

Bifurcations in Planar Radiating Diffusion Flames Dynamics

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1 Introduction

The interest in detecting *unstable* combustion conditions is continuously increasing together with the need to reduce pollutant emissions. Indeed, this achievement is pursued by moving the operative conditions of combustion appliances towards conditions that, while are beneficial with respect to the emissions, are often more prone to the loss of stability of a stationary behaviour, sometimes leading to complete extinction, like blow-off or quenching. It is clearly emerged from previous investigations that an oscillatory behavior can be observed before instabilities linked with flame extinction [1]. Several examples of this behavior are reported in the literature related with extinctions due to heat losses [1–3]. [4] identified the bifurcation point before extinction as a subcritical bifurcation of oscillating solutions. [5] classified different ways to extinction involving supercritical and subcritical Hopf bifurcations. [6] performed a linear stability analysis with respect to the Damköhler number and the radiative heat release coefficient. It has been shown how the S-shaped diagram evolves into a double branched structure with the presence of an island. More recently, the theoretical studies have been sided by the experimental investigation of a quasi 1D planar diffusion flame configuration [7, 8].

For the systematic analysis of the system dynamics, numerical bifurcation theory provides an arsenal of algorithms and software packages, such as AUTO and MATCONT, for performing tasks such as the continuation of stable or unstable steady states and limit cycles, as well as the detection of critical points [9–12]. These packages are invaluable tools for performing systematic analysis for small to medium scale systems, however their applicability is most-often limited by the dimensionality of the system. Matrix free methods offer the possibility to overcome these limitations.

In [13], by systematically tracing these branches of oscillating solutions by employing timestepping/matrix free methods [14–17], we found the exact location of homoclinic bifurcations which marks the abrupt disappearance of the oscillating solutions with respect to the Damköhler number. The chosen model was a relatively simple one, describing the dynamics of a planar counterflow flame with radiative heat losses, already well investigated by several authors [4–6, 18, 19]. A still open question regards the relevance that these solutions have with respect to a real diffusion flame. Two aspects need consideration: the simplifying assumptions adopted and the range of parameters values at which the dynamical

features are detected. Therefore, a new investigation is currently carried on by adopting a different non-dimensionalization of the model equations that allows to relax some constraints artificially imposed in the previous formulation and to easily connect the computed solutions to parameter values admissible in real experimental configurations.

2 Mathematical model

The equations describing the evolution of planar 1D diffusion flames have been derived by Matalon et al. [1,20]. Several investigations adopted the same model with only few differences [6,18,19]. Under the hypotheses of a planar, constant density flow, the model equations for the diffusion flame with radiative heat losses, assuming a one-step reaction, include the energy balance equation, written as:

$$\rho C_p \frac{\partial T^*}{\partial t^*} = \alpha \frac{\partial^2 T^*}{\partial x^{*2}} + Q \rho B \exp \left(-\frac{E_a}{\mathcal{R} T^*} \right) Y_f^* Y_{ox}^* - 4\sigma K_p (T^{*4} - T_b^{*4}) \quad (1)$$

and the fuel and oxidizer species Y_i^* , $i = f, ox$ balance equations, written in the form:

$$\rho \frac{\partial Y_i^*}{\partial t^*} = \rho \mathcal{D} \frac{\partial^2 Y_i^*}{\partial x^{*2}} + \nu_i \rho B \exp \left(-\frac{E_a}{\mathcal{R} T^*} \right) Y_f^* Y_{ox}^* \quad (2)$$

In these equations, C_p is the specific heat, assumed constant, α the thermal diffusivity, ν_{ox} the stoichiometric coefficient of oxidant per unit of fuel, normalized with respect to $\nu_f = 1$, Q the heat released per unit of fuel, B the frequency coefficient of the reaction, E_a the activation energy, $\mathcal{R}$ the universal gas constant, σ the Stefan-Boltzmann constant, and K_p is the Planck mean absorption constant, also assumed constant.

