

AN ASYMPTOTIC FRACTIONAL DIFFERENTIAL MODEL OF SPHERICAL FLAME

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ABSTRACT. This paper is devoted to the analysis and numerical simulation of a model of initiation of a small spherical flame by a point source derived by G. Joulin. This asymptotical model for large activation energies gives the radius of the flame as the solution of a nonlinear Abel integral equation of the second type. The analysis (existence, uniqueness, qualitative comportement and power threshold) and one step numerical simulation use both classical integral equation tools and diffusive representation.

RÉSUMÉ. Cet article est consacré à l'analyse et à l'approximation d'un modèle asymptotique d'initiation de flamme sphérique du à G. Joulin. Ce modèle asymptotique pour de grandes énergies d'activation détermine le rayon de la flamme comme solution d'une équation d'Abel non linéaire de deuxième espèce. L'étude de ce modèle des points de vue existence, unicité, seuil d'énergie et la simulation numérique par méthode à un pas utilisent l'approche classique de ce type de problème et une représentation diffusive de l'opérateur non linéaire.

1. THE ASYMPTOTICAL MODEL OF SPHERICAL FLAME ([5])

The model under consideration deals with the initiation of a quasi-steady nearly adiabatic spherical flame in a mixture of reactive species by a ponctual source.

The mixture is assumed to be initially homogeneous at rest and the burning process is modelled by a one reactant exothermic reaction of Arrhenius type slow enough and isobaric.

The reduced mass density ρ is taken as a constant and using spherical coordinates and adimensionalisation of the classical balance laws, the dimensionless temperature change θ and mass fraction y of the (light) reactant are solutions of

$$\begin{cases} \rho \left(\frac{1}{\beta^2} \partial_t \theta + U \partial_x \theta \right) = \frac{1}{x^2} \partial_x (x^2 \partial_x \theta) + W \\ \rho \left(\frac{1}{\beta^2} \partial_t y + U \partial_x y \right) = \frac{1}{Le x^2} \partial_x (x^2 \partial_x y) - W, \end{cases} \quad (1.1)$$

with β the dimensionless activation temperature taken as the large parameter of the model, Le the Lewis number and $W = W(\beta)$ the reduced chemical rate.

The reactive zone is considered as a thin sheet located at $R(t)$ with jump relations associated with matched expansions:

$$\left(\frac{\theta - 1}{Le}, y \right) = \sum \frac{(\theta_i, y_j)}{\beta^j}.$$

The dimensional source strength is denoted $Eq(t)$, $q = O(t)$ (t the slow time scale). Then W is taken 0 and the system is supplemented with the boundary condition:

$$\beta(x^2 \partial_x \theta)(t, 0) = -Eq(t). \quad (1.2)$$

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Neglecting $O(\frac{1}{\beta^2})$ terms outside the reactive sheet, integration of 1-D Laplace equation associated with jump relations give for the quasi steady zone $x = O(1)$:

$$2R(\tau) \ln(R(\tau)) + Eq(\tau) = R(\tau)[K(\tau) - L(\tau)], \quad x \ll \beta, \quad (1.3)$$

K, L two constants of integration depending on time.

For $X = x/\beta = O(1)$ (far-field) expansions

$$\beta\theta = T(X, \tau) + O(1/\beta), \quad \beta \frac{1-y}{Le} = Y(\tau) + O(1/\beta)$$

give

$$\partial_\tau(T, Y) = X^{-2} \partial_X(X^2 \partial_X(T, Y/Le)). \quad (1.4)$$

Matching procedures and the hypothesis q switched on at $\tau = 0$ provides boundary and initial conditions for this diffusion equation:

$$XT = XY = \frac{R(t)}{Le} \quad \text{as } X \rightarrow 0 \quad \text{and} \quad T(X, 0) = Y(X, 0) = 0.$$

Finally, a two terms matching of the solution of this diffusion problem, expressed using the heat kernel, with that of the quasi-steady zone gives:

$$K(t) - L(t) = \frac{1 - \sqrt{Le}}{Le\sqrt{\pi}} \int_0^t \frac{R'(s)}{\sqrt{t-s}} ds,$$

which combined with (1.3) defines the evolution equation for R :

$$2(R \ln(R) + Eq) = \frac{R(1 - \sqrt{Le})}{Le\sqrt{\pi}} \int_0^t \frac{R'}{\sqrt{\tau-s}} ds,$$

associated with the initial condition $R(0) = 0$.

The determination of the radius R reduces by a linear change in time to the resolution of the non linear fractional differential equation:

$$2(R \ln(R) + Eq) = R \frac{1}{\sqrt{\pi}} \int_0^\tau \frac{R'}{\sqrt{\tau-s}} ds = RD^{1/2} R. \quad (1.5)$$

2. LOCAL EXISTENCE

With f the function defined over $\mathbb{R}^+ \times \mathbb{R}_*^+$ by:

$$f(t, r) = \ln(r) + \frac{Eq(t)}{r}, \quad (2.1)$$

the problem 1.5 is equivalent thanks to the initial condition to the nonlinear singular Abel equation:

$$R(t) = I^{1/2}(f(s, R(s))) = \frac{1}{\sqrt{\pi}} \int_0^t \frac{f(s, R(s)) ds}{\sqrt{t-s}}, \quad R(0) = 0, \quad (2.2)$$

associated with the constraint of positivity on its life interval.

The search for an ansatz to R in a neighbourhood of 0 gives two different comportements following the values of β :

PROPOSITION 2.1. *Assume $q(t) \sim q_0 t^\beta$ as $t \rightarrow 0$.*

Then the problem (2.2) admits a positive solution on a neighbourhood $[0, T_0[$ of 0 iff $\beta < 1/2$.

In this case the solution is unique and $C^{3/2}([0, T_0])$ regular with

$$R(t) \sim \sqrt{B\left(\frac{3-2\beta}{4}, \frac{1}{2}\right)} t^{1/4} \sqrt{Eq(t)} \quad \text{as } t \rightarrow 0.$$

Proof. If $\beta < 1/2$ when $R(t) = R_0 t^\alpha$ is substituted in (2.2),

$$R_0 t^\alpha \sim \frac{E q_0 t^{\beta+1/2-\alpha}}{R_0 \sqrt{\pi}} \int_0^t \frac{ds}{s^{\alpha-\beta} \sqrt{1-s}}$$

and the positivity of R_0 is equivalent to $\beta < 1/2$.

