

Université de Montréal

MODÉLISATION ASYMPTOTIQUE POUR LA  
SIMULATION AUX GRANDES ÉCHELLES DE  
LA COMBUSTION TURBULENTE  
PRÉMÉLANGÉE

par

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SIMULATION AUX GRANDES ÉCHELLES DE  
LA COMBUSTION TURBULENTE  
PRÉMÉLANGÉE**

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# RÉSUMÉ

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Cette thèse est constituée de trois articles destinés à la publication dans des journaux spécialisés plus un chapitre d'introduction et un chapitre supplémentaire. Étant donné les différences de style de rédaction imposées par les journaux dans lesquels les articles ont été ou seront publiés, chacun des trois articles constitue un chapitre indépendant.

On se propose de développer et d'évaluer une stratégie rigoureuse de modélisation et de simulation numérique en combustion turbulente prémélangée. On s'intéresse à l'approche connue sous l'appellation *simulations aux grandes échelles* (en anglais, *large eddy simulations*, ou *LES*). Comme le nom l'indique, seules les grandes échelles  $\gamma$  sont résolues tandis que l'effet des échelles non-résolues (dites *sous-grille*) est modélisé. L'originalité du projet présenté ici est qu'il est basé sur une approche asymptotique rigoureuse selon la théorie de l'homogénéisation de la combustion turbulente prémélangée de Majda et Souganidis (1994). Voici les grandes lignes de la démarche suivie pour transformer l'approche théorique abstraite en un outil de calcul pratique.

Dans le chapitre d'introduction, on justifie l'intérêt relié à la combustion prémélangée en donnant quelques exemples pratiques. On rappelle en quoi consiste la philosophie de la stratégie de simulations aux grandes échelles. On résume la théorie de Majda-Souganidis et on donne quelques outils numériques génériques pour les équations de type Hamilton-Jacobi dont on se servira dans la suite.

Dans le chapitre 2, on utilise l'approche rigoureuse pour proposer un modèle de paramétrisation de l'augmentation de la vitesse d'une flamme prémélangée dans le cas d'un cisaillement qui dépend du temps. On démontre l'existence de deux régimes limites selon lesquels une flamme turbulente prémélangée se propage : un

régime lent où l'augmentation de vitesse due à la turbulence est importante et un régime rapide avec très peu d'augmentation de vitesse. En particulier, on explique le phénomène de flexion (*bending effect*) comme étant la transition du régime lent au régime rapide. Cette transition est bien connue des expérimentalistes mais c'est la première fois qu'une explication théorique réussit à la décrire de façon quantitative.

La théorie de Majda-Souganidis est très abstraite et sa mise en œuvre nécessite le développement de nouveaux outils numériques pour les équations aux dérivées partielles de type Hamilton-Jacobi. Dans les équations homogénéisées, l'effet des petites échelles est représenté par un problème aux valeurs propres non linéaire connu sous le nom de *problème cellulaire*. Dans le chapitre 3, on développe une approche numérique pour résoudre ce problème. On transforme cette équation de type Hamilton-Jacobi en un système de lois de conservation dont la solution est le gradient de la fonction propre. La solution de ce problème non-linéaire est obtenue par un processus itératif d'évolution dans le pseudo-temps. Pour garantir la convergence vers l'état stationnaire, on construit un schéma numérique qui préserve le gradient en utilisant la technique des grilles décalées (en anglais, *staggered grids*).

Dans le chapitre 4, on analyse qualitativement la dynamique d'un front de flamme prémélangée soumise à un écoulement bi-dimensionnel de type Childress-Soward (combinaison de tourbillons et cisaillements). En particulier on généralise d'une manière qualitative les résultats du chapitre 2 qui avaient été obtenus dans le cas d'un cisaillement instationnaire. Ceci nous permet entre autre de démystifier et comprendre qualitativement le rôle de ce type d'écoulement sur le comportement (en particulier géométrique) de la flamme.

Finalement dans le chapitre 5, on démontre à l'aide d'un exemple toute l'utilité de l'approche asymptotique rigoureuse pour évaluer les fondements de la méthode de simulations aux grandes échelles basée sur le modèle des flammelettes comme



modèle sous-grille. Un certain nombre de questions soulevées lors de calculs pratiques sont abordées dans le contexte du modèle idéalisé. En exploitant les outils théoriques et numériques mis au point dans le cadre de cette thèse, il est possible d'apporter des réponses définitives à des questions d'intérêt pratique restées jusque là sans réponse.

## MOTS CLÉS

Combustion turbulente prémélangée, régime des flammelettes, modélisation asymptotique, homogénéisation, équations de Hamilton-Jacobi, vitesse de combustion turbulente, temps de résidence de la flamme, schéma conservatif qui préserve le gradient, simulations aux grandes échelles, méthode des iso-surfaces.

# SUMMARY

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This dissertation consists of three articles intended for publication in specialized journals plus one introductory chapter and an additional chapter. Because of the differences in style of drafting imposed by the journals in which the articles were or will be published, each of the three articles constitutes an independent chapter.

We develop and evaluate a rigorous strategy of modeling and numerical simulation in turbulent premixed combustion. We are interested in the approach known by the name *large eddy simulations* (LES) where only the large scales are resolved while the effect of the unresolved scales (known as *sub-grid scales*) is modeled. The originality of the project presented here is that it is based on a rigorous asymptotic approach according to the homogenization theory of turbulent premixed combustion of Majda and Souganidis (1994). Here is the broad outline of the steps followed to transform the abstract theoretical approach into a practical computational tool.

In the introductory chapter, we review the subject of turbulent premixed combustion and give some practical examples for motivation. We recall the philosophy of the large eddy simulations strategy. We summarize the theory of Majda-Souganidis and give some generic numerical tools for Hamilton-Jacobi equations which will be useful for the subsequent chapters.

In chapter 2, we use the rigorous approach to propose a parameterization model for the turbulent speed enhancement of a premixed flame subject to a time-dependent shear flow. We show the existence of two limiting regimes according to which a turbulent premixed flame propagates : a slow regime where the speed enhancement due to turbulence is significant and a fast regime with very little

speed enhancement. In particular, we explain the phenomenon of *bending* as being the transition from the slow regime to the fast regime. This transition is well-known by experimentalists but it is the first time that a theoretical explanation succeeds in describing it in a quantitative fashion.

The implementation of abstract theory of Majda-Souganidis requires the development of new numerical tools for partial differential equations of Hamilton-Jacobi type. In the homogenized equations, the effect of the small scales is represented by a nonlinear eigenvalue problem known as *cell-problem* whose numerical resolution is challenging. In chapter 3, we develop a new approach to solve this cell-problem. We transform this Hamilton-Jacobi equation into a system of conservation laws for the eigenfunction gradient. The solution of this non-linear problem is obtained by an iterative process of marching to steady state in the pseudo-time. To guarantee convergence to steady state, we rely on the staggered grids technique to build a *gradient-preserving* numerical scheme.