3 Methodology

Limit cycles are computed as fixed points of a Poincare map using a shooting formulation. We employ a well-tested initial value solver (LSODE) [21], for which numerical accuracy for the time integration of the system, as well as variational equations (which are important for bifurcation detection and continuation), can be easily adjusted [22]. If we consider that the evolution of the system is described through an autonomous non-linear system:

$$\frac{dx(t)}{dt} = f(x(t), \lambda),$$

with λ a system parameter, which serves as the bifurcation parameter, then to compute a periodic solution, one seeks for solutions which satisfy:

$$\mathbf{R} \equiv x(0) - x(T) = \mathbf{0}, \quad (3)$$

where T the period of oscillation. Newton-Raphson iteration is employed to solve the non-linear set of equations above, and the Jacobian matrix is:

$$\frac{\partial \mathbf{R}}{\partial x(0)} = \mathbf{I} - \frac{\partial x(T)}{\partial x(0)},$$

where $\mathbf{I}$ is the identity matrix and $\frac{\partial x(T)}{\partial x(0)}$ is the state transition matrix of the system, describing the sensitivity of the “final” state $x(T)$ with respect to the “initial” state $x(0)$. The state transition matrix is computed from the variational matrix $\mathbf{V}(t) \equiv \frac{\partial x(t)}{\partial x(0)}$, the evolution of which is given by:

$$\frac{d}{dt} \mathbf{V} = \left[\frac{\partial f}{\partial x} \right] \cdot \mathbf{V},$$

with initial conditions:

$$\mathbf{V}(0) = \frac{\partial x(t)}{\partial x(0)} \Big|_{t=0} = \mathbf{I}$$

In its current form the Newton-Raphson problem is ill-posed; due to the translational (in time) invariance of the periodic solutions (any point on the limit cycle satisfies Eq.3), we single out one point on the limit cycle, applying an additional algebraic constraint (also called pinning condition), which has the general form:

$$g(x, \lambda, T) = 0,$$

and allows the computation of the unknown period of oscillation T . We can examine the dependence of the obtained periodic solutions on the system parameter λ , through the application of parameter continuation techniques such as the pseudo arc-length continuation method [23].

4 Some relevant results

The nondimensional form of equations (1) and (2) can be written as [6, 18, 19]:

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} + DY_o Y_f e^{-T_a/T} - RD(T^4 - T_o^4) \quad (4)$$

$$L \frac{\partial Y_o}{\partial t} = \frac{\partial^2 Y_o}{\partial x^2} - DY_o Y_f e^{-T_a/T} \quad (5)$$

$$L \frac{\partial Y_f}{\partial t} = \frac{\partial^2 Y_f}{\partial x^2} - DY_o Y_f e^{-T_a/T}, \quad (6)$$

where $T = T(x, t)$ is the temperature, Y_o is the oxidizer mass fraction and Y_f denotes the fuel mass fraction of the mixture. L is the Lewis number (same for both the fuel and the oxidizer), and R is the ratio of the characteristic chemical and radiation time scales. Above D is the Damköhler number, and T_a is the activation temperature. The following boundary conditions are assumed at the porous walls:

$$\text{at } x = -1 : T = T_o, \quad Y_f = 1, \quad Y_o = 0 \quad (7)$$

$$\text{at } x = +1 : T = T_o, \quad Y_f = 0, \quad Y_o = 1. \quad (8)$$

A typical example of the complete characterization of branches of limit cycles solutions computed with the proposed procedure is reported in Fig.1, for the case $T_a = 1$, $R = 0.2$ and $R = 0.233$. With respect to previously published results, some new features are detected. Two stable steady branches exist on the upper part of the diagram, in [6] observed only for lower valued of the parameter R ($R = 0.1$). Furthermore, the full branch of stable periodic solutions between the Hopf points at $D = 1823.9$ and $D = 10471$ has been successfully computed. Stable and unstable branches of steady state solutions are depicted with solid black and broken lines respectively. The periodic solution branch is marked by the open circles. The amplitude of limit cycles is represented by the dotted line with the open circles. Full circles and triangles are used to point out turning and Hopf points respectively. Clearly, no extinction occurs along this interval. The bifurcation diagram for $R = 0.233$ shows again the existence of a region of D values, where stable periodic solutions are present. This region is located within the homoclinic bifurcation point at $D = 2742$ and a supercritical Hopf point at $D = 5957$. In the vicinity of $D = 2742$ the period tends to infinity marking the location of a homoclinic bifurcation. Similar results are obtained for the case of activation temperature, $T_a = 1.2$ and different R values. In particular, the parametric dependence of $T[0]$ with D for $R = 0.01$ is shown in Fig.2 (left). A region of unstable solutions marked