The existence of a positive R under the form $R_0 t^{\beta/2+1/4}(1+\rho(t))$ is then proved using the fixed point theorem in C^0 endowed with the weighted supremum norm $y \rightarrow \sup \frac{|y(t)|}{t^{1/8}}$.

If $\beta > 1/2$, the consideration of $R(t) = R_0 t^\alpha$ gives a negative righthandside for (2). ■

3. DIFFUSIVE FORMULATION, GLOBAL EXISTENCE, POWER-THRESHOLD

Obstructions to global existence of the solution initiated in Prop. 2.1 are a priori relevant of non lipschitz comportement of $f(t, \cdot)$ in neighbourhoods of 0 and ∞ . In fact non global solutions are the ones which tend to 0 in finite time and then with an infinite negative slope.

That kind of result can be established either in the context of Volterra equations or using the interpretation of its solution as the trace on $x = 0$ of a radiation-diffusion problem on $]0, \infty[$ particularly well fitted to comparison theorems and numerical simulations.

This problem, more conveniently formulated as a diffusion one with a (Dirac-) measure valued right-handside is closely related to the initial problem, itself of this type.

PROPOSITION 3.1. *The function R over $[0, T[$ is a solution of (2.2) in this interval iff there exists u solution of the Cauchy problem in $[0, T[\times \mathbb{R}$:*

$$\partial_t u - \partial_x^2 u = 2f(\cdot, u(0))\delta_0, \quad u(0, \cdot) = 0. \quad (3.1)$$

Then R is given by $R(t) = u(t, 0)$.

Proof. One verifies readily that any (necessarily continuous) solution of the Cauchy problem is such that

$$u(t, 0) = \frac{1}{\sqrt{\pi}} \int_0^t \frac{f(s, u(0, s)) ds}{\sqrt{t-s}}.$$

Conversely, if R is solution of (2.2) the function u defined using the heat kernel as:

$$u(t, x) = \frac{1}{\sqrt{4\pi}} \int_0^t e^{-x^2/4(t-s)} \frac{2f(s, R(s))}{\sqrt{t-s}} ds$$

is a solution of the Cauchy problem (3.1). ■

The following proposition [2] then gives existence and uniqueness results for (2.2) as consequences of analysis of the semi-linear Cauchy problem (3.1) with right-handside in $L^2(0, T; H^{-1}(\mathbb{R}))$ [7].

PROPOSITION 3.2. *Let q in $C^\infty(\mathbb{R}^+)$ be such that $q(t) > 0$ any t in $]0, t_0[$ and $q(t) = 0$ if $t \geq t_0$.*

(i) *If $t_0 = \infty$, then (3.1) has a unique global solution positive on \mathbb{R}_*^+ . Moreover $u(\cdot, 0)$ is C^∞ on \mathbb{R}_*^+ .*

(ii) *If t_0 is finite, then (3.1) has a unique maximal solution defined on $[0, t_{max}[$ which is even, C^∞ on $]0, t_{max}[\times \mathbb{R}_*^+$ and positive on $]0, t_{max}[$.*

Moreover $t \rightarrow u(t, 0)$ is C^∞ on $[0, t_{max}[$ and in the cases $t_{max} < \infty$, $\liminf_{t \rightarrow t_0} u(t) = 0$.

The more involved following theorem [2] asserts the existence of a critical level of excitation which separates comportements of developement and collapse or asymptotic extinction of the flame following q is compactly supported or not. Its proof, is based upon diffusive formulation and, in this context, on the non increase of the number of zeros of solutions of (3.1) ([1]).

THEOREM 3.3. *Assume the function q to be positive on \mathbb{R}_+^* .*

There exists an energy threshold $E_{cr}(q) > 0$ such that $\lim_{t \rightarrow +\infty} R_E(t) = +\infty$, 1 or 0, following E is greater, equal or less than E_{cr} .

Assume the function q to be positive on $]0, t_0[$ and zero elsewhere.

Then there exists $E_{cr}(q) > 0$ such that, if $E \geq E_{cr}(q)$, then the preceding conclusions hold and if $E < E_{cr}(q)$, the lifespan $[0, t_{max}[$ of R , is bounded with $\lim_{t \rightarrow t_{max}} R(t) = 0$.

This theorem is completed by the study of the asymptotic comportement of R near infinity in the cases of developement and extinction and near the quenching time in the corresponding case.

THEOREM 3.4. *Let us assume $E > E_{cr}(q)$. Then there exists $k > 0$ such that $r_e(t) \sim k\sqrt{t} \ln t$ as $t \rightarrow +\infty$.*

Assume $E < E_{cr}(q)$. Then there exists $k > 0$ such that $R_E(t) \sim k\sqrt{t_{max} - t}$ as $t \rightarrow t_{max}$.

Assume $E = E_{cr}(q)$. Then there exists $k > 0$ such that $R_E(t) - 1 \sim \frac{k}{\sqrt{t}}$ as $t \rightarrow +\infty$.

4. NUMERICAL SIMULATION USING DIFFUSIVE REPRESENTATION

Approximation for (2.2) under consideration based upon time-discretization of the Cauchy problem (3.1) formulated either in the $t - x$ or, using Fourier transformation, time-frequency variables may also be considered as a discrete time model of the phenomenon.

Here two approaches may be considered.

1) Introduction of a cut-off-discretization of the spatial or frequency domain leads to a finite dimensional non hereditary recursive system [9], [10].

2) For semi-discretization of time-frequency formulation, by this particularly fitted to computation, elimination of the implicit state variable $u(n\tau, \cdot)$ leads to a discrete hereditary model which keeps the main features of the semi-discrete model.