In chapter 4, we qualitatively analyze the dynamics of a premixed flame front subject to a two-dimensional flow of Childress-Soward type (combination of shears and eddies). In particular we generalize in a qualitative fashion the results of chapter 2. This descriptive study enables us to demystify and understand qualitatively the role of this type of flows on the (topological) behavior of the flame.

Finally in chapter 5, through a specific setup, we demonstrate the utility of the rigorous asymptotic approach to evaluate the basis of the large eddy simulations strategy based on the flamelet sub-grid model. A certain number of questions raised during practical computations are addressed in the context of the idealized model. By exploiting the theoretical and numerical tools developed within the framework of this thesis, it is possible to bring final answers to practical questions remained until now without answer.

**KEY WORDS**

Turbulent premixed combustion, flamelet regime, asymptotic modeling, homogenization, turbulent burning speed, flame residence time, gradient-preserving scheme, large eddy simulations, level-set method.

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*Il y a des signes qui ne trompent pas,  
qui sont évidents mais qu'on ne peut pas expliquer.*

Mouloud Feraoun dans *La Terre et le Sang*.

---

*À Aldjia*

*À Mohand*

*À La mémoire de mes parents*

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---

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# Chapitre 1

---

## INTRODUCTION

### 1.1. MOTIVATION

Dans ce travail on se propose de développer et évaluer une stratégie de modélisation et de simulation numérique en combustion turbulente prémélangée. La motivation pratique de cette recherche est le développement de codes capables de prédire d'une façon précise et économique le comportement de la flamme.

La combustion turbulente est parmi les sujets les plus difficiles en mécanique des fluides [4, 5, 8, 16, 31, 46] à cause de l'interaction permanente entre la chimie (la flamme) et l'écoulement turbulent. L'intérêt pratique que suscite cette question—notamment en industrie (voir ci-après) a fait que des chercheurs dans plusieurs disciplines tels que des physiciens, des ingénieurs et des mathématiciens s'y intéressent [8, 16, 17, 44, 50, 46, 63, 64, etc.]

On retrouve, par exemple, les flammes turbulentes prémélangées dans les moteurs à allumage par étincelles (moteurs équipés de bougies d'allumage : moteurs de voitures à essence) et les centrales électriques [31, 54]. Dans ce type de moteur, le combustible est d'abord mélangé avec de l'air par la turbulence pendant un intervalle de temps suffisamment long pour qu'on puisse considérer que le mélange est homogène jusqu'au niveau moléculaire. La mixture ainsi obtenue est acheminée vers l'intérieur de la chambre de combustion (le cylindre). Une étincelle est alors provoquée au sein du mélange. Cette étincelle résulte en un noyau avec une température suffisamment élevée pour que la réaction chimique ait lieu. Puisque la réaction est exothermique, le phénomène s'auto-entretient, ce qui donne naissance

à un front de flamme qui éventuellement va se propager d'une façon turbulente à travers tout le mélange.

La turbulence a plusieurs impacts sur la manière dont la flamme se propage. Les chercheurs s'intéressent à plusieurs aspects du problème, allant de la dimension fractale du front jusqu'à l'extinction de la flamme [23] par la turbulence. Parmi toutes ces questions très importantes, un problème essentiel est celui d'expliquer et prédire l'augmentation de la vitesse de propagation du front sous l'effet de la turbulence [1, 8, 16, 17, 24, 25, 26, 44, 50, 46, 47, 63, 64, etc]. Cette augmentation est en général perçue comme un effet positif de la turbulence sur la combustion prémélangée (en tout cas, en ce qui concerne la combustion dans les moteurs, un contre-exemple serait la prévention des incendies ou des explosions accidentelles). La compréhension systématique de ce phénomène contribuera à aider l'industrie à réaliser des processus de combustion efficaces et peu polluants.

Dans le régime des flammellettes, qui est un régime rencontré très fréquemment en pratique, le front d'une flamme prémélangée est une interface très mince qui sépare les gaz brûlés et non brûlés (le mélange frais). Le front se propage de façon irréversible vers les gaz frais au fur et à mesure que la combustion transforme les gaz frais en gaz brûlés. En présence d'un écoulement turbulent, le front se plisse et ceci se traduit par une augmentation de la surface de réaction et donc de la vitesse de combustion (c'est-à-dire la vitesse de propagation du front) [31, 44, 63]. Les plissements, qui sont en fait le résultat de la déformation de la flamme par l'écoulement turbulent, apparaissent à toutes les échelles de cet écoulement ; dans la figure 1.1 on fait l'esquisse d'un tel front de flamme turbulente en présence de tourbillons à deux échelles, une beaucoup plus grande que l'autre. Les plissements de la flamme sont ainsi formés par la superposition de plissements causés par les grands tourbillons qui sont donc à l'échelle de ces grands tourbillons et de petits plissements associés aux petits tourbillons<sup>1</sup>.

---

<sup>1</sup>Ici, le champ de vitesse est formé par la superposition de tourbillons variant sur deux échelles. La ligne pointillée désigne le plissement du front de la flamme quand il est soumis

En pratique, on ne s'intéresse qu'au comportement de la flamme aux grandes échelles, i.e., une flamme où tous les petits plissements ont été "filtrés". Ainsi, dans un calcul numérique destiné à prédire ce comportement aux grandes échelles, on peut espérer ne pas devoir résoudre les plissement dûs aux tourbillons aux petites échelles, ce qui serait très coûteux en terme de résolution. Cependant, ces petits plissements ont un impact non-négligeable sur le comportement de la flamme aux grandes échelles qui ne peut être ignoré dans la simulation, à savoir, l'augmentation de la vitesse de propagation due à ces tourbillons sous-grille et la déformation éventuelle du front aux grandes échelles qui en résulte.

Un modèle ad-hoc fréquemment utilisé par les ingénieurs est de considérer que l'augmentation de la vitesse de combustion par la turbulence est proportionnelle aux plissements de la flamme. Ce modèle est basé sur l'idée que tant que les plus petites échelles de la turbulence demeurent plus grandes que l'épaisseur de la flamme, cette dernière ne serait pas affectée par la turbulence et sa structure transverse resterait essentiellement identique au profil observé dans le cas laminaire. L'augmentation de vitesse ne résulterait alors que de la seule augmentation de la surface de réaction à cause des plissements qui sont à leur tour proportionnels à l'intensité de l'écoulement. Cette interprétation ad hoc a été utilisée depuis longtemps pour élaborer à l'aide d'arguments purement géométriques des modèles permettant de paramétriser l'effet des petits tourbillons en fonction de leur l'intensité. Les premiers modèles allant dans ce sens remontent à Damköhler (1939), voir [44, 63]. Néanmoins, une théorie mathématique a été récemment introduite par Majda et Souganidis [46] (1994). Cette nouvelle théorie démontre clairement, du moins dans le cas d'un certain type de réaction (KPP), qu'en général les arguments géométriques ne suffisent pas à eux seuls pour paramétriser l'effet de la turbulence sur la combustion prémélangée mais on doit tenir compte aussi

---

aux tourbillons à grande échelle seulement, tandis que la ligne continue superposée sur celle-ci représente le front plissé simultanément par les grands et les petits tourbillons

d'autres facteurs comme celui du mélange chaud-froid causé par la turbulence du côté froid de la flamme.

