Equations aux dérivées partielles/ Partial Differential Equations
Problèmes Mathématiques de la Mécanique/Mathematical Problems in Mechanics

Mathematical justification of a nonlinear integro-differential equation for the propagation of spherical flames

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Abstract. This note is devoted to the justification of an asymptotic model for quasisteady three-dimensional spherical flames proposed by G. Joulin [7]. The paper [7] derives, by means of a three-scale matched asymptotic expansion, starting from the classical thermo-diffusive model with high activation energies, an integro-differential equation for the flame radius. In the derivation, it is essential for the Lewis Number - i.e. the ratio between thermal and molecular diffusion - to be strictly less than unity. In this note, we give the main ideas of a rigorous proof of the validity of this model, under the additional restriction that the Lewis number is close to 1.

Justification mathématique d'une équation intégro-différentielle non linéaire pour un modèle de flamme sphérique

Abstract. Nous donnons dans cette note les grandes lignes de la justification mathématiquement rigoureuse d'un modèle intégro-différentiel non linéaire d'évolution du rayon d'une flamme sphérique initialement proposé par G. Joulin dans [7]. Cette équation est obtenue dans le cadre du modèle thermo-diffusif tridimensionnel aux hautes énergies d'activation, avec nombre de Lewis strictement plus petit que 1. Nous montrons dans cette note la validité du modèle sous la restriction supplémentaire que le nombre de Lewis est assez proche de 1.

Version française abrégée

Considérons le modèle thermo-diffusif tridimensionnel pour la propagation des flammes prémélangées. Dans l'hypothèse de la chimie simple $A \to B$ et des hautes énergies d'activation, celui-ci s'écrit [2], [4]:

$$\left\{\begin{array}{rl} T_t - \Delta T = & Y f_\varepsilon(T) \\ Y_t - \dfrac{\Delta Y}{Le} = & -Y f_\varepsilon(T) \end{array}\right. \qquad ((t,x) \in I\!R_+ \times I\!R^3) \tag{0.1}$$

auquel nous adjoignons les conditions aux limites suivantes:

$$T(t, r = +\infty) = 0, \qquad Y(t, r = +\infty) = 1. \tag{0.2}$$

Les notations sont classiques: $T(t,x)$ est la température, $Y(t,x)$ la fraction massique du réactant. Le réel $Le > 0$ est le nombre de Lewis, i.e. le rapport des diffusions thermiques et moléculaires. La fonction $f_\varepsilon(T)$ est le terme d'Arrhénius classique $f_\varepsilon(T) = \dfrac{1}{\varepsilon^2} \exp \dfrac{T - Le^{-1}}{\varepsilon}$ pour T proche de

Le^{-1}. Le réel $\varepsilon > 0$ représente l'inverse de l'énergie d'activation normalisée. On suppose de plus que f_ε s'annule pour $T \leq \theta$, avec $0 < \theta < Le^{-1}$.

On fait dans toute cette Note l'hypothèse de la symétrie sphérique. *Dans une importante contribution à la compréhension de (0.1)-(0.2), G. Joulin [7] identifie une échelle de temps caractéristique de l'ordre de ε^{-2} lorsque $Le < 1$. Il obtient de façon formelle, via un développement asymptotique à trois échelles, une équation asymptotique pour $\rho_\varepsilon(\tau) := R_\varepsilon(\tau/\varepsilon^2)$, où $R_\varepsilon(t)$ est le rayon de la flamme à l'instant t - i.e. le plus petit rayon pour lequel $T(t,.) - Le^{-1}$ est d'ordre $\varepsilon Log\varepsilon$:*

$$(1 - \sqrt{Le})\partial_{1/2}\rho = 2LeLog(\sqrt{Le^3}\rho) + \phi(\tau) \tag{0.3}$$

où $\phi(\tau)$ est un terme de forçage dépendant de la donnée initiale. L'opérateur $\partial_{1/2}$ est la dérivée fractionnaire classique: pour une fonction $\rho(\tau)$ de classe C^1, on note

$$\partial_{1/2}\rho(\tau) = \frac{1}{\sqrt{\pi}} \int_0^\tau \frac{\dot{\rho}(s)}{\sqrt{\tau - s}}\, ds. \tag{0.4}$$

Nous décrivons dans cette Note le résultat suivant, dont les preuves détaillées feront l'objet d'un article ultérieur.