With U the space-Fourier transform of the solution u of (1), the solution R of (1) is given by:

$$\begin{cases} R(t) = I(U(t)) = \int_{\xi} U(t, \xi) d\xi \\ \partial_t U + 4\pi^2 \xi^2 U = 2f(t, I(U(t))) = 2 \left(\ln(I(u(t))) + \frac{Eq(t)}{I(U(t))} \right). \end{cases} \quad (4.1)$$

The fully implicit Euler semi-discretisation with step $\tau > 0$ of (4.1):

$$\frac{U^n - U^{n-1}}{\tau} + 4\pi^2 \xi^2 U^n = 2 \left(\ln(I(U^n)) + \frac{Eq(t)}{I(U^n)} \right), \quad U^0 = 0 \quad (4.2)$$

is fitted to the initial singularity while implicitation of the second order term needs no supplementary computation.

Easy improvements correspond to the use of higher order approximation (e.g. Runge-Kutta) method instead of Euler scheme.

PROPOSITION 4.1. *The sequence $(R^n) = (u^n(0)) = I(U^n)$ is recursively defined by:*

$$\begin{cases} R^n = \alpha^n + \sqrt{\tau}g^n, & n \geq 1 \\ \alpha^n = \int_{\mathbb{R}} \frac{U^{n-1}}{1 + 4\pi^2\xi^2\tau} d\xi = \sqrt{\tau} \sum_{k=1}^{n-1} \theta_{n-k+1} g^k, & U^0 = 0 \\ g^n = \ln(\alpha^n + \sqrt{\tau}g^n) + \frac{Eq(n\tau)}{\alpha^n + \sqrt{\tau}g^n}, & n \geq 1, \end{cases}$$

where $\theta_{p+1} = \frac{2p-1}{2p} \theta_p = \frac{C_{2p-1}^p}{2^{2p-1}} \theta_1$ and $\theta_1 = 1$.

Remark. *The Euler implicit scheme for the equivalent formulation:*

$$\partial_t(e^{4\pi^2\xi^2t}U(t)) = 2e^{4\pi^2\xi^2(t-\tau)}f(t, I(u(t))), \quad U(0) = 0$$

leads to the recursive formula:

$$U^n = \sum_{k=1}^n e^{-4\pi^2\xi^2(n+1-k)\tau} \cdot 2f(k\tau, I(U^k)), \quad R^n = I(U^n) = \frac{\tau}{\sqrt{\pi}} \sum_{k=1}^n \frac{f(k\tau, I(U^k))}{\sqrt{(n+1)\tau - k\tau}},$$

i. e. to the right rectangle formula for (1).

The determination of the sequence (R^n) consists in successive resolutions of the equation (4.3-a) and actualisations (4.3-b):

$$\begin{cases} \Phi(g^n) = g^n - \ln(\alpha^n + \sqrt{\tau}g^n) - \frac{Eq(n\tau)}{\alpha^n + \sqrt{\tau}g^n} = 0 & \text{(a)} \\ \alpha^n = \sqrt{\tau} \sum_{k=1}^{n-1} \theta_{n+1-k} g^k. & \text{(b)} \end{cases} \quad (4.3)$$

As $\text{sgn}(\partial_g^2\Phi_n(g)) = \text{sgn}((\alpha^n + \sqrt{\tau}g) - 2Eq^n)$, Φ_n is concave on $] -\frac{\alpha_n}{\sqrt{\tau}}, \frac{2Eq^n + \alpha_n}{\sqrt{\tau}}[$ and convex on $] \frac{2Eq^n + \alpha_n}{\sqrt{\tau}}, \infty[$ hence, except if $R^n = 2Eq^n$, a monotone convergence of Newton iterations for initial values $g_0^n = g^{n-1}$ near from g^n (τ small enough).

PROPOSITION 4.2. *The equation (4.3-a) admits*

- no solution if $q^n = 0$ and $\alpha_n < \sqrt{\tau}(1 - \ln\sqrt{\tau})$,
- one maximal solution $g^n = \sup\{g; \Phi_n(g) < 0\}$ in any other case.

Non maximal solutions g are such that $\alpha_n + \sqrt{\tau}g \leq \sqrt{\tau}$ independently of α_n .

Proof. If $Eq^n > 0$, $\Phi_n(g) \rightarrow \pm\infty$ as $g \rightarrow \infty$ or $-\frac{\alpha_n}{\sqrt{\tau}}$ and the conclusion follows monotonicity properties of Φ_n .

If $Eq^n = 0$, the function Φ_n is minimal with value $1 - \ln\sqrt{\tau} - \frac{\alpha_n}{\sqrt{\tau}}$ at $1 - \frac{\alpha_n}{\sqrt{\tau}}$.

The last assertion is a consequence of inequalities $\alpha_n + \sqrt{\tau}(1 - \frac{\alpha_n}{\sqrt{\tau}})$, $\alpha_n + \sqrt{\tau}g_+^n \leq \sqrt{\tau}$, g_+^n the upper zero of Φ'_n . ■

Non maximal solutions (if there), obviously non intrinsic, are considered as parasite values and neglected in the sequel.

The occurrence $\alpha_n < \sqrt{\tau}(1 - \ln\tau)$, when $Eq^n = 0$, delimits the life interval of the flame and defines the (eventual) discrete quenching time $n_q\tau$.

The analysis of the sequence (R^n) is based upon evaluations related to the sequence (θ_n) and estimates related to the recursive equation (4.3-a). Such estimates are mainly dependant on sign properties of this function:

If $Eq^n \geq \frac{1}{e} f(n\tau, \cdot)$, decreasing on $]0, Eq^n[$ and increasing on $]Eq^n, \infty[$, is non negative. Otherwise it admits 2 zeros $\alpha_-(Eq^n) < \alpha_+(Eq^n)$ such that

$$0 < \alpha_-(Eq^n) < \frac{Eq^n}{-\ln(Eq^n)} < Eq^n < \alpha_+(Eq^n) < 1.$$

We summarize:

PROPOSITION 4.3. *The solution g^n of equation (4.3-a) satisfies:*

- If $Eq^n = 0$ and $\alpha_n \geq \sqrt{\tau}(1 - \ln \tau)$, $1 - \frac{\alpha_n}{\sqrt{\tau}} < g^n < \frac{\alpha_n \ln(\alpha_n)}{\alpha_n - \sqrt{\tau}}$
- If $Eq^n > 1/e$, $g^n \geq \ln(Eq^n) + 1$
- If $\frac{\sqrt{\tau}}{4} < Eq^n < \frac{1}{e}$:

- for $\alpha_n \leq \alpha_-(Eq^n)$, $0 < g^n < \frac{\alpha_-(Eq^n) - \alpha_n}{\sqrt{\tau}}$ and $\alpha_n \leq r^n \leq \alpha_-(Eq^n)$,

- for $\alpha_-(Eq^n) \leq \alpha_n \leq \alpha_+(Eq^n)$, $\frac{\alpha_-(Eq^n) - \alpha_n}{\sqrt{\tau}} \leq g^n \leq 0$ and $\alpha_-(Eq^n) \leq r^n \leq \alpha_n$,

- for $\alpha_n \geq \alpha_+(Eq^n)$, $g^n \geq \frac{\alpha_+(Eq^n) - \alpha_n}{\sqrt{\tau}}$ and $r^n \geq \alpha_+(Eq^n)$.