Dans ce travail, on se base sur cette théorie pour paramétriser d'une façon rigoureuse l'augmentation de vitesse due à la turbulence pour le cas d'un cisaillement instationnaire qu'on généralise ensuite, du moins d'une manière qualitative, à des écoulement synthétique plus élaborés. De plus, on démontre à l'aide d'un cas test, la faisabilité dans un cadre global d'une stratégie de *simulation aux grandes échelles* [42] (voir ci-dessous) qui se sert de cette théorie rigoureuse pour modéliser les petites échelles sous-grille en utilisant une base de données.

#### Simulation aux grandes échelles en combustion prémélangée.

Un des domaines les plus actifs dans la recherche en combustion turbulente prémélangée est celui de l'élaboration de stratégies de calcul numérique efficaces capables de représenter les effets de toutes les échelles de la turbulence sur la flamme. Comme il a été mentionné ci-haut, la difficulté majeure réside dans le fait que la flamme très mince interagit simultanément avec les multiples échelles de la turbulence. En pratique, il n'est pas nécessaire (mais aussi impossible) de résoudre toutes les petites échelles que représentent l'épaisseur de la flamme et les petits tourbillons. Lors d'une simulation aux grandes échelles (LES : en anglais, large eddy simulation) [8, 9, 10, 42], sur une grille de calcul donnée où seules les échelles qui sont de la taille de cette grille ou plus grandes sont résolues, l'effet des petites échelles est remplacé par un modèle.

### 1.2. CAS LAMINAIRE : RÉGIME DES FLAMMELETTES ET MÉTHODE DES ISO-SURFACES

Sous le régime des flammelettes, l'épaisseur de la flamme est infiniment mince. La flamme est représentée par une interface qui sépare les gaz brûlés et non brûlés. La vitesse normale avec laquelle cette interface avance vers le mélange frais est, dans le cas laminaire, le résultat de la balance entre l'effet de diffusion de la

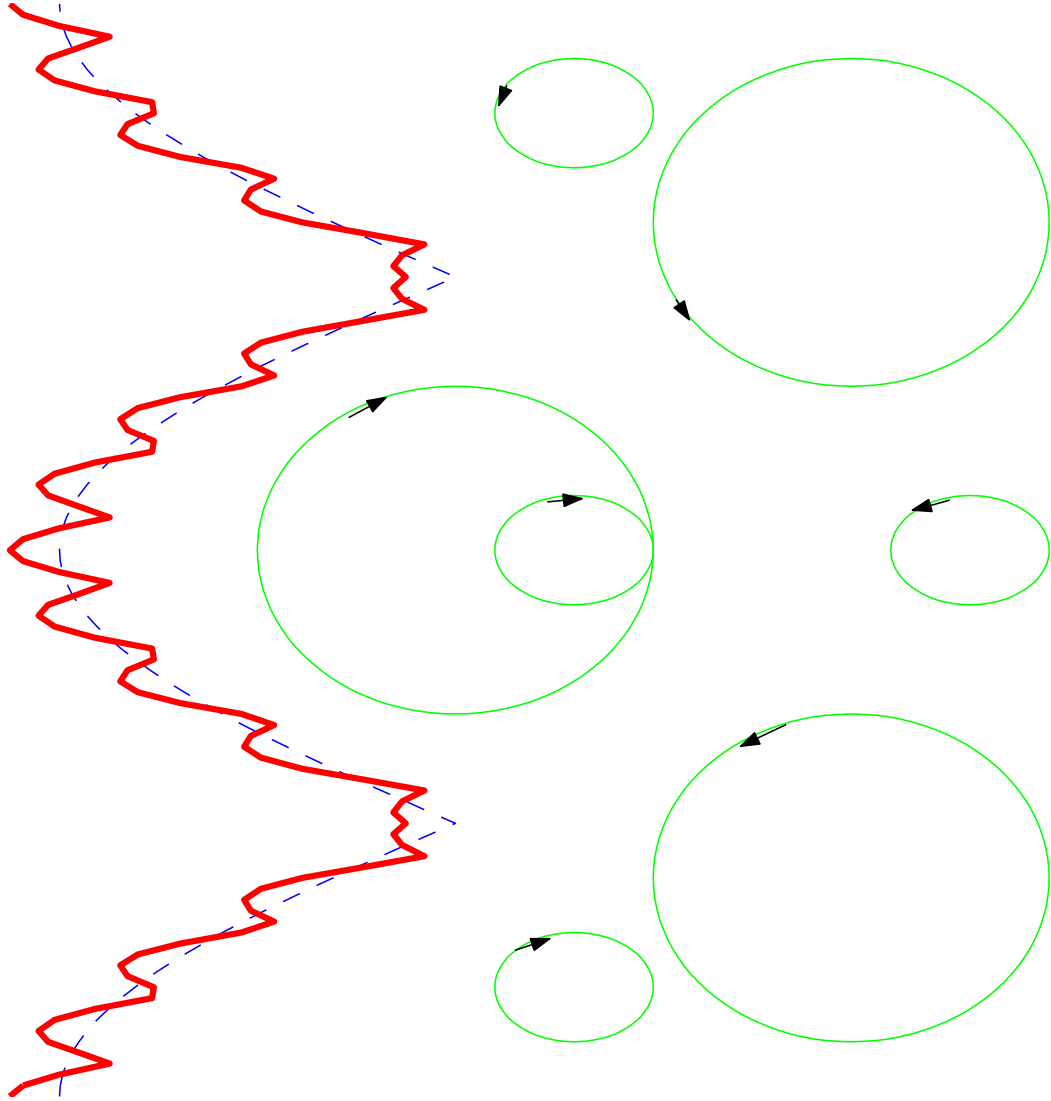


FIG. 1.1. Esquisse d'un front de flamme plissé sous l'effet d'un champ de vitesse qui varie sur deux échelles.

température et celui de la réaction chimique. Cette vitesse est connue sous le nom de vitesse de combustion laminaire et est notée  $S_L$ . Le front de flamme obéit donc au principe d'Huygens (connu en optique) et avance normalement à lui-même avec la vitesse  $S_L$ . En présence d'un écoulement,  $\bar{\mathbf{v}}$ , la vitesse absolue  $V$  du front de la flamme est donnée par

$$V = S_L \mathbf{n} + \bar{\mathbf{v}}$$



où  $\mathbf{n}$  est la normale au front dirigé du côté brûlé.