RESULTAT PRINCIPAL. On choisit $Le = 1 - \delta$ avec $0 < \delta < 1$, et $\varepsilon > 0$ petit, indépendamment de δ. Notons $\tau = \varepsilon^2 t$. Il existe: $\delta_0 > 0$, $\varepsilon_0 > 0$, une classe de données initiales $(T_0^\varepsilon, Y_0^\varepsilon)_{0<\varepsilon\leq\varepsilon_0}$, et une fonction $\phi_\varepsilon(\tau)$ proche de la fonction $\phi(\tau)$ de (0.3), une solution $\rho(\tau)$ de (0.3) de temps de vie $\tau_{max} > 0$ tels que:
- si $0 < \delta < \delta_0$, $0 < \varepsilon < \varepsilon_0$, et $0 < \tau_0 < \tau_{max}$,
- et si $(T^\varepsilon(t,r), Y^\varepsilon(t,r))$ est la solution de (0.1) issue de $(T_0^\varepsilon, Y_0^\varepsilon)$,
on a $|R_\varepsilon(\tau/\varepsilon^2) - \rho(\tau)| = O(\varepsilon)$ pour $\tau \in [0, \tau_0]$.

La démonstration de ce résultat utilise les trois ingrédients suivants:

- l'existence et l'analyse de stabilité d'une classe particulière de solutions stationnaires de (0.1) (flammes en boules de Zeldovich);

- la construction, en suivant les idées développées dans [7], d'une solution approchée $(T_J^\varepsilon, Y_J^\varepsilon)$ de (0.1)-(0.2) dont le rayon vérifie (0.3) à ε près,

- une analyse précise de la distance entre la solution $(T_J^\varepsilon, Y_J^\varepsilon)$ et la solution $(T^\varepsilon, Y^\varepsilon)$ de (0.1) de donnée initiale $(T_0^\varepsilon, Y_0^\varepsilon)$, à l'aide du premier point et d'estimations sur l'opérateur d'évolution engendré par la version linéarisée de (0.1) autour de $(T_J^\varepsilon, Y_J^\varepsilon)$.

English version

1. INTRODUCTION. In an important contribution [7], G. Joulin derives, in a formal way, a nonlinear integro-differential equation describing the evolution of the radius of a spherical flame, in the context of the thermo-diffusive model for flame propagation with high activation energies. The goal of this note is to give the main steps of a mathematically rigorous proof of this derivation. One of the motivations for doing this - besides the fact that the model has an interest of its own - is that Joulin's derivation can be carried out for a large class of models; see for instance [3] or [8]. Hence it can be expected that the methods devised here have some degree of generality.

We consider the evolution equations for a gaseous mixture with simple chemistry $A \to B$ in the whole space $\mathbb{R}^3$ [2], [4]:

$$\left\{ \begin{aligned} T_t - \Delta T &= Y f_\varepsilon(T) \\ Y_t - \frac{\Delta Y}{Le} &= -Y f_\varepsilon(T) \end{aligned} \right. \qquad ((t,x) \in \mathbb{R}_+ \times \mathbb{R}^3) \tag{1.1}$$

to which we append the following conditions at $|x| = +\infty$:

$$T(t, r = +\infty) = 0, \qquad Y(t, r = +\infty) = 1. \tag{1.2}$$

The notations are classical: $T(t,x)$ is the temperature, $Y(t,x)$ is the mass fraction of the reactant A. The number $Le > 0$ is the Lewis number, i.e. the ratio between thermal and molecular diffusion. The function $f_\varepsilon(T)$ is the classical Arrhenius term

$$f_\varepsilon(T) = \frac{1}{\varepsilon^2} \exp \frac{T - Le^{-1}}{\varepsilon} \tag{1.3}$$

for T close to Le^{-1}. To avoid the cold boundary difficulty, the function f_ε is assumed to vanish for $T \leq \theta$, with $0 < \theta < Le^{-1}$. The only slight difference with the most classical expressions is that, here, the flame temperature has been normalized to Le^{-1}.