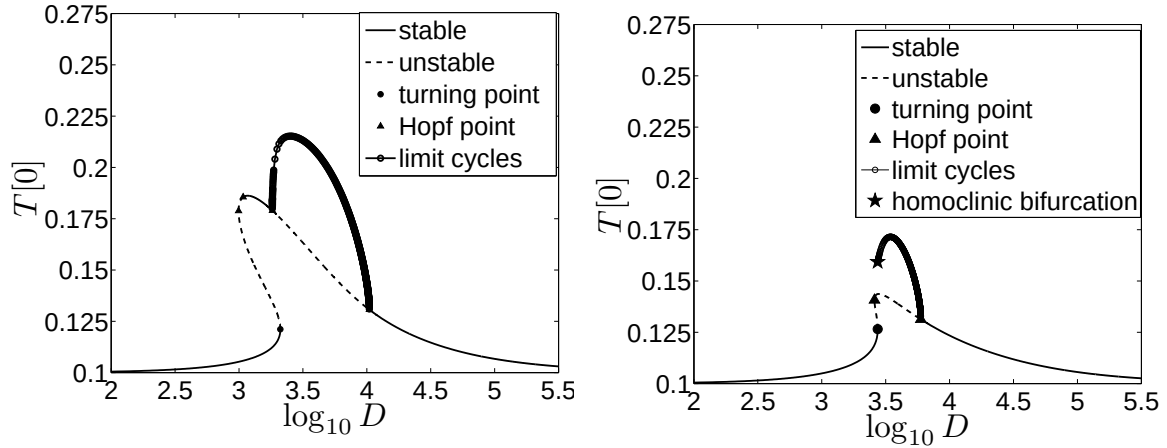


Figure 1: Parametric dependence of temperature at $x = 0$ with respect to the Damköhler parameter. Parameter set values: $T_a = 1.0$; $R = 0.2$ (left), $R = 0.233$ (right).

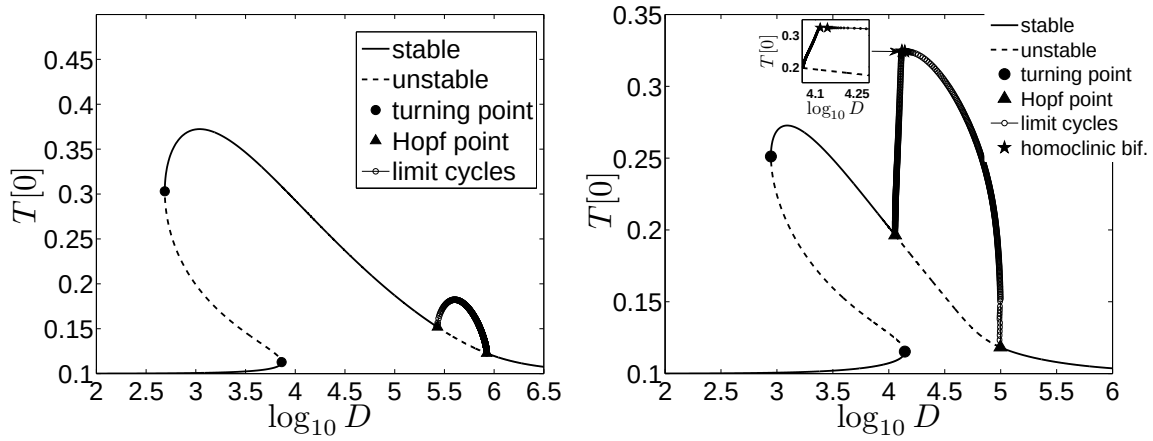


Figure 2: Parametric dependence of temperature at $x = 0$ with respect to the Damköhler parameter. Parameter set values: $T_a = 1.2$; $R = 0.01$ (left), $R = 0.04$ (right).

by the turning points at $D = 488$ and $D = 7290$ is revealed while the Hopf points at $D = 269272$ and $D = 842922$ define a region of stable periodic solutions. The dependence of $T[0]$ with respect to D when R is increased to $R = 0.04$ is depicted in Fig.2(right). A region of unstable solutions is pinpointed by the turning points at $D = 884$ and $D = 13900$. The Hopf points are located at $D = 11373$ and $D = 99467$. In this case the homoclinic bifurcation occurs well inside the ignited region.