Williams [63] a introduit la méthode des iso-surfaces, connue aussi en théorie de l'image [2, 58, 59], qui consiste à représenter le front de la flamme comme le niveau zéro d'une fonction  $G(\mathbf{x}, t)$  telle que

$$\begin{aligned} G(\mathbf{x}, t) &> 0 && \text{dans la zone brûlée,} \\ G(\mathbf{x}, t) &< 0 && \text{dans la zone non brûlée,} \\ G(\mathbf{x}, t) &= 0 && \text{sur l'interface qui désigne le front de la flamme.} \end{aligned} \quad \text{Voir la figure 1.2.}$$

On a

$$\mathbf{n} = -\frac{\nabla G}{|\nabla G|}$$

$G$  vérifie l'équation de type Hamilton-Jacobi suivante.

$$G_t + \mathbf{V} \cdot \nabla G = S_L |\nabla G|, \quad (1.2.1)$$

i.e, tous les niveaux de la fonction  $G$  se déplacent à la même vitesse ; la vitesse du front de la flamme.

L'équation (1.2.1) est connue en combustion sous le nom de l'équation  $G$ .

**Remarque 1.2.1.** *En raison de son caractère géométrique, l'équation  $G$  (1.2.1) n'est valable que lorsque l'écoulement,  $\bar{\mathbf{v}}$ , est constant (voir la section suivante) mais en pratique elle est généralisée d'une façon ad-hoc pour les écoulements non constants, puis pour les écoulements turbulents en remplaçant  $S_L$  par un modèle de combustion turbulente,  $S_T$  [4, 5, 8, 9, 22, 23, 63, 64, etc].*

Malgré l'apparence très simple de l'équation (1.2.1), sa résolution numérique, surtout dans le régime turbulent, peut s'avérer très difficile. La solution  $G$  n'est pas lisse. Ses courbes de niveaux (surfaces de niveaux en 3D) présentent des points de rebroussement (*cusps*) qui sont des singularités pour le gradient de  $G$ . Ces singularités étant difficiles à traiter numériquement, les premiers numériciens qui se sont intéressés à cette équation y ajoutaient de la viscosité numérique de façon à lisser la solution [3, 4] avec des résultats plutôt imprécis. Dans ce travail, on se sert des schémas essentiellement non oscillatoires (ENO) d'ordre supérieur [53] pour les équations de Hamilton-Jacobi (voir ci-dessous) afin de pouvoir capturer ces

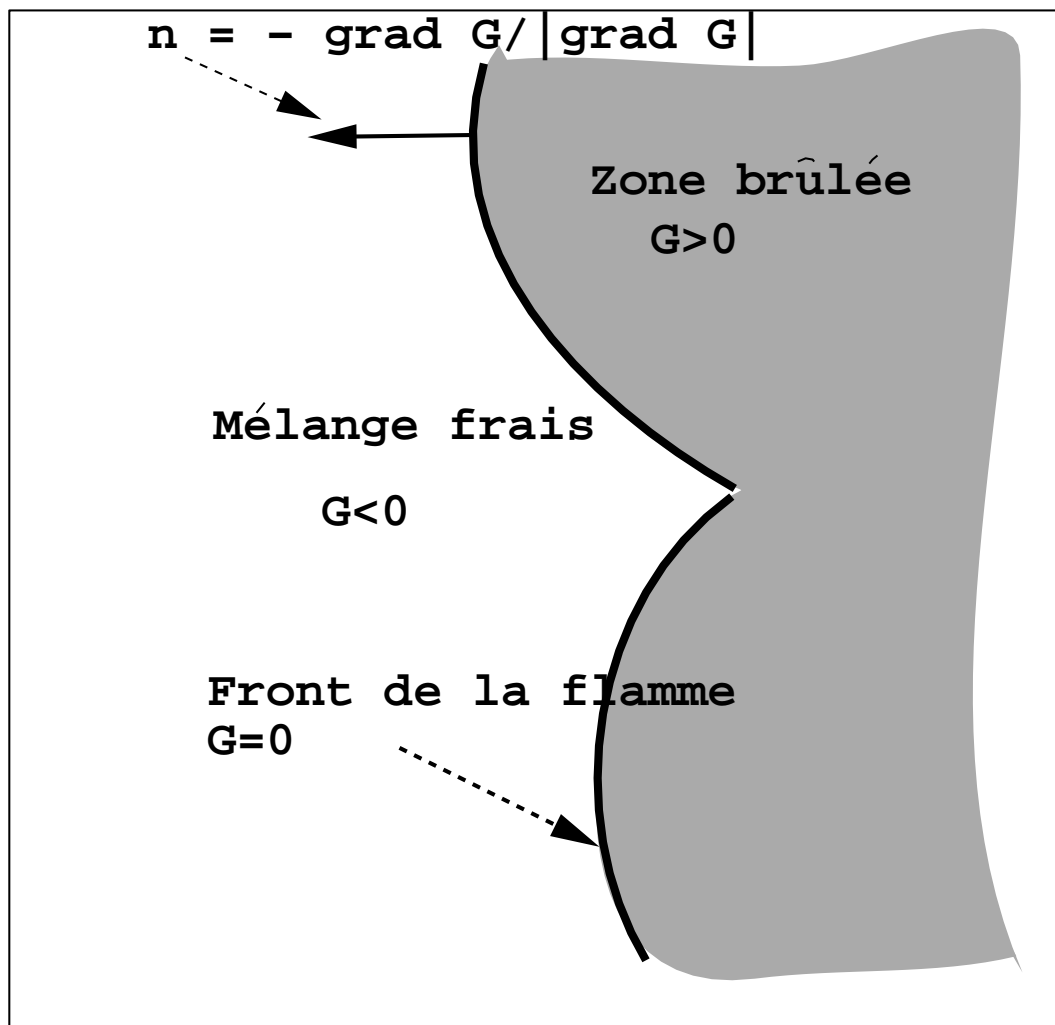


FIG. 1.2. Méthode des iso-surfaces pour suivre le front d'une flamme.

singularités en ajoutant une viscosité numérique locale aussi petite que possible ce qui garantit une grande précision dans les zones où la solution est lisse.

### 1.3. THÉORIE DE L'HOMOGENÉISATION DE LA COMBUSTION TURBULENTE PRÉMÉLANGÉE (MAJDA & SOUGANIDIS 1994)

La théorie de Majda et Souganidis utilise la méthode de l'homogénéisation et le concept de solutions de viscosité pour les équations de Hamilton-Jacobi [18, 19, 21, 27, 28] pour généraliser le régime des flammelettes connu dans le

cas laminaire au cas turbulent. On considère une flamme prémélangée en présence d'un écoulement variant sur deux échelles séparées; l'échelle intégrale et une échelle intermédiaire entre l'échelle intégrale et l'épaisseur de la flamme. On s'intéresse au comportement asymptotique de la flamme quand son épaisseur ainsi que l'échelle intermédiaire de l'écoulement tendent vers zéro.

Le front de la flamme homogénéisée est donné par la solution d'une *inégalité variationnelle* couplée avec un problème aux valeurs propres non-linéaire – *le problème cellulaire* – qui représente l'effet de l'échelle intermédiaire.