Under the condition $t^{1/2-\varepsilon} = O(Eq(t))$, $g^1 = g^1(\tau) \sim \frac{\sqrt{Eq(\tau)}}{\tau^{1/4}}$ as τ tends to 0.

Proof. The assertions follow the study of the sign of $\Phi_n(g^n)$ in the different cases.

As a significative exemple the last one is a consequence of, given $c > 0$,

$$\operatorname{sgn} \left(\Phi_1 \left(\frac{c\sqrt{Eq(\tau)}}{\tau^{1/4}} \right) \right) = \operatorname{sgn} \left((c - 1/c) \frac{\sqrt{Eq(\tau)}}{\tau^{1/4}} - \ln \left(\frac{c\sqrt{Eq(\tau)}}{\tau^{1/4}} \right) \right) = \operatorname{sgn}(c - 1/c)$$

for τ small enough. ■

The discrete scheme enjoys the same consequences of comparison principles (on which the proof of existence of a threshold was based) as the problem (3.1). These properties are narrowly associated with the existence of a diffusive formulation:

PROPOSITION 4.4. *The dependances of (u^n) , (α_n) and (R^n) on (Eq^n) are monotone.*

Proof. Let $(u_i^n)_{n \leq n_i}$, $i = 1, 2$ the sequence associated with $(E_i q_i^n)$ where $E_1 q_1^n \leq E_2 q_2^n$ any n .

Let $w^n = u_1^n - u_2^n$ and $\omega_n = \operatorname{supp} w_+^n$. Then using w_+^n as a test function in the equation verified by w^n :

$$\begin{aligned} \|w_+^n\|^2 - \int_{\omega_n} (w_+^{n-1})^2 dx + \int_{\omega_n} (w_+^n - w_+^{n-1})^2 dx + 2\tau \int_{\omega_n} |\partial_x w_+^n|^2 dx &\leq \frac{4\tau}{u_2^n(0)} (w_+^n(0))^2, \\ \left(1 - \frac{4\tau}{u_2^n(0)^2}\right) \|w_+^n\|^2 + \int_{\omega_n} (w_+^n - w_+^{n-1})^2 dx &\leq \int_{\omega_n} (w_+^{n-1})^2 dx, \end{aligned}$$

and, as long as $u_2^n(0) > 2\sqrt{\tau}$ (see Proposition 4.3), $w_+^n = 0$. The other comparison results derive from $R^n = u^n(0)$, and from the interpretation of α_n as value at $x = 0$ of the solution of

$$v - \partial_x^2 v = u^{n-1}.$$

■

The dependance of estimates for the sequence (R^n) on estimates for (g^n) may be emphasized:

PROPOSITION 4.5. *There exists two positive constants c_{\pm} such that any pair (G_-, G_+) of C^1 -positive functions such that $G_-(n\tau) \leq g^n = g_\tau^n \leq G_+(n\tau)$, given $n\tau$, one has, up to an $O(\tau)$ term:*

$$c_- \int_0^{n\tau} \frac{G_-(s) ds}{\sqrt{n\tau - s}} \leq r^n \leq c_+ \int_0^{n\tau} \frac{G_+(s) ds}{\sqrt{n\tau - s}}.$$

Proof. From classical asymptotics, with C the Euler constant and ζ the Riemann function:

$$-\ln(\sqrt{n}) - \frac{C}{2} - \frac{\zeta(2)}{4} - o(1) < \ln(\theta_n) < -\ln(\sqrt{n}) - \frac{C}{2} - o(1)$$

so that, any n : $\frac{c_-}{\sqrt{n}} < \theta_n < \frac{c_+}{\sqrt{n}}$ and the conclusion follows:

$$\left| \tau \sum_{k=1}^n \frac{G_{\pm}(k\tau)}{\sqrt{(n+1)\tau - k\tau}} - \int_0^{n\tau} \frac{G_{\pm}(s)}{\sqrt{(n+1)\tau - s}} \right| \leq \tau \cdot (n\tau) \cdot \sup |G'_{\pm}|.$$

■

5. GENERIC EVOLUTIONS AND APPROXIMATION

Keeping in mind the fact that, when $\text{supp } q = \mathbb{R}_+$, any solution (R^n) is global, we shall be only concerned with cases of compactly supported excitations Eq and in fact by excitations such that, any n in the domain of (R^n) , g^n , hence (α_n) is nonnegative, so that, any n , $\alpha_{n+1} \leq \alpha_n + \frac{1}{2}g^n$.

PROPOSITION 5.1. *If Eq is such that:*

- $Eq(t) \geq 1/e$ on $[T_1, T_2]$,
- $Eq(t)$ is increasing and $Eq(t) < 1/e$ on $[0, T_1]$,
- $Eq(t) \geq At^{1/2-\varepsilon}$ near 0,
- then $g^n \geq 0$ for $n\tau \leq T_2$ and $g^n < Eq^n$ for $n\tau \leq T_1$.

Proof. From equality $\Phi_1 \left(\frac{\sqrt{Eq^1}}{\tau^{1/4}} \right) = -\ln \left(\tau^{1/4} \sqrt{Eq^1} \right)$, $\alpha_2 < \frac{1}{2}\tau^{1/4} \sqrt{Eq^1}$ so that $\alpha_2 < \alpha_-(Eq^1) < \alpha_-(Eq^2)$ and $g^2 > 0$.