In the whole work, the assumption of spherical symmetry will be made. This allows us to define, for all time $t > 0$, the radius of the flame $R_\varepsilon(t)$; namely: the smallest $r > 0$ such that $T(t,x) = Le^{-1} + 100\varepsilon \mathrm{Log}\varepsilon$ if $|x| = r$. The paper [7] derives, by means of a three-scale formal matched asymptotic expansion, an asymptotic equation for $\rho_\varepsilon(\tau) := R_\varepsilon(\tau/\varepsilon^2)$; namely:

$$(1 - \sqrt{Le})\partial_{1/2}\rho = 2Le\mathrm{Log}(\sqrt{Le^3}\rho) + \phi(\tau) \tag{1.4}$$

where $\phi(\tau)$ is a forcing term depending on the initial datum. The operator $\partial_{1/2}$ is the classical fractional derivative of order $1/2$; for a C^1 function $\rho(\tau)$ it is defined by (0.4).

It appears that equation (1.4) can be locally ill-posed for $Le > 1$, whereas it is always locally well-posed when $Le < 1$ - a deeper analysis [1] reveals that the only obstacle for global well-posedness is finite time quenching, which is indeed shown to be possible. We shall explain why it is essential to have $Le < 1$ in the course of the note. It is to be noted that the situation differs drastically from the case $Le = 1$. See [5] for a general multi-dimensional study, and the references therein.

The plan of the note is therefore to state the main result - Section 2 -, then to give a stability result explaining why one must have $Le < 1$ - Section 3 -. Subsequently, following Joulin's idea, we construct an approximate solution to (1.1)-(1.2) - Section 4 -, whose radius satisfies (1.4) up to $O(\varepsilon)$ errors. Finally we explain why the true and approximate solutions are ε^2-close to each other.

2. THE ZELDOVICH FLAME BALL AND MAIN RESULT. The Zeldovich flame ball is a particular nondegenerate steady solution of (1.1). Namely: if w is a parameter, we look for a solution $(T_w^\varepsilon, Y_w^\varepsilon)$ of

$$\left\{ \begin{array}{rl} -\Delta T = & Y f_\varepsilon(T) \\ -\dfrac{\Delta Y}{Le} = & -Y f_\varepsilon(T) \end{array} \right. \qquad (\mathbb{R}^3) \tag{2.1}$$

$$T(r = +\infty) = \varepsilon w, \qquad Y(r = +\infty) = 1. \tag{2.2}$$

PROPOSITION 1. *For any given $M > 0$ large enough, there is $\varepsilon_0 > 0$ such that, for all $\varepsilon \leq \varepsilon_0$, Problem (2.1)-(2.2) has a unique solution $(T_w^\varepsilon, Y_w^\varepsilon)$, which is C^2 with respect to w - in the topology of $C^2(\mathbb{R}^3)$, and whose radius is between $\dfrac{1}{M}$ and M. If $R_{\varepsilon,w}$ is the radius of this solution we have* $\lim_{\varepsilon \to 0} R_{\varepsilon,w} = \sqrt{Le^{-3}} \exp(-w/2)$.

MAIN RESULT. *Set $Le = 1 - \delta$ with $0 < \delta < 1$. Let $(T^\varepsilon(t,r), Y^\varepsilon(t,r))$ be a solution of (1.1), with initial datum $(T_0^\varepsilon, Y_0^\varepsilon)$ such that*

[i] there exist $w_0 \in \mathbb{R}$, $\nu \in (0,1)$ and a constant $C > 0$, such that:

$$|(T_0^\varepsilon, Y_0^\varepsilon)(x) - (T_{w_0}^\varepsilon, Y_{w_0}^\varepsilon)(x)|_\infty \leq C\varepsilon^3 \quad \text{for } |x| \leq \varepsilon^{-\nu},$$

[ii] $(T_0^\varepsilon, Y_0^\varepsilon)$ converges to $(0,1)$ at least as fast as $|x|^{-1}$ as $|x| \to +\infty$.