### 1.3.1. Le modèle utilisé

Lorsque l'échelle intégrale,  $L$ , est très grande devant l'épaisseur de la flamme (zone de réaction),  $l_F$ , le nombre de Lewis (rapport de la viscosité thermique sur la viscosité moléculaire) est égal à un, la chimie est réduite à une seule réaction et les expansions thermiques sont ignorées (flamme froide), le champ de température  $T$  est gouverné par l'équation de réaction-diffusion-advection suivante :

$$\begin{aligned} T_t + \mathbf{V} \cdot \nabla T - \epsilon \kappa \Delta T + \epsilon^{-1} f(T) &= 0, \text{ dans } \mathbb{R}^N \times (0, +\infty) \\ T &= T_0, \text{ sur } \mathbb{R}^N \times \{0\} \end{aligned} \quad (1.3.1)$$

où  $N = 1, 2$  ou  $3$ ,  $V$  est le champ de vitesse de l'écoulement,  $\epsilon = \frac{l_F}{L} \ll 1$ ,  $\kappa > 0$ , est la viscosité thermique et le taux de réaction  $f$  vérifie les conditions suivantes :

$$\begin{aligned} f &> 0 && \text{dans } (-\infty, 0) \cup (1, +\infty), \\ f &< 0 && \text{dans } (0, 1), \\ f'(0) &= \inf_{T > 0} \frac{f(T)}{T} < 0, \end{aligned}$$

i.e.,  $f$  une réaction de type KPP (exemple :  $f(T) = -KT(1 - T)$ ,  $K > 0$ ).  $G_0 = \overline{\{T_0 \neq 0\}}$  est le support de  $T_0$  qui est supposé compact. Dans (1.3.1) la

température  $T$  est normalisée tel que

$$\begin{aligned}
0 \leq T \leq 1, \\
\{T = 0\} & \quad \text{représente la région des gaz non brûlés (le mélange frais),} \\
\{T = 1\} & \quad \text{désigne la région brûlée,} \\
\{0 < T < 1\} & \quad \text{correspond à la zone de réaction.}
\end{aligned}
\tag{1.3.2}$$

La vitesse (relative) avec laquelle la réaction avance vers le mélange frais en absence de turbulence, appelée vitesse de combustion laminaire, est une fonction du taux de réaction du côté froid (entre  $T > 0$  et  $T = 0$ ) [24, 25, 26, 46], elle est donnée par

$$S_L = 2(-\kappa f'(0))^{1/2}. \tag{1.3.3}$$

Afin de respecter les notations dans [46], nous présentons les résultats de cette section dans le cas général de  $\mathbb{R}^N$  pour  $N = 1, 2, 3$ , bien que dans ce travail nous nous limitons au cas  $N = 2$  au plus.

Dans la suite, on suppose que le champ de vitesse,  $\mathbf{V}$ , varie sur deux échelles séparées, l'échelle intégrale (qui est d'ordre un) et une échelle beaucoup plus petite que l'échelle intégrale mais plus grande que l'épaisseur de la flamme,  $\epsilon$ , i.e.

$$\mathbf{V} = \mathbf{V}(\mathbf{x}, t, \epsilon^{-\alpha}\mathbf{x}, \epsilon^{-\alpha}t), 0 < \alpha \leq 1.$$

où  $\mathbf{V}(\mathbf{x}, t, \mathbf{y}, \tau)$  est borné continu, lipshitzien et périodique en ses deux dernières variables  $(\mathbf{y}, \tau)$  de période  $Q \times I \subset \mathbb{R}^N \times \mathbb{R}$ ,  $Q = [0, P]^N$ ,  $I = [0, T]$ ,  $P, T > 0$  (typiquement  $P = T = 1$ ). On s'intéresse au comportement asymptotique de la solution de (1.3.1) quand  $\epsilon$  tend vers zéro, i.e, au comportement de la flamme à grande échelle lorsque à la fois l'épaisseur de la flamme,  $\epsilon$ , et l'échelle intermédiaire de l'écoulement,  $\epsilon^\alpha$ , sont très petites—des échelles sous-grille pour une simulation numérique qui se limite aux grandes échelles.

### 1.3.2. Homogénéisation : problème asymptotique quand $\epsilon$ tend vers zéro

Afin d'élucider ce qui se passe du côté froid de la flamme (le mélange chaud et froid dû à la turbulence qui sert à accélérer la combustion dans le cas de réaction KPP), on fait le changement de variables ci-dessous pour capturer la décroissance exponentielle de la température,

$$T = \exp(\epsilon^{-1} Z^\epsilon).$$

L'équation dans (1.3.1) devient :

$$\left\{ \begin{array}{ll} Z_t^\epsilon - \epsilon \kappa \Delta Z^\epsilon - \kappa |\nabla Z^\epsilon|^2 + \mathbf{V}(\mathbf{x}, t, \epsilon^{-\alpha} \mathbf{x}, \epsilon^{-\alpha} t) \cdot \nabla Z^\epsilon + \frac{f(T)}{T} = 0 & \text{dans } \mathbb{R}^N \times (0, \infty) \\ Z^\epsilon = \epsilon \log(T_0) & \text{sur } \text{int}G_0 \times \{0\} \\ Z^\epsilon(x, t) \downarrow -\infty, \text{ quand } t \rightarrow 0 & \text{pour } x \in \mathbb{R}^N \setminus \bar{G}_0 \end{array} \right. \quad (1.3.4)$$

Dans le cas laminaire, ce changement de variable peut être schématisé par la figure 1.3 : en passant de  $T$  à  $Z^\epsilon$  on ramène la courbe  $T$  qui est concave du côté froid et convexe du côté chaud de la flamme à la courbe  $Z^\epsilon$  qui est toujours convexe.  $Z^\epsilon$  a une limite asymptotique (quand  $\epsilon \rightarrow 0$ ) continue ce qui n'est pas le cas de  $T$  qui convergerait vers la fonction constante par morceaux qui vaut zéro à gauche et un à droite.

La flamme se définit par rapport à  $Z^\epsilon$  par

$$\begin{aligned} -\infty &\leq Z^\epsilon \leq 0, \\ \{Z^\epsilon = 0\} &\text{ dans la zone brûlée,} \\ \{-\infty < Z^\epsilon < 0\} &\text{ dans la zone de réaction,} \\ \{Z^\epsilon = -\infty\} &\text{ dans la zone non brûlée.} \end{aligned} \quad (1.3.5)$$

Ce changement de variable sert en quelque sorte à "étirer" la zone de réaction du côté froid.