Let us suppose $0 < \alpha_k < \alpha_-(Eq^k)$ hence $g^k > 0$, $k\tau = \tau \dots, n\tau < T_1$. Then

$$\Phi_n \left(\frac{\alpha_-(Eq^n) - \alpha_n}{\sqrt{\tau}} \right) = \frac{\alpha_-(Eq^n) - \alpha_n}{\sqrt{\tau}} > 0 \text{ and } 0 < g^n < \frac{\alpha_-(Eq^n) - \alpha_n}{\sqrt{\tau}}, \text{ so}$$

that

$$\alpha_{n+1} < \alpha_n + \frac{1}{2\sqrt{\pi}}(\alpha_-(Eq^n) - \alpha_n) < \alpha_-(Eq^n) < \alpha_-(Eq^{n+1}).$$

For $T_1 \leq n\tau \leq T_2$, one gets $g^n > \ln(Eq^n) + 1 \geq 0$.

$$\text{As } \ln(\sqrt{\tau}\sqrt{Eq^1}) + \frac{\sqrt{Eq^1}}{\sqrt{\tau}} > 0, \alpha^1 = \sqrt{\tau}g^1 < \alpha_-(Eq^1) \text{ and } 0 < g^1 < \frac{\alpha_-(Eq^1) - \alpha_1}{\sqrt{\tau}},$$

so that

$$0 < \alpha_2 < \frac{\alpha_1 + Eq^1}{2} < Eq^2.$$

Let us suppose $0 < \alpha_k < \alpha_-(Eq^k) < Eq^k < 1/e$, $k = 1, \dots, n$.

Then $0 < g^n < \frac{\alpha_-(Eq^n) - \alpha_n}{\sqrt{\tau}}$ and

$$0 < \alpha_{n+1} < \alpha_-(Eq^n) < \alpha_-(Eq^{n+1}), \quad g^{n+1} < \alpha_-(Eq^n) < Eq^{n+1}.$$

■

Generic evolutions correspond to (so called generic) excitations Eq with support $[0, T_e]$ such that:

1. $t^{1/2-\varepsilon} = O(Eq(t))$ as $t \rightarrow 0$,
2. $Eq(t) \geq \frac{1}{e}$ on $[T_1, T_2]$,
3. Eq is increasing on $[0, T_1]$,
4. $\sum_k \frac{\ln(Eq^k + 1)}{\sqrt{n_e + 1 - k}} \geq 1$.

PROPOSITION 5.2. *For generic evolutions, two sufficient conditions for $\alpha_{n+1} \geq \alpha_n$ (hence for $R^{n+1} \geq R^n$) are given by:*

$$\begin{aligned} \sqrt{\tau}(\ln(Eq^n) + 1) &\geq \frac{\alpha_n}{2} \text{ if } Eq^n \geq 1/e, \\ \sqrt{\tau}\alpha_n^2 - \alpha_n \ln\left(\frac{3\alpha_n}{2}\right) &\leq \frac{4Eq^n}{3} \text{ if } Eq^n \geq \frac{\sqrt{\tau}}{4}. \end{aligned}$$

Proof. For a non negative sequence (g^n) , $\alpha_{n+1} - \alpha_n \geq -\frac{\alpha_n}{4} + \frac{\sqrt{\tau}g^n}{2}$ and a sufficient condition for $\alpha_{n+1} \geq \alpha_n$ is, when $Eq^n \geq \frac{\sqrt{\tau}}{4}$, $\frac{3\sqrt{\tau}\alpha_n^2}{2} - \frac{3\alpha_n}{2} \ln\left(\frac{3\alpha_n}{2}\right) - Eq^n \leq 0$. ■

The asymptotic comportement of R^1 may be globalized:

PROPOSITION 5.3. *For generic evolutions, there exists two positive constants C_{\pm} and t_0 such that, if $n\tau \leq t_0$,*

$$C_-(n\tau)^{1/4} \sqrt{Eq(n\tau)} \leq R^n \leq C_+(n\tau)^{1/4} \sqrt{Eq(n\tau)}$$

Proof. Let us suppose $Cs^{1/4} \sqrt{Eq(s)} \leq Eq(s) < 1/e$ on $[0, t_0]$ and (Proposition 4.3) for $k = 1, \dots, n$:

$$\lambda C(n\tau)^{1/4} \sqrt{Eq(k\tau)} \leq R^k \leq C(n\tau)^{1/4} \sqrt{Eq(k\tau)}. \quad (5.1)$$

Then, as under the last condition $\partial_{R^k} g^k \leq 0$,

$$\begin{aligned} \ln\left(\lambda C(k\tau)^{1/4} \sqrt{Eq(k\tau)}\right) + \frac{\sqrt{Eq(k\tau)}}{C(k\tau)^{1/4}} &\leq g^k \leq \ln\left(\lambda C(k\tau)^{1/4} \sqrt{Eq(k\tau)}\right) + \\ &+ \frac{\sqrt{Eq(k\tau)}}{\lambda(k\tau)^{1/4}}. \end{aligned}$$

The sufficient condition for (5.1), $k = n$:

$$\begin{aligned} \lambda C(k\tau)^{1/4} \sqrt{Eq(k\tau)} - \sqrt{\tau}f\left(n\tau, \lambda C(k\tau)^{1/4} \sqrt{Eq(k\tau)}\right) &\geq \alpha_n \geq \\ \geq C(k\tau)^{1/4} \sqrt{Eq(k\tau)} - \sqrt{\tau}f\left(n\tau, \lambda C(k\tau)^{1/4} \sqrt{Eq(k\tau)}\right) \end{aligned}$$

is then implied by

$$\begin{aligned} \lambda \left(C^2(n\tau)^{1/4} - \frac{\sqrt{\tau}}{(n\tau)^{1/4}} \right) &\geq \sqrt{\tau} \sum \theta_{n+1-k} \sqrt{\frac{Eq(k\tau)}{Eq(n\tau)}}, \\ \lambda \left(C^2(n\tau)^{1/4} - \frac{\sqrt{\tau}}{(n\tau)^{1/4}} \right) &\leq \sqrt{\tau} \sum \theta_{n+1-k} \sqrt{\frac{Eq(k\tau)}{Eq(n\tau)}} + \eta(\lambda, C), \end{aligned}$$

where $\eta(\lambda, C) = \frac{1}{\sqrt{Eq(n\tau)}} \left[\sqrt{\tau} \ln \lambda C(n\tau)^{1/4} + \sqrt{\tau} \sum \theta_{n+1-k} \ln \left(C(k\tau)^{1/4} \sqrt{Eq(k\tau)} \right) \right]$,

which are fulfilled under conditions λC and λ respectively large and small enough. ■

PROPOSITION 5.4. *Let us consider the generic excitation Eq with $\text{supp } Eq = [0, T_e]$ then discrete quenching occurs iff there exists $n\tau > T_e$ with $\alpha_n < 1$.*

If any n such that $n\tau > T_e$, $\alpha_n \geq 1 + \eta$, $\eta > 0$, then the solution is global and $\alpha_n \rightarrow \infty$ as $n \rightarrow \infty$.