Set $\tau = \varepsilon^2 t$. There exist $\delta_0 > 0$, $\varepsilon_0 > 0$, and a smooth function $\phi(\tau)$, determined by the limiting behaviour of the rescaled initial data at infinity, such that:
- if $0 < \delta < \delta_0$ and $0 < \varepsilon < \varepsilon_0$,
- and if $\rho(\tau)$ is the solution of (1.4) with the initial datum $\rho(0) = \sqrt{Le^{-3}}\exp(-w_0/2)$ and lifetime τ_{max},
then we have

$$\forall \tau_0 \in (0, \tau_{max}), \qquad \sup_{0\le\tau\le\tau_0} |R_\varepsilon(\tau/\varepsilon^2) - \rho(\tau)| = O(\varepsilon).$$

3. LINEAR STABILITY ANALYSIS FOR THE ZELDOVICH FLAME BALL. The method that is devised in [7] to derive (1.4) is to notice that, when $Le < 1$, one can identify a slow time scale of the order $\dfrac{1}{\varepsilon^2}$. This allows an explicit computation of the temperature and mass fraction at finite distance; the slow motion of the flame is then controlled by the temperature field at $|x| = +\infty$: if the flame were really steady, then the temperature - resp. the mass fraction - would not, in general, be 0 - resp. 1 - at $|x| = +\infty$, thus violating the conditions (1.2). This imposes the introduction of a large spatial scale, and the computation of the variations of the temperature and mass fraction on this large scale yields, to the first order in ε, an evolution equation for the radius of the flame.

One way to interpret this $\dfrac{1}{\varepsilon^2}$ time scale is to relate it to the growth rate of a spherically symmetric disturbance, and our task is to prove this growth rate is at most of order ε^2.

The basic problem to investigate is therefore the linear (in)stability of the Zeldovich flame ball. Namely, we look at the problem

$$\mathcal{L}^\varepsilon(u,v) = \begin{pmatrix} -\Delta u - f'_\varepsilon(T_0)Y_0 u - f_\varepsilon(T_0)v \\ -\dfrac{\Delta v}{Le} + f'_\varepsilon(T_0)Y_0 u + f_\varepsilon(T_0)v \end{pmatrix} = \lambda(u,v), \qquad (u,v) \in L^2(I\!R^3). \tag{3.1}$$

THEOREM 1. *[i] Assume $Le = 1-\delta$, $\delta > 0$. There exists $\delta_0 > 0$ such that, for all $\delta \in (0,\delta_0)$, the following is true: there exist three constants $m > 0$, $M > 0$ and $\theta \in (0, \dfrac{\pi}{2})$, possibly depending on δ, such that the only eigenvalue of (3.1) outside the set*

$$\{\lambda \in C : \ \arg(\lambda + M) \le \theta, \quad \mathrm{Re}\lambda \ge m\}$$

is a complex number $\varepsilon^2\lambda_\varepsilon$ such that

$$\lim_{\varepsilon\to 0} \lambda_\varepsilon = -\left(\frac{1+\sqrt{Le}}{\delta}\right)^2 R_0^2 Le^6 e^{2w_0}.$$

[ii] Assume $Le = 1+\delta$, $\delta > 0$. There exists $\delta_0 > 0$ and two smooth positive functions $k_\varepsilon(\delta)$ and $\underline{k}(\delta)$ defined on $(0,\delta_0]$ such that $k_\varepsilon(\delta) \ge \underline{k}(\delta)$ for $0 < \delta < \delta_0$, and such that $(-\dfrac{k_\varepsilon(\delta)}{\varepsilon^2})$ is an eigenvalue to (3.1).

The proof is a bootstrap process inspired from [6].

REMARK. *Part [i] is a first step to the proof of Joulin's equation: the growth rate of the disturbance of the Zeldovich flame ball is of order ε^2. Joulin's construction consists in devising, at each time step, solutions that are quasisteady –i.e. Zeldovich flame balls up to terms of order ε^2. These quasisteady solutions can be expected to have the same stability properties as the Zeldovich flame balls, as we will see in Section 5 below.*

Part [ii] of this theorem explains why Joulin's derivation cannot work in the case $Le > 1$.