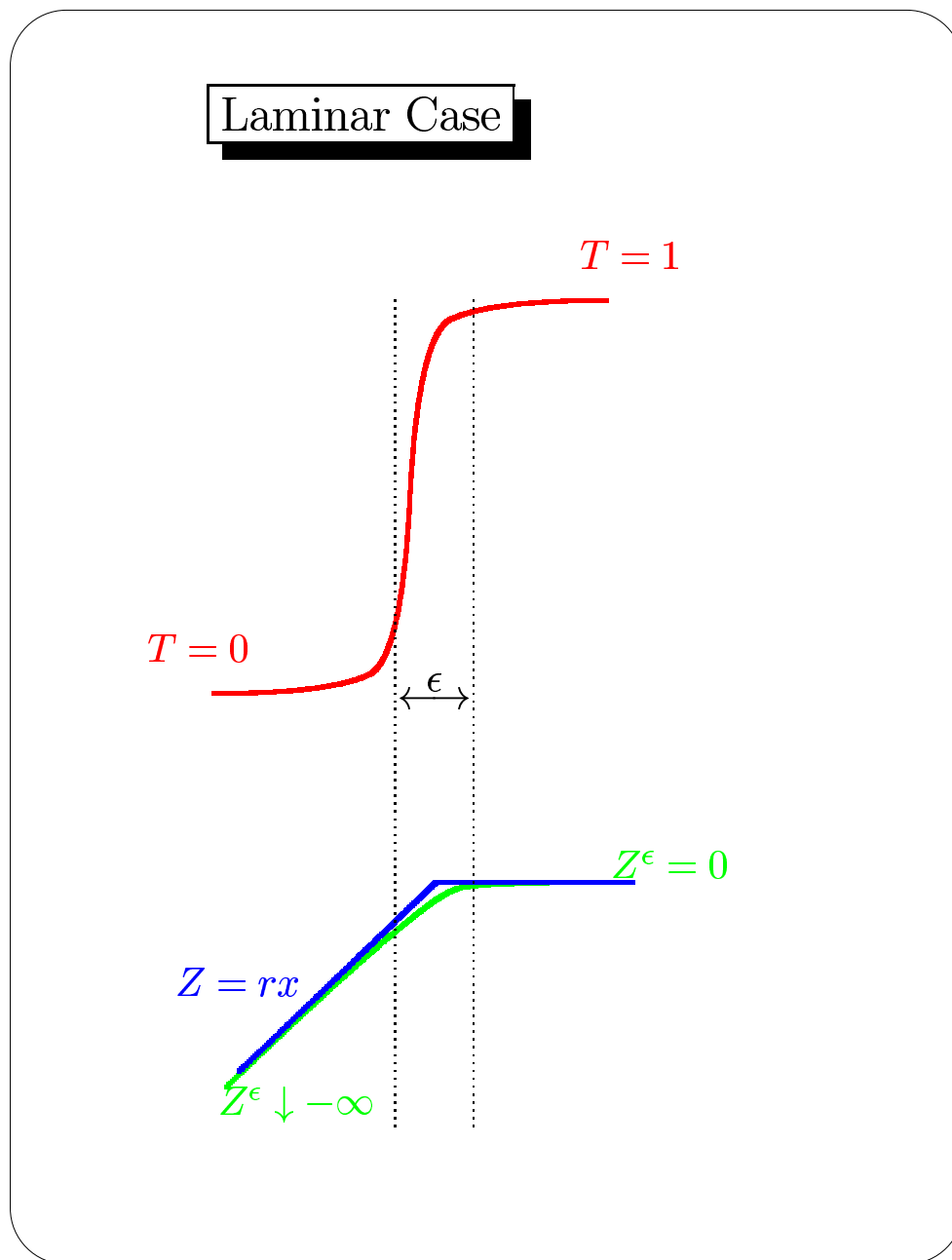


FIG. 1.3. Changement de variable  $T \rightarrow Z^\epsilon$  pour la théorie de l'homogénéisation dans le cas laminaire.

Le théorème suivant, qui est le résultat principal dans [46], donne la limite asymptotique de  $Z^\epsilon$  quand  $\epsilon$  tend vers zéro.

**Théorème 1.3.1 (Homogénéisation [46]).** *Soit  $Z^\epsilon$  la solution de (1.3.4). Supposons que  $f$  est de type KPP et que  $0 \leq T_0 \leq 1$ . Alors*

$$Z^\epsilon \longrightarrow Z \text{ quand } \epsilon \rightarrow 0$$

et

$$T^\epsilon \longrightarrow \begin{cases} 0 & \text{dans } Z < 0 \\ 1 & \text{dans } Z = 0 \end{cases} \text{ quand } \epsilon \rightarrow 0$$

où  $Z \in \mathcal{C}(\mathbb{R}^N \times [0, +\infty))$  est l'unique solution de viscosité de l'inéquation variationnelle

$$\begin{cases} \max(Z_t - H(x, t, \nabla Z) + f'(0), Z) = 0 & \text{dans } \mathbb{R}^N \times (0, \infty) \\ Z(x, 0) = \begin{cases} 0 & \text{si } x \in G_0 \\ -\infty & \text{si } x \in \tilde{G}_0^c \end{cases} \end{cases} \quad (1.3.6)$$

où  $H$  est l'unique valeur propre du problème cellulaire

$$w_\tau - a(\alpha)\kappa\Delta w - \kappa|\mathbf{p} + \mathbf{D}w|^2 + \mathbf{V}(\mathbf{x}, t, \mathbf{y}, \tau) \cdot (\mathbf{p} + \mathbf{D}w) = -H(\mathbf{x}, t, \mathbf{p}) \text{ dans } Q \times I, \quad (1.3.7)$$

pour tout  $(\mathbf{x}, t, \mathbf{p}) \in \mathbb{R}^N \times (0, \infty) \times \mathbb{R}^N$  avec  $w \in \mathcal{C}^{0,1}(\mathbb{R}^N \times (0, \infty))$ , périodique sur  $Q \times I$ , est la fonction propre.  $a$  est une constante telle que  $a(\alpha) = 0$ , si  $0 < \alpha < 1$  et  $a(1) = 1$ . Le symbole  $\mathbf{D}$  désigne le gradient par rapport à  $\mathbf{y}$ .

De plus,  $H$  est continue lipschitzienne sur  $\mathbb{R}^N \times (0, \infty) \times B(0, R)^2$  pour tout  $R > 0$ , convexe en  $p$ ,

$$\lim_{|\mathbf{p}| \rightarrow \infty} \frac{H(\mathbf{x}, t, \mathbf{p})}{|\mathbf{p}|} = \infty \text{ uniformément en } (\mathbf{x}, t) \text{ (coercivité)}$$

et vérifie

$$\kappa|\mathbf{p}|^2 - |\mathbf{V}|_\infty|\mathbf{p}| \leq H(\mathbf{x}, t, \mathbf{p}) \leq \kappa|\mathbf{p}|^2 + |\mathbf{V}|_\infty|\mathbf{p}| \quad (1.3.8)$$

---

<sup>2</sup> $B(0, R)$  désigne la boule ouverte de centre zéro et de rayon  $R$  pour la topologie euclidienne dans  $\mathbb{R}^N$

**Remarque 1.3.1.** a) La frontière de  $\{Z < 0\}$  avec  $Z$  la solution de (1.3.6) représente le front de la flamme à grande échelle (Fig. 1.4) tandis que les iso-niveaux de la solution  $w$  de (1.3.7) sont associés aux perturbations possibles de la flamme par l'écoulement à la petite échelle,  $\epsilon^\alpha$  (voir le chapitre 4).

b) D'une part le théorème 1.3.1 constitue un résultat important du point de vue théorique car il définit d'une façon précise le front de flamme à grande échelle tout en clarifiant l'effet des petites échelles de la turbulence. D'autre part, lorsqu'il est couplé avec un résultat de régularité ([46], théorème 1.2) garantissant le caractère non fractale du front à grande échelle, il constitue une preuve rigoureuse justifiant l'utilisation du modèle des flammes lors d'une simulation numérique en combustion prémélangée : l'existence d'une interface infiniment mince se substituant à la flamme d'épaisseur sous grille.

