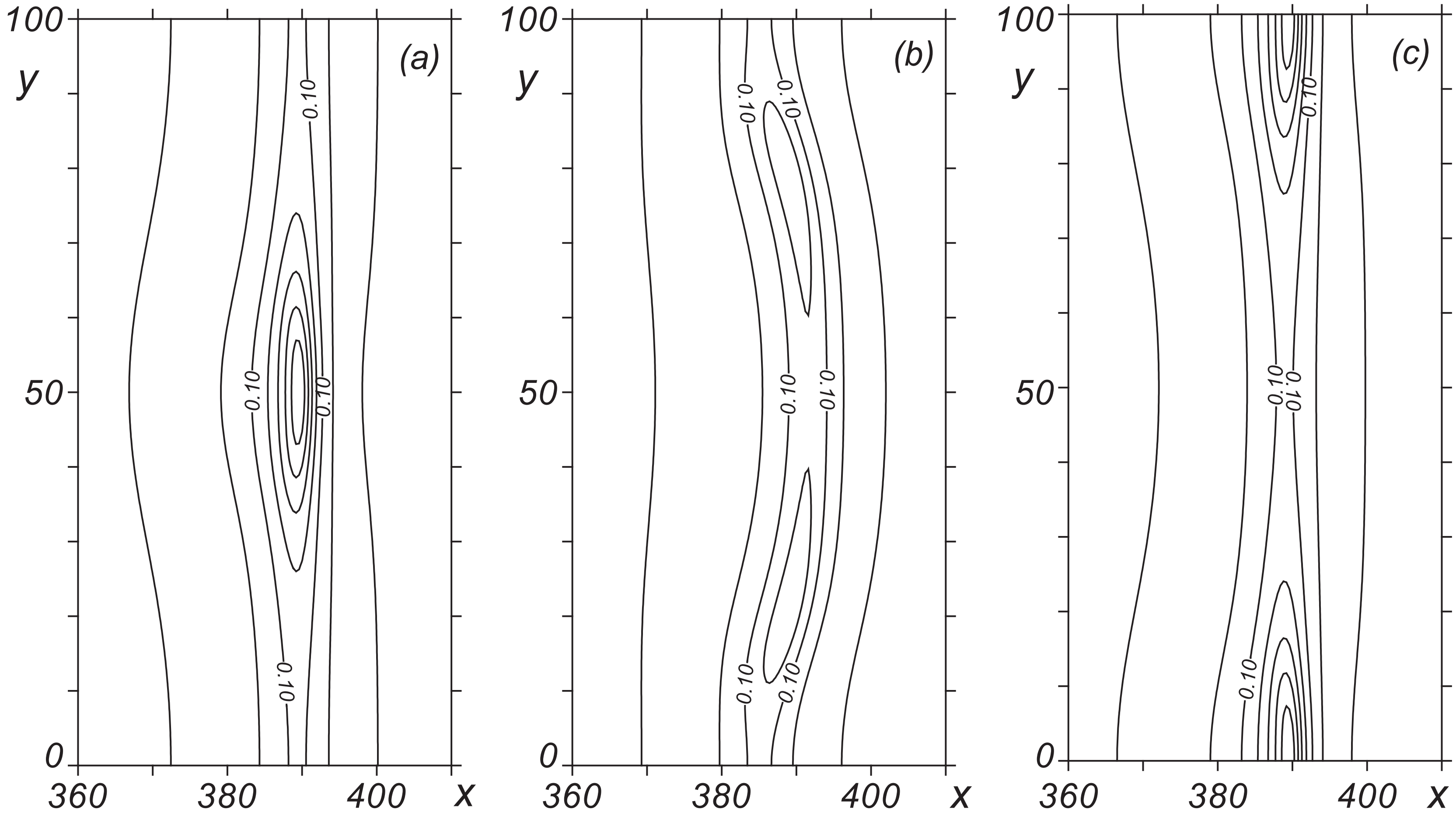


Wave instability



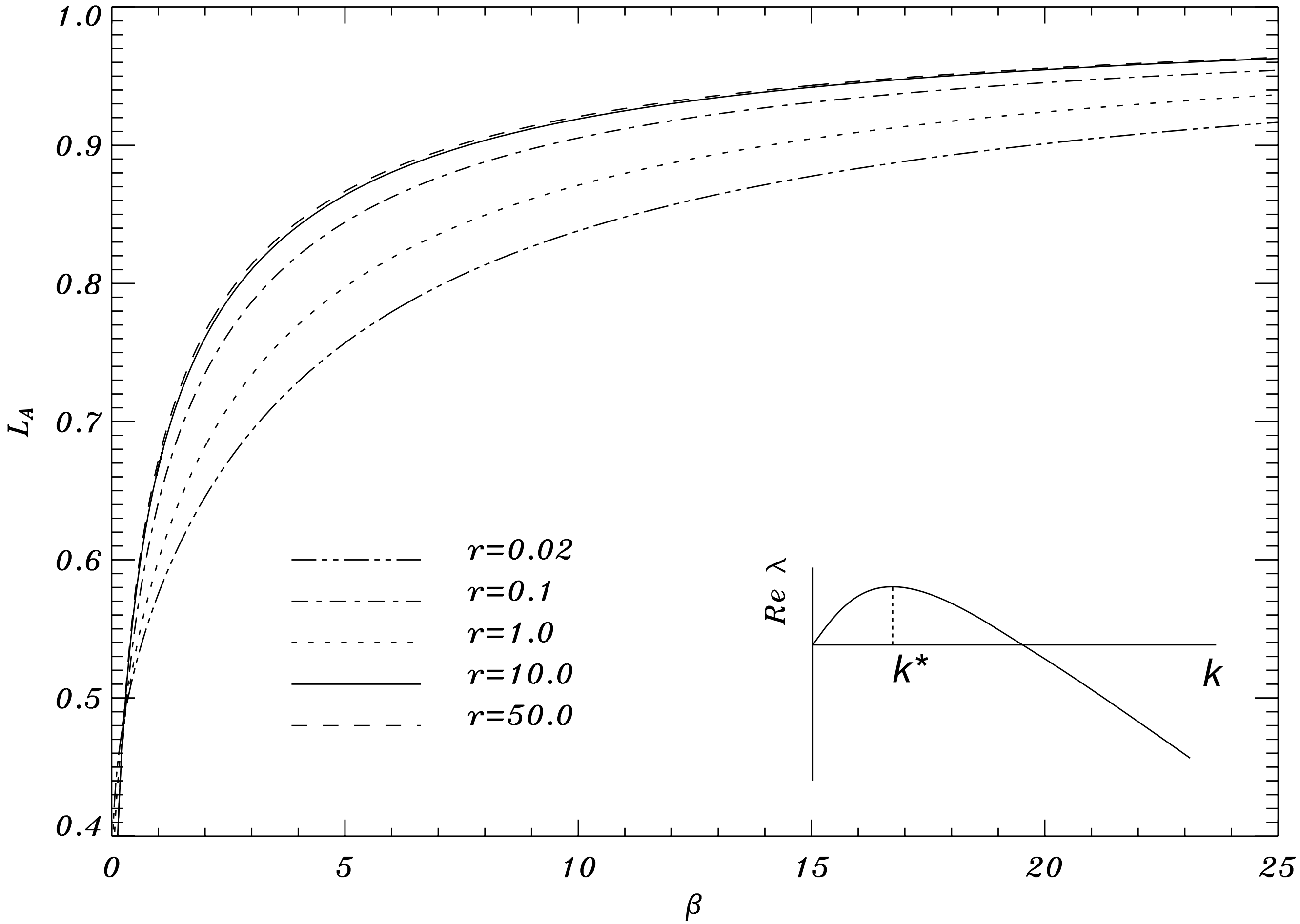
Neutral stability boundary in the L_A vs. β plane for $L_B = 1$, $u_a = 0$ and $r = 0.02$, 0.1, 1, 10, 50 plotted with curves 1, 2, 3, 4, and 5, respectivelly.