4. CONSTRUCTION OF AN APPROXIMATE SOLUTION. Consider $\nu > 0$ as small as needed. Joulin's idea is to assume that there is a solution (T_J, Y_J) of

$$\left\{ \begin{array}{l} \mathbf{1}_{\{|x|\geq \varepsilon^{-\nu}\}}\, T_t - \Delta T = Y f_\varepsilon(T) \\ \mathbf{1}_{\{|x|\geq \varepsilon^{-\nu}\}}\, Y_t - \dfrac{\Delta Y}{Le} = -Y f_\varepsilon(T) \end{array} \right. \tag{4.1}$$

which indeed expresses the fact that there is a slow time scale. Equation (1.4) comes out as an asymptotic compatibility condition for the derivatives of T and Y at $|x| = \varepsilon^{-\nu}$. Here we do not attempt to prove that this problem has an exact solution, all the more as what we are interested in is the full system (1.1). Instead, we construct an approximate solution to (4.1), which is given in the following theorem:

THEOREM 2. *Let $w_0 \in I\!R$, $\varepsilon > 0$ and $R_0 = R_{\varepsilon,w_0}$. Let (T_0, Y_0) be the Zeldovich flame ball $(T^\varepsilon_{w_0}, Y^\varepsilon_{w_0})$ in $B(0,\varepsilon^{-\nu})$ and let T_0, Y_0 be radially symmetric and continuous in $I\!R^3$ with $|x|T_0(x)$, $|x|Y_0(x)$ bounded and satisfying, for $\overline{T}_0(x) = \frac{1}{\varepsilon}T_0(\frac{x}{\varepsilon})$, $\overline{Y}_0(x) = \frac{1}{\varepsilon}\Big(Y_0(\frac{x}{\varepsilon}) - 1\Big)$, that*

$$\begin{array}{ll} & i)\ \ || \, |x|\overline{T}_0(x)||_{L^\infty(|x|>\varepsilon^{1-\nu})},\ || \, |x|\overline{Y}_0(x)||_{L^\infty(|x|>\varepsilon^{1-\nu})} \leq C \quad \textit{independent of } \varepsilon \\ & ii)\ \ || \, |x|\overline{T}_0(x)||_{C^{3+\alpha}(\varepsilon^{1-\nu}\leq|x|\leq\varepsilon^{1-\nu}+r_0)},\ || \, |x|\overline{Y}_0(x)||_{C^{3+\alpha}(\varepsilon^{1-\nu}\leq|x|\leq\varepsilon^{1-\nu}+r_0)} \leq C \\ & \qquad \textit{with } C,\ r_0 > 0,\ 0<\alpha<1 \textit{ independent of } \varepsilon \\ (4.2) & iii)\ \ \dfrac{\partial^2}{\partial r^2}\big(|x|\overline{T}_0(x)\big)\big|_{|x|=\varepsilon^{1-\nu}+0} = \dfrac{\partial^2}{\partial r^2}\big(|x|\overline{Y}_0(x)\big)\big|_{|x|=\varepsilon^{1-\nu}+0} = 0 \\ & iv)\ \ \varepsilon^{1-\nu}([\overline{T}_0)_r + \dfrac{(\overline{Y}_0)_r}{Le}]|_{|x|=\varepsilon^{-\nu}+0} = -\big[2Log(\sqrt{Le^3}\ R_0) + w_0\big] \\ & v)\ \ |x|\overline{T}_0(x), |x|\overline{Y}_0(x) \quad \textit{converge uniformly on compact subsets of } |x|>0 \\ & \qquad \textit{as } \varepsilon\to 0. \end{array}$$

There exist $\tau_{max} > 0$ independent of ε and a solution $(T^\varepsilon_J, Y^\varepsilon_J)$ to

$$\left\{ \begin{array}{l} T_t - \Delta T = Y f_\varepsilon(T) + F_1(t,x) + \mu_1 \\ Y_t - \dfrac{\Delta Y}{Le} = -Y f_\varepsilon(T) + F_2(t,x) + \mu_2 \end{array} \right. \qquad \big((0,\tau_{max}/\varepsilon^2)\times I\!R^3\big) \tag{4.3}$$