**Remarque 1.3.2.** La solution  $Z$  de l'inéquation variationnelle (1.3.6) est donnée par la formule de dualité de Fenchel :

$$Z(x, t) = \sup \left\{ \min_{0 \leq a \leq t} \int_0^a [-f'(0) - H^*(\Phi(s), t - s, \Phi'(s))] ds, \right. \\ \left. \Phi : [0, \infty) \rightarrow \mathbb{R}^N, \text{ absolument continue, } \Phi(0) = x, \Phi(t) \in G_0 \right\} \quad (1.3.9)$$

où  $H^*(\mathbf{x}, t, \mathbf{q}) = \sup_{\mathbf{p} \in \mathbb{R}^N} \{\mathbf{p} \cdot \mathbf{q} - H(\mathbf{x}, t, \mathbf{p})\}$  est le conjugué de la fonction convexe  $H$  avec  $H$  vérifie (1.3.7) [28, 46]. Exceptés les cas simples tel celui d'un simple cisaillement ou d'un écoulement localement rotationnel ([26]) pour lesquels les solutions analytiques pour (1.3.7) sont connues (voir [46] et [26] respectivement), (1.3.9) est pratiquement inutile ici ; en plus de la difficulté pour résoudre numériquement (1.3.7) nous avons la double évaluation du supremum sur des espaces infinis (l'ensemble des fonctions absolument continues,  $\Phi : [0, \infty) \rightarrow \mathbb{R}^N$ , telles que  $\Phi(0) = x, \Phi(t) \in G_0$ , pour calculer  $Z(\mathbf{x}, t)$  et l'ensemble  $\mathbf{p} \in \mathbb{R}^N$  pour calculer  $H(\mathbf{x}, t, \mathbf{p})$  respectivement).



### 1.3.3. Principe d’Huygens, bornes géométriques pour le front, vitesse de combustion

Dans cette sous-section, on s’intéresse à la question de la validité du principe d’Huygens selon lequel le front de la flamme se déplace normalement à lui même avec une vitesse qui dépend seulement de sa position et non de ce qui se passe en avant ou en arrière. Dans ce cas, le front de la flamme peut être représenté par le niveau zéro de la solution de l’é.d.p.<sup>3</sup> géométrique

$$u_t = F(\mathbf{x}, t, \nabla u)$$

où la vitesse de propagation est donnée par  $F$  qui est une fonction définie de  $\mathbb{R}^N \times (0, \infty) \times \mathbb{R}^N$  dans  $\mathbb{R}$  et vérifie

$$F(\mathbf{x}, t, s\mathbf{p}) = sF(\mathbf{x}, t, \mathbf{p}), \forall s > 0.$$

Selon la théorie M-S [46], la réponse à cette question est en général négative. Des contre-exemples très simples ont été donnés dans ([46] et [26]). Mais, dans le cas où le champ de vitesse  $\mathbf{V}$  est donné par

$$\mathbf{V}(\mathbf{x}, t, \mathbf{y}, \tau) = \bar{\mathbf{v}}(\mathbf{x}, t) + \lambda v(\mathbf{y}, \tau) \tag{1.3.10}$$

avec  $\mathbf{v}$  périodique, incompressible, de moyenne nulle et de norme max égale à un où  $\lambda$  est un paramètre positif qui sert à fixer l’intensité de la “turbulence”, il a été démontré dans [46] que le front de la flamme à grande échelle est borné supérieurement et inférieurement par deux fronts, i.e, le front est cerné entre deux fronts,  $\{\bar{u} = 0\}$  et  $\{\underline{u} = 0\}$ , voir la figure 1.4, qui obéissent au principe d’Huygens. De plus il existe un front géométrique,  $\{u = 0\}$ , qui se situe entre la borne inférieure,  $\{\underline{u} = 0\}$ , et le front de la flamme lui-même. Ce front géométrique intermédiaire se propage normalement à lui-même avec la même vitesse que le front effectif, i.e, la vitesse (locale) de combustion. (En effet, la quantité  $F$  définie en (1.3.11), théorème 1.3.2 ci-dessous, représente la vitesse avec laquelle le front

<sup>3</sup>équation aux dérivées partielles

de la flamme  $\partial\{Z < 0\}$  se déplace car (1.3.6) peut être réécrite sous la forme  $\max(Z_t - F(\mathbf{x}, t, \nabla Z), Z) = 0$  (voir [46] démonstration de la proposition 2.3). Dans le cas où le champ de vitesse à grande échelle est constant, i.e.,

$$\bar{\mathbf{v}}(x, t) = \bar{\mathbf{v}} = \text{constante} \in \mathbb{R}^N,$$

le front de la flamme lui-même obéit au principe d'Huygens, il est donc confondu avec le front  $\{u = 0\}$ .

Les é.d.p. géométriques qui gouvernent les fronts  $\bar{u}$  et  $\underline{u}$  sont données d'une façon explicite. Par contre, la vitesse de propagation,  $F$  (qui est aussi la vitesse de combustion (locale) de la flamme) qui régit l'é.d.p. pour  $\{u = 0\}$  fait intervenir le problème cellulaire (1.3.7) ainsi qu'un problème de minimisation. Ci-dessous, on donne en premier lieu les résultats reliés à  $\{u = 0\}$  et à la vitesse de combustion,  $F$ .

**Théorème 1.3.2 (Principe d'Huygens).** *Soit*

$$H^*(\mathbf{x}, t, \mathbf{q}) = \sup\{\mathbf{p} \cdot \mathbf{q} - H(\mathbf{x}, t, \mathbf{p})\}$$

la conjuguée (transformée de Fenchel) de la fonction convexe  $H$ , où  $H$  est donné par (1.3.7). On pose

$$F(\mathbf{x}, t, \mathbf{p}) = \max_{\mathbf{q}/H^*(\mathbf{x}, t, \mathbf{q}) = -f'(0)} \mathbf{p} \cdot \mathbf{q} = \inf_{s > 0} \{-sf'(0) + sH(\mathbf{x}, t, \frac{\mathbf{p}}{s})\} \quad (1.3.11)$$

On considère l'é.d.p. géométrique :

$$\begin{cases} u_t = F(\mathbf{x}, t, \nabla u) & \text{dans } \mathbb{R}^N \times (0, \infty) \\ u = g & \text{sur } \mathbb{R}^N \times \{0\} \end{cases} \quad (1.3.12)$$

où  $g$  est uniformément continue, positive sur  $G_0$  (zone brûlée) et négative sur  $\mathbb{R}^N \setminus \bar{G}_0$  (zone non brûlée). Dans le cas où  $V$  est donné par (1.3.10), la solution  $u$  de cette é.d.p. donne alors une borne inférieure pour le front de la flamme aux grandes échelles. Plus précisément on a :

$$\{\mathbf{x} : Z(\mathbf{x}, t) = 0\} \supseteq \{x : u(x, t) = 0\}$$

i.e. la partie de  $\mathbb{R}^N$  où  $u > 0$  reste à l'intérieur de la zone brûlée, voir la figure 1.4.