Proof. i) Under the hypothesis $g^n > 0$ and $\alpha_n > 0$, any $n, n\tau \leq T_e$.

Let $n = \min\{k; k\tau > T_e, \alpha_k < 1\}$. If $\alpha_n \leq 1 - \eta$, $g^n \leq -\frac{\alpha_n}{\alpha_n - \sqrt{\tau}} \eta$, $a_{n+1} < a_n - \frac{\sqrt{\tau}}{2} \eta$ and as g^n is increasing with respect to α_n , by induction $\alpha_{n+k} < \alpha_n - k \frac{\sqrt{\tau}\eta}{2}$, hence quenching occurs before $n + \frac{2\alpha_n}{\sqrt{\tau}\eta}$.

ii) Here, any $n > [T_e/\tau]$:

$$\alpha_n > \sqrt{\tau} \sum_{k=[T_e/\tau]}^n \theta_{n+1-k} \ln(1+\eta) > \sqrt{\tau} \sum_{k=[T_e/\tau]}^n \frac{c_- \ln(1+\eta)}{\sqrt{n+1-k}} > \int_{T_e}^{n\tau} \frac{c_- \ln(1+\eta) ds}{\sqrt{n\tau-s}}.$$

■

As direct consequences of Proposition 5.4:

- For generic compactly supported excitations such that $Eq \leq 1/e$, quenching occurs (in finite time).
- For standard excitations one has the decomposition:

$$\mathbb{R}_+ = \{E; n_q < \infty\} \cup \{E; \liminf_{n \rightarrow \infty} \alpha_n = 1\} \cup \{E; R^n \rightarrow \infty \text{ as } n \rightarrow \infty\}$$

where $\{E; n_q < \infty\} = [0, E_-[$, $\{E; R^n \rightarrow \infty \text{ as } n \rightarrow \infty\} =]E_+, \infty[$, and $\{E; \liminf_{n \rightarrow \infty} \alpha_n = 1\} = \{E; \omega(0) \neq \emptyset\}$.

6. ERROR ESTIMATE FOR STANDARD EVOLUTIONS

The error estimate is derived from that of the semi-discretisation of the reaction-diffusion problem (3.1) and strongly dependant on monotonicity of the nonlinearity in neighbourhoods of its singularities (mainly $t = 0$). Estimates on intervals where the nonlinearity is Lipschitz are easily deduced and correspond only to a modification of the coefficient of amplification. We consider here only estimates near the origin.

Let $f'(t)$ stand for the derivative of $t \rightarrow f(t, I(U(t)))$ and let (U^n) be the solution of the semi-discrete approximation of problem (4.1):

$$\frac{U^n - U^{n-1}}{\tau} + 4\pi^2 \xi^2 U^n = 2f(n\tau, I(U^n)), \quad U^0 = 0. \quad (6.1)$$

The sequence (W^n) defined by $W^n = U(n\tau) - U^n$ satisfies:

$$(1 + 4\pi^2 \xi^2 \tau)W^n = W^{n-1} + \tau \varepsilon^n + 2\tau(f(n\tau, I(U(n\tau))) - f(n\tau, I(U^n))), \quad W^0 = 0, \quad (6.2)$$

with (ε^n) the truncation error:

$$\varepsilon^n = \frac{1}{\tau} \int_{(n-1)\tau}^{n\tau} (U'(s) - U'(n\tau)) ds. \quad (6.3)$$

PROPOSITION 6.1. *There exists an even function α on \mathbb{R}*

$$\frac{2}{2-\tau} \left(1 + 4\pi^2 \xi^2 \frac{\tau}{2-\tau}\right) \leq \frac{1}{\alpha} \leq \frac{4}{2-\tau} \left(1 + 4\pi^2 \xi^2 \frac{\tau}{2-\tau}\right),$$

such that any n with $U^n, U(n\tau) \leq Eq(n\tau)$:

$$I\left(\frac{|W^n|^2}{\alpha}\right) \leq \frac{1}{(1-\tau/2)^{2(n-n_0)}} I\left(\frac{|W^{n_0}|^2}{\alpha}\right) + \tau \sum_{k=n_0+1}^n \frac{1}{(1-\tau/2)^{2(n+1-k)}} I\left(\frac{|\varepsilon^k|^2}{1+4\pi^2 \xi^2}\right).$$

Proof. Under the hypothesis, because then $f(n\tau, \cdot)$ is decreasing, any positive α, β :

$$I((2-\alpha + \tau(8\pi^2 \xi^2 - \beta))|W^n|^2) \leq I\left(\frac{|W^{n-1}|^2}{\alpha}\right) + \tau I\left(\frac{|\varepsilon^n|^2}{\beta}\right).$$

The choice $\beta = 1 + 4\pi^2 \xi^2$, $K = (1 - \tau/2)^2$ gives:

$$2-\alpha + \tau(8\pi^2 \xi^2 - \beta) = \frac{K}{\alpha} \text{ for } \alpha = \frac{1}{2}(2-\tau + 4\pi^2 \xi^2 \tau) \left(1 - \sqrt{1 - \left(\frac{2-\tau}{2-\tau + 4\pi^2 \xi^2 \tau}\right)^2}\right),$$

so that:

$$4 \frac{2-\tau + 4\pi^2 \xi^2}{(2-\tau)^2} \geq \frac{1}{\alpha} \geq 2 \frac{2-\tau + 4\pi^2 \xi^2}{(2-\tau)^2}.$$