where the functions F_1, F_2 are supported on $[0,\tau_{max}/\varepsilon^2)\times B(0,\varepsilon^{-\nu})$ and, for all $\tau_0 \in (0,\tau_{max})$, we have: $|F_i(t,x)| \leq \overline{C}\varepsilon^2$ for $0\leq t\leq \tau_0/\varepsilon^2$, $i=1,2$; moreover μ_1 and μ_2 are measures supported on $[0,\tau_{max}/\varepsilon^2)\times\partial B(0,\varepsilon^{-\nu})$ such that, for all $\tau_0\in(0,\tau_{max})$ and for every $\psi\in C([0,\tau_{max}/\varepsilon^2]\times I\!R^3)$,

$$\Big|\int \psi\, d\mu_i\Big| \leq \overline{C}\varepsilon^{2-\nu}|Log^2\varepsilon|\ ||\psi||_{L^\infty([0,\tau_0/\varepsilon^2]\times\partial B(0,\varepsilon^{-\nu}))}.$$

The constant $\overline{C}$ may depend on τ_0.

Moreover, for every $\tau_0\in(0,\tau_{max})$, the couple of functions $(T^\varepsilon_J, Y^\varepsilon_J)$ is continuous in $[0,\tau_0/\varepsilon^2]\times I\!R^3$, $C^{2,1}((0,\tau_0/\varepsilon^2]\times\{|x|\leq\varepsilon^{-\nu}\})$, $C^{2,1}((0,\tau_0/\varepsilon^2]\times\{|x|\geq\varepsilon^{-\nu}\})$. The rescaled radius $\rho^\varepsilon_J(\tau)$ of $(T^\varepsilon_J, Y^\varepsilon_J)$ satisfies equation (1.4) with a forcing term ϕ_ε, depending on the rescaled initial datum at $|x| = +\infty$, that converges uniformly as $\varepsilon\to 0$.

REMARKS. *1. The function $(T^\varepsilon_J, Y^\varepsilon_J)$ constructed in Theorem 2 is a solution to (4.1) in $|x|<\varepsilon^{-\nu}$ and in $|x|>\varepsilon^{-\nu}$, with a jump of the gradient at $|x|=\varepsilon^{-\nu}$ of order $\varepsilon^{2+\nu}|Log^2\varepsilon|$. The time derivatives T_t and Y_t in $|x|<\varepsilon^{-\nu}$ are of order ε^2.*

2. The real number τ_{max} is the lifetime of the solution $\rho(\tau)$ to (1.4) with forcing term

$$\phi(\tau) = \lim_{\varepsilon\to 0}\phi_\varepsilon(\tau)$$

and initial datum $\rho(0) = \sqrt{Le^{-3}}\exp(-w_0/2)$.

3. Conditions iii) and iv) in Theorem 2 are compatibility conditions. Indeed, Problem (4.1) leads *to a singularly perturbed fractional derivative system, whose structure will be studied somewhere else.*

5. CONCLUSION. Set $(u, v) = (T^\varepsilon, Y^\varepsilon) - (T^\varepsilon_J, Y^\varepsilon_J)$ where $(T^\varepsilon, Y^\varepsilon)$ is the solution of the full system (1.1)-(1.2) with initial datum satisfying the assumptions of Section 2. Define - as in Section 3 - $\mathcal{L}^\varepsilon_J(\varepsilon^2 t)$ the linear operator around the approximate solution $(T^\varepsilon_J, Y^\varepsilon_J)$. Then (u, v) verifies

$$(\dot{u}, \dot{v}) + \mathcal{L}^\varepsilon_J(\varepsilon^2 t)(u, v) = F_\varepsilon(u, v) + (\mu_1, \mu_2)$$

where F_ε has quadratic behaviour around $(u, v) = (0, 0)$; the measures μ_i being defined in Theorem 2 and of order $\varepsilon^{2-2\nu}$ at most. A detailed analysis of the properties of the evolution operator generated by $\mathcal{L}^\varepsilon_J(\varepsilon^2 t)$ and a classical stability argument yields that (u, v) is of size $\varepsilon^{2-2\nu}$ at most.

The detailed proofs and discussion will appear in a forthcoming paper.

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Acknowledgement. C.L. and N.W were supported by Grants: ANPCYT - PICT 03-05009 and CONICET - PIP 0660/98. J.-M. R. was supported by the CNRS "Young researcher Grant" titled "Combustion diphasique". Both teams are grateful to their home institutions for several fruitful meetings.