5 A new non dimensionalization

In order to distinct the role played by the heat loss and the chemical production, the appearance of the Da number in front of both the chemical production term and the radiative heat transfer, as it occurs in eq. (4), should be avoided. Therefore it is here proposed to define different non-dimensional groups that arises by assuming the following definitions for the dimensional variables:

$$t^* = t t_c = \frac{d_c^2}{D} t, \quad x^* = d_c x, \quad T^* = \frac{Q Y_{f,s}}{C_p} T, \quad Y_i^* = Y_{f,s}^* Y_i \quad (9)$$

By grouping all dimensional quantities, the following three non dimensional group arise:

$$Le = \frac{\alpha}{\rho C_p D} \quad , \quad Da = \frac{BY_{f,s}d_c^2}{D} \quad , \quad Le \kappa = \frac{\alpha}{\rho C_p D} \frac{4d_c^2 \sigma K_p}{\alpha} \left(\frac{QY_{f,s}}{C_p} \right)^3 \quad (10)$$

The first two groups correspond to the definition of the Lewis number (here assumed to be the same for both the fuel and the oxidizer) and the Damköhler number. The last group can be interpreted as the enhancement of heat transfer due to the contribution of the radiative heat transfer. Adopting these definitions, the non dimensional form of the model equations become:

$$\frac{\partial T}{\partial t} = Le \frac{\partial^2 T}{\partial x^2} + Da \exp\left(-\frac{T_a}{T}\right) Y_f Y_{ox} - Le \kappa (T^4 - T_b^4) \quad (11)$$

$$\frac{\partial Y_{ox}}{\partial t} = \frac{\partial^2 Y_{ox}}{\partial x^2} - \nu_{ox} Da \exp\left(-\frac{T_a}{T}\right) Y_f Y_{ox} \quad (12)$$

$$\frac{\partial Y_f}{\partial t} = \frac{\partial^2 Y_f}{\partial x^2} - Da \exp\left(-\frac{T_a}{T}\right) Y_f Y_{ox}, \quad (13)$$

This model allows for the independent assignment of the fuel and oxidizer at the boundary: boundary conditions at the porous walls depend upon the stoichiometric fuel-oxidizer ratio $Y_{f,s}$ being therefore possible to modify the mixture strength. At the two boundaries pure fuel and pure oxidizer are fed, respectively, on $x = -1$ and $x = 1$. Therefore the boundary conditions can be expressed as:

$$\begin{aligned} \text{at } x = -1 : \quad T &= T_b, \quad Y_{f,b} = 1/Y_{f,s}, \quad Y_{ox,b} = 0 \\ \text{at } x = +1 : \quad T &= T_b, \quad Y_{f,b} = 0, \quad Y_{ox,b} = 1/Y_{f,s}. \end{aligned}$$

Stoichiometric conditions inside the channel, where the flame is expected to anchor, are identified by $Y_f = 1$ and having assumed equal diffusivities for fuel and oxidizer, it is located at $x = 0$.

6 Preliminary results and conclusions

A systematic exploration of the solution behaviour in the parameter space has been started to investigate the possibility of the occurrence of the behaviour previously reported but in ranges relevant to real diffusion flames. Fig. 3 shows results obtained with values of the main parameters corresponding to values for all the coefficients typical of a real flames. The behaviour of the bifurcation diagram confirms the occurrence of limit cycles close to the extinction point. By increasing the radiative heat loss parameter κ , a different behavior is detected: the unstable branch disappears and the transition from not-ignited to ignited solutions occurs crossing a region of stable limit cycles for Da between 537031 and 1076465.

References

- [1] S. Cheatham, M. Matalon, Proc. Combust. Inst., 26(1996), 1063-1070.
- [2] E.W. Christiansen, S.D. Tse, C. K. Law, Combust. Flame, 134(2003), 327-337.
- [3] P. Papas, M. Rais, P.A. Monkewitz, A.G. Tomboulides, Comb. Theory Model, 7(2003), 603-633.
- [4] C.J. Sohn, S.H. Chung, J.S. Kim, Combust. Flame 117 (1999), 404-12.
- [5] C.H. Sohn, J.S. Kim, S.H. Chung, K. Marut, Combust. Flame, 123(2000), 95-106.