One gets now by induction:

$$I\left(\frac{|W^n|^2}{\alpha}\right) \leq \frac{1}{K^{n-n_0}} I\left(\frac{|W^{n_0}|^2}{\alpha}\right) + \tau \sum_{k=n_0+1}^n \frac{1}{K^{n+1-k}} I\left(\frac{|\varepsilon^k|^2}{1+4\pi^2\xi^2}\right).$$

Error estimate is then a consequence of evaluation of the truncation error ($|\varepsilon^n|$). ■

LEMMA 6.2. *Let f be C^1 on $[t_0, N\tau]$ and U denote the solution of*

$$\frac{d}{dt}u + 4\pi^2\xi^2u = 2f, \quad u(0) = 0.$$

Then the semi-discretization error of truncature:

$$\varepsilon^n = \frac{1}{\tau} \int_{(n-1)\tau}^{n\tau} (U'(n\tau) - U'(s)) ds$$

satisfies the estimate:

$$|\varepsilon^n| \leq \chi\tau \frac{e^{-\chi((n-1)\tau-\theta)}}{2(1+\chi\tau/2)^2} |u'(\theta)| + 4\tau \left[\frac{\chi((n-1)\tau-\theta)}{1+\chi((n-1)\tau-\theta)/2} + 1 \right] \frac{\sup |f'(\sigma)|}{(1+\chi\tau)}.$$

Proof. With $\chi = 4\pi^2\xi^2$ and f' the derivative of $t \rightarrow f(t, I(U(t)))$, the derivative U' of U , as a solution on $]0, T[$ of the equation (2.4), satisfies, any positive t_0 :

$$U'(t) = e^{-\chi(t-\theta)}U'(\theta) + \int_{t_0}^t e^{-\chi(t-s)}f'(s) ds.$$

It follows the decomposition of ε^n :

$$\begin{aligned} \varepsilon^n &= \frac{1}{\tau} \int_{(n-1)\tau}^{n\tau} (A_1^n(s) + A_2^n(s) + A_3^n(s)) ds, \\ |A_1^n(s)| &= (e^{-\chi(s-\theta)} - e^{-\chi(n\tau-t_0)})|U'(t_0)|, \\ |A_2^n(s)| &= 2 \left| \int_{t_0}^s e^{-\chi(n\tau-\sigma)} - e^{-\chi(s-\sigma)} f'(\sigma) d\sigma \right|, \\ |A_3^n(s)| &= 2 \left| \int_s^{n\tau} e^{-\chi(n\tau-\sigma)} f'(\sigma) d\sigma \right|. \end{aligned}$$

Direct integration of these functions give:

$$\begin{aligned} |\varepsilon^n| &\leq \chi\tau e^{-\chi((n-1)\tau-t_0)} \frac{1 - e^{-\chi\tau} - \chi\tau e^{-\chi\tau}}{(\chi\tau)^2} |u'(t_0)| + \\ &\quad + 4\tau \frac{\chi\tau - 1 + e^{-\chi\tau}}{(\chi\tau)^2} \sup |f'(\sigma)| \end{aligned}$$

and from inequalities for positive c :

$$\begin{aligned} 0 \leq \frac{1 - e^{-c}}{c} &\leq \frac{1}{1+c/2}, \quad 0 \leq \frac{e^{-c} + c - 1}{c^2} \leq \frac{1}{1+c}, \\ \frac{1 - e^{-c} - ce^{-c}}{c^2} &\leq \frac{1}{2(1+c/2)^2}, \\ \frac{|\varepsilon^n|^2}{1+\chi} &\leq \tau \frac{\chi}{1+\chi} \frac{\chi\tau e^{-2\chi((n-1)\tau-\theta)}}{2(1+\chi\tau/2)^4} |y'(\theta)|^2 + \\ + \frac{4\tau^2}{1+\xi} &\left[\left(\frac{\chi((n-1)\tau-\theta)}{1+\chi((n-1)\tau-\theta)/2} \right)^2 + 1 \right] \left(\frac{\sup |f'(\sigma)|}{1+\chi\tau} \right)^2. \end{aligned}$$

■

THEOREM 6.3. *Let Eq a generic excitation.*

Any positive $t_0 < n\tau < T$, one has the asymptotical majoration:

$$\begin{aligned} & |R(n\tau) - R^n|^2 \leq \\ & \leq \sqrt{\frac{2}{\tau}} \left[e^{(n-n_0)\tau} I \left(\frac{|W^{n_0}|^2}{\alpha} \right) + \frac{\tau^2}{2} I \left(\frac{\chi^2}{1+\chi} |U'(t_0)|^2 \right) + 16(n-n_0)\tau^2 \sup |f'(\sigma)|^2 \right]. \end{aligned}$$

Proof. The previous lemma furnishes:

$$\frac{|\varepsilon^n|^2}{1+\chi} \leq \frac{\tau^2 \chi^2 e^{-2\chi(n-1-n_0)\tau}}{2(1+\chi)(1+\chi\tau/2)^4} |U'(t_0)|^2 + \frac{38\tau^2}{(1+\chi)(1+\chi\tau)^2} \sup |f'(\sigma)|^2,$$

which, combined with Proposition 6.1 gives the estimate

$$\begin{aligned} I \left(\frac{|W^n|^2}{\alpha} \right) & \leq \frac{1}{(1-\tau/2)^{2(n-n_0)}} I \left(\frac{|W^{n_0}|^2}{\alpha} \right) + \\ & + I \left(\frac{\tau^2 \chi^2}{2(1+\chi)(1+\chi\tau/2)^4} \tau \sum_{k=0}^{n-n_0-1} \left(\frac{e^{-\chi\tau}}{1-\tau/2} \right)^{2k} |U'(t_0)|^2 \right) + \\ & + 32\tau^2 \tau \sum_{k=0}^{n_0-1} \frac{1}{(1-\tau/2)^{2k}} \sup |f'(\sigma)|^2 I \left(\frac{1}{1+\chi} \right), \end{aligned}$$

and up to a $\tau^2.o(1)$ term,

$$\begin{aligned} & I \left(\frac{|W^n|^2}{\alpha} \right) \leq \\ & \leq e^{(n-n_0)\tau} I \left(\frac{|W^{n_0}|^2}{\alpha} \right) + \frac{\tau^2}{2} I \left(\frac{\chi^2}{1+\chi} |U'(t_0)|^2 \right) + 16(n-n_0)\tau \tau^2 \sup |f'(\sigma)|^2. \end{aligned}$$