Pulsating waves



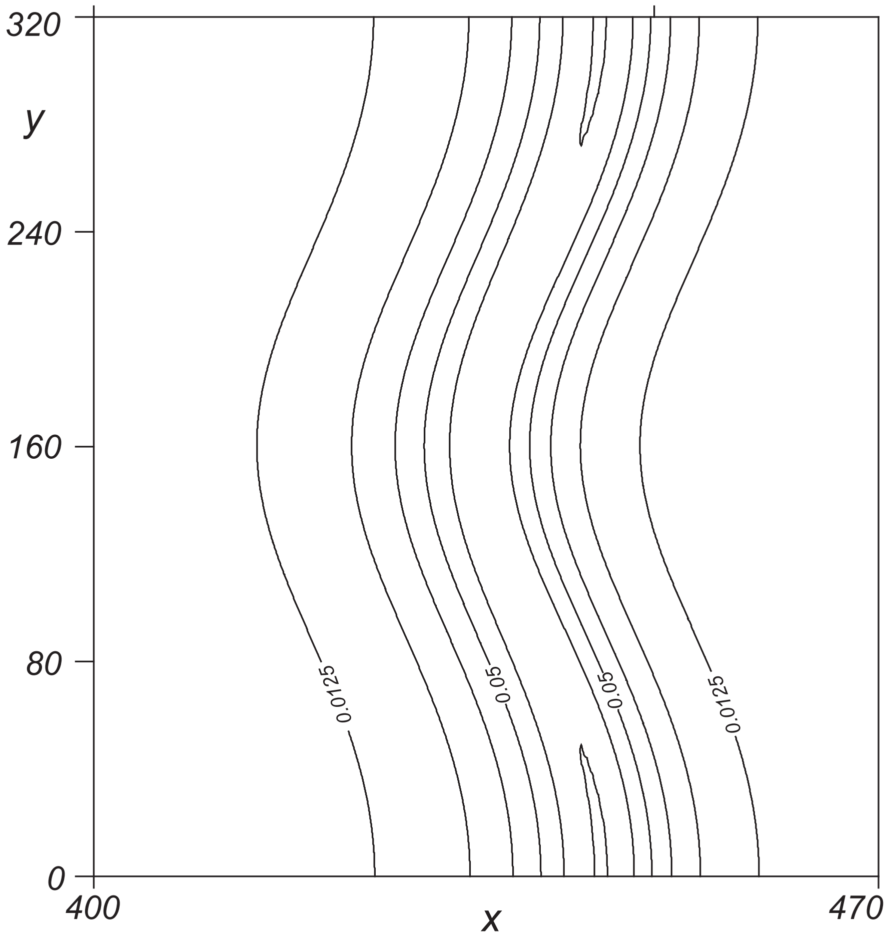
Contour plots of the radical concentration profiles, $w(x, y)$, sampled at three successive moments of time $t_1 = 80$ in panel (a), $t_2 = 145$ in panel (b), and $t_3 = 190$ in panel (c) for $L_A = 10$, $L_B = 1$, $b = 7.5$, and $r = 0.1$.

Cellular instability



Stability diagram on the L_A vs. β plane for $L_B = 1$, $u_a = 0$ and various values of $r = 0.02$, 0.1, 1, 10, and 50.

Cellular waves



Contour plots of the radical concentration profiles, $w(x, y)$, for $L_A = 0.81$, $L_B = 1$, $\beta = 9.5$, $r = 0.1$.

Conclusions

- The stability of combustion waves in the Zeldovich-Liñán model is investigated in the adiabatic limit by using the Evans function method and by direct integration of the governing PDEs. The neutral stability boundary is found in the L_A vs β plane. The effect of variation of parameters is delineated.
- It is demonstrated that for the case of $L_A > 1$, the combustion wave loses stability with respect to wave perturbations. For the case of $L_A < 1$, the combustion wave loses stability with respect to cellular perturbations.
- It is demonstrated that as the critical parameter values for the onset of instability are crossed, either pulsating or cellular two-dimensional solutions emerge. The properties of these solutions are studied.
- Further investigation is required to validate the results with respect to experimental data for hydrogen-oxygen flames. Of special interest is to undertake such comparison for the predictions of the limits of stability and emergence of pulsating and cellular flames with complex dynamics.

- V.V. Gubernov, A.V. Kolobov, A.A. Polezhaev, H.S. Sidhu, Stability of combustion waves in the Zeldovich–Liñán model, Combustion and Flame 159 (2012) 1185-1196
- V.V. Gubernov, A.V. Kolobov, A.A. Polezhaev, H.S. Sidhu, Pulsating instabilities in the Zeldovich–Liñán model, Journal of Math. Chemistry 49 (2011) 1054-1070