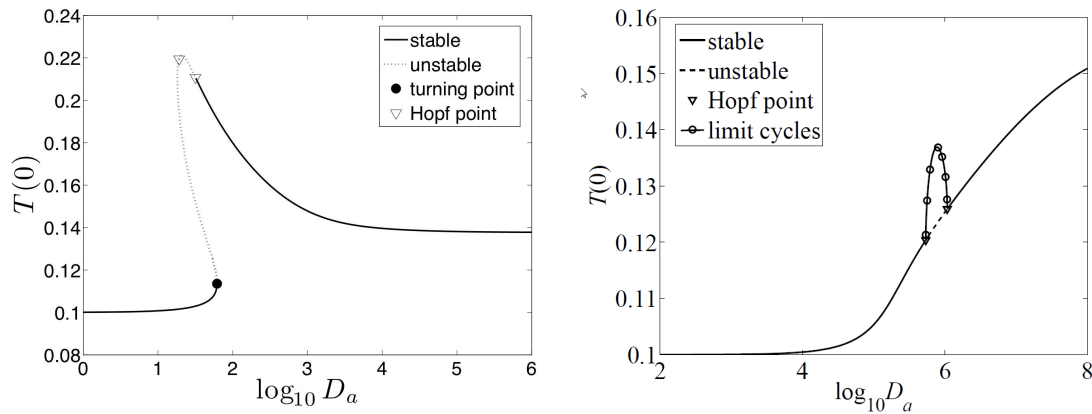


Figure 3: Parametric dependence of temperature at $x = 0$ with respect to the newly defined Damköhler parameter. Parameter set values: $Le = 0.97$, $\kappa = 1000$, $T_a = 1.2$, $T_b = 0.1$, $Y_f = 0.06$, $\nu_{ox} = 5$ and $\kappa = 1000$, (left); $Le = 1$, $T_a = 1.2$, $T_b = 0.1$, $Y_f = Y_{ox} = 1$, $\nu_{ox} = 1$ and $\kappa = 8000$ (right).

- [6] M. Miklavcic, A.B. Moore, I.S. Wichman, *Combust. Theory Model*, 9 (2005), 403-16.
- [7] , E. Robert, P.A. Monkewitz, *Proc. Combust. Inst.*, 32 (2009), 987-994.
- [8] , E. Robert, P.A. Monkewitz, *Combust. Flame*, 160 (2013), 546-556.
- [9] E. Doedel, L.S. Tuckerman, Eds., *Numerical methods for bifurcation problems and large-scale dynamical systems*, IMA Vol. in Math. Appl., 119, Springer-Verlag, 2000.
- [10] A. Dhooge, W. Govaerts, Yu.A. Kuznetsov, *ACM Trans. Math. Software* 29 (2003) 141-164.
- [11] E. J. Doedel, W. Govaerts, Yu. A. Kuznetsov, A. Dhooge, *Int. J. Bif. Chaos* 15 (2005) 841-860.
- [12] J.F.W. Govaerts, Yu.A. Kuznetsov, A. Dhooge, *SIAM J. Sci. Comp.* 27 (2005) 231-252.
- [13] M.E. Kavousanakis, L. Russo, F.S. Marra, C. Siettos, *Combust. Theory Mod.*, (2013) in press.
- [14] G.M. Shroff, H.B. Keller, *SIAM J. Num. Anal.* 30 (1993) 1099-1120.
- [15] C.T. Kelley, I.G. Kevrekidis, L. Qiao, *SIAM J. Sci. Comp.* 19 (2004) 1188-1209.
- [16] K. Lust, D. Roose, A. Spence, A.R. Champneys, *SIAM J. Sci. Comp.* 19 (1998) 1188-1209.
- [17] M. Kavousanakis, L. Russo, C. I. Siettos, A. G. Boudouvis, G. C. Georgiou, *J. Non-Newtonian Fluid Mechanics* 151 (2008) 59-68.
- [18] M. Miklavcic, *Combust. Theory Model.*, 11 (2007), 103-112.
- [19] H. Gotoda, T. Miyano, I.G. Shepherd, *Phys. Rev. E* 81 (2010) 026211-10.
- [20] Kukuck, S., Matalon, M., *The Onset of Oscillations in Diffusion Flames*, *Combust. Theory Modelling*, 5(2001), 217-240.
- [21] A.C. Hindmarsh, *ACM-SIGNUM Newsl.* 25 (1980), 10-11.
- [22] J.R. Leis, M.A. Kramer, *ACM Trans. Math. Software*, 14 (1988), 61-67.
- [23] H.B. Keller, *Numerical solution of bifurcation and non-linear eigenvalue problems*, P.H. Rabinowitz, Editor, *Applications of Bifurcation Theory*, Academic Press, New York, 1977, p. 359-384.