On the other hand,

$$|I(W^n)|^2 \leq I \left(\frac{|W^n|^2}{\alpha} \right) I(\alpha) \leq \frac{(2-\tau)^{3/2}}{2\sqrt{\tau}} I \left(\frac{|W^n|^2}{\alpha} \right).$$

■

The subsequent simulations are related to the typical cases of generic evolutions:

- $q(t) = t^{0.3}(1-t)$, $t_{\max} = 10$, 500 steps, $E = 7.7$ (Fig. 1): quenching,
- $q(t) = t^{0.3}(1-t)$, $t_{\max} = 40$, 1000 steps, $E = 7.8$ (Fig. 2): development,
- $q(t) = t^{0.3}$, $t_{\max} = 40$, 1000 steps, $E = 7.7$ (Fig. 3),
- $q(t) = t^{0.3}$, $t_{\max} = 40$, 1000 steps, $E = 7.8$ (Fig. 4).

It is worth to be noticed that, in these cases, the substitution of asymptotics to the solution of the scheme during the very initiation (from two to six steps) of the flame does not perturb notably the subsequent evolution.

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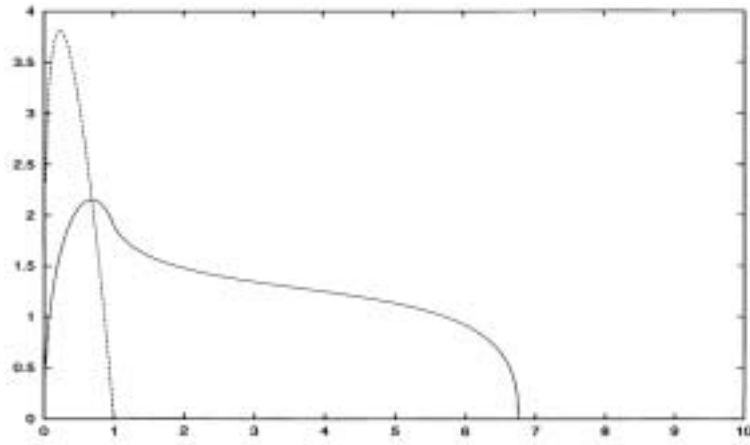


FIGURE 1. Excitation (dots) - Radius

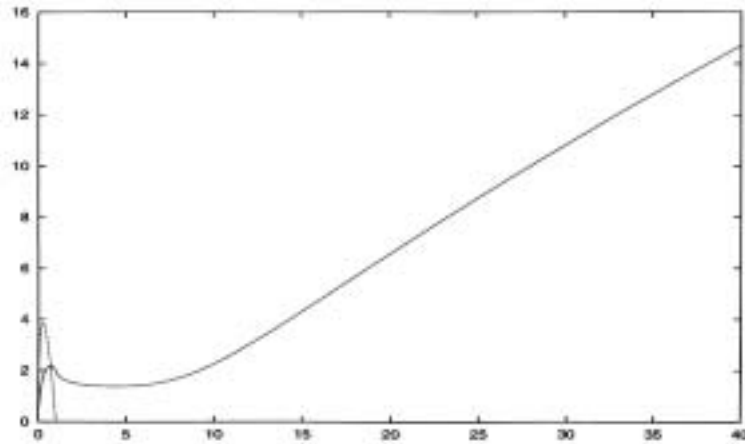


FIGURE 2. Excitation (dots) - Radius

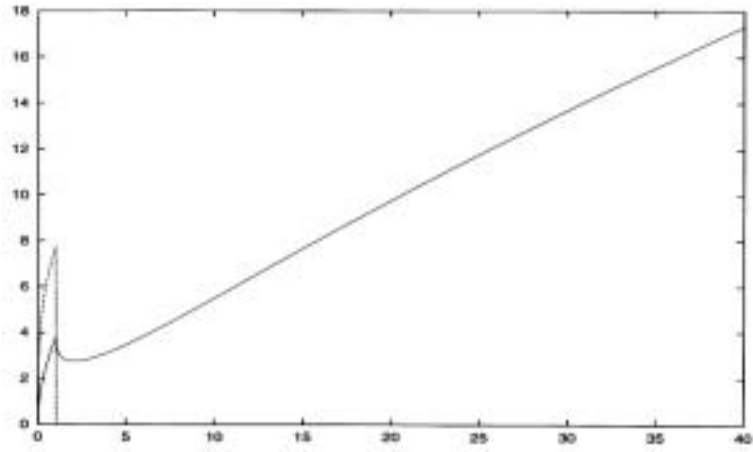


FIGURE 3. Excitation (dots) - Radius

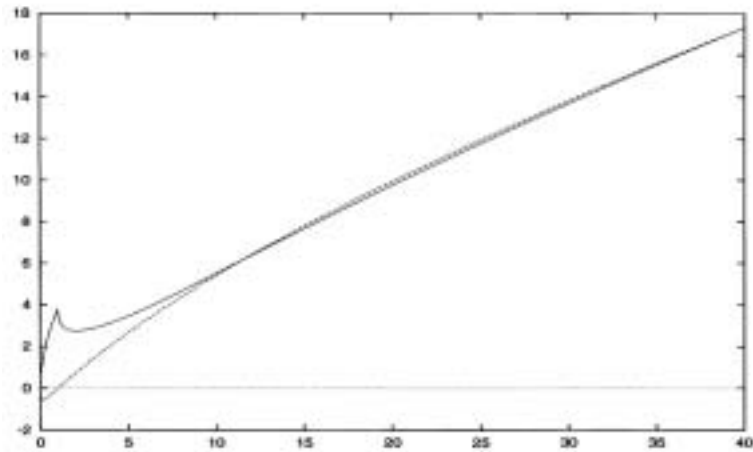


FIGURE 4. Radius asymptot. (dots) - Radius