Si de plus le champ de vitesse à grande échelle est constant, i.e.  $\bar{\mathbf{v}} = \text{constante}$ , alors le niveau zéro de  $u$  représente le front à grande échelle. Plus précisément, en plus de l'inclusion ci-dessus, on a

$$\{x : Z(x, t) < 0\} \supseteq \{x : u(x, t) < 0\}$$

i.e. la courbe  $\{\mathbf{x} : u(\mathbf{x}, t) = 0\}$  est confondue avec la frontière de  $\{\mathbf{x} : Z(\mathbf{x}, t) < 0\}$ ,  $\partial\{\mathbf{x} : Z(\mathbf{x}, t) < 0\}$ .

**Remarque 1.3.3.** La vitesse de propagation du front  $\{u = 0\}$  est donnée par :

$$F(\mathbf{x}, t, \mathbf{n}),$$

où  $\mathbf{n}$  est la normale unitaire au front.

Pour parvenir au résultat donnant les deux bornes  $\bar{u}$  et  $\underline{u}$ , on pose

$$\begin{aligned} \underline{H}(\mathbf{x}, t, \mathbf{p}) &= \kappa|\mathbf{p}|^2 - \bar{\mathbf{v}} \cdot \mathbf{p} \\ \bar{H}(\mathbf{x}, t, \mathbf{p}) &= \kappa|\mathbf{p}|^2 - \bar{\mathbf{v}} \cdot \mathbf{p} + \max_{Q \times I}(-\lambda \mathbf{v} \cdot \mathbf{p}) \\ \overline{\overline{H}}(\mathbf{x}, t, \mathbf{p}) &= \kappa|\mathbf{p}|^2 + \sum_{i=1}^N (|\bar{\mathbf{v}}_i|_\infty + |\lambda| |\mathbf{v}_i|_\infty) |\mathbf{p}_i| \end{aligned}$$

On a le résultat suivant [46].

$$\underline{H}(x, t, p) \leq H(x, t, p) \leq \bar{H}(x, t, p) \leq \overline{\overline{H}}(x, t, p) \quad (1.3.13)$$

Par ailleurs, en intégrant (1.3.7) sur la période  $Q \times I$  et en divisant par la mesure de la période,  $|Q \times I|$ , grâce à l'incompressibilité de  $\mathbf{v}$ , à la  $Q \times I$ -périodicité et au fait que les moyennes périodiques de  $\mathbf{v}(\mathbf{y}, \tau)$  et de  $w(\mathbf{y}, \tau)$  sont nulles, en utilisant le théorème de la divergence, on trouve

$$H(\mathbf{x}, t, \mathbf{p}) = \kappa \left( |\mathbf{p}|^2 + \frac{1}{|Q \times I|} \int_{Q \times I} |\mathbf{D}w|^2 dy d\tau \right) - \bar{\mathbf{v}} \cdot \mathbf{p}. \quad (1.3.14)$$

D'où, avec (1.3.13), la moyenne quadratique  $\langle |\mathbf{D}w|^2 \rangle$  est bornée supérieurement par  $\max_{Q \times I}(-\lambda v \cdot p)$ .

**Remarque 1.3.4.** *Le fait que le hamiltonien  $H$  soit donné explicitement par (1.3.14) en fonction de la norme du gradient de  $w$  est exploité dans les chapitres 2 et 3 afin de construire une méthode numérique pour résoudre le problème (1.3.7). On résout d'abord une équation pour le gradient  $\mathbf{D}w$  seul sans la valeur propre  $H$  puis on calcule a posteriori  $H$  en utilisant (1.3.14). Pour trouver une équation vérifiée par le gradient  $\mathbf{D}w$  seul il suffit par exemple de prendre la dérivée de (1.3.7) par rapport à  $\mathbf{y}$ .*

Soient  $\overline{\overline{Z}}, \overline{Z}, Z$  et  $\underline{Z}$  les solutions de l'inéquation variationnelle (1.3.6) quand le hamiltonien est donné par  $\overline{\overline{H}}, \overline{H}, H$  et  $\underline{H}$  respectivement. Les seconds membres pour les é.d.p. géométriques correspondantes aux hamiltoniens  $\overline{\overline{H}}, \overline{H}$  et  $\underline{H}$  sont donnés par

$$\begin{aligned} \overline{\overline{F}}(\mathbf{x}, t, \mathbf{p}) &= \inf_{s>0} \{-sf'(0) + s\overline{\overline{H}}(\mathbf{x}, t, \frac{\mathbf{p}}{s})\} \\ &= 2\sqrt{-f'(0)\kappa}|\mathbf{p}| + \sum_{i=1}^N (|\bar{\mathbf{v}}_i|_\infty + \lambda|\mathbf{v}_i|_\infty)|\mathbf{p}_i| \end{aligned} \quad (1.3.15)$$

$$\begin{aligned} \overline{F}(\mathbf{x}, t, \mathbf{p}) &= \inf_{s>0} \{-sf'(0) + s\overline{H}(\mathbf{x}, t, \frac{\mathbf{p}}{s})\} \\ &= 2\sqrt{-f'(0)\kappa}|\mathbf{p}| - \bar{\mathbf{v}} \cdot \mathbf{p} + \max_{\mathbf{y}}(-\lambda\mathbf{v}(\mathbf{y} \cdot \mathbf{p})) \end{aligned} \quad (1.3.16)$$

$$\begin{aligned} \underline{F}(\mathbf{x}, t, \mathbf{p}) &= \inf_{s>0} \{-sf'(0) + \lambda\underline{H}(\mathbf{x}, t, \frac{\mathbf{p}}{s})\} \\ &= 2\sqrt{-f'(0)\kappa}|p| - \bar{v} \cdot p \end{aligned} \quad (1.3.17)$$

respectivement.

**Théorème 1.3.3 (Bornes géométriques sur le front).** *Soit,  $\overline{\overline{u}}, \overline{u}$  et  $\underline{u}$  les solutions de l'é.d.p. géométrique (1.3.12) quand  $F$  est respectivement remplacée par les fonctionnelles,  $\overline{\overline{F}}, \overline{F}$  et  $\underline{F}$ , données par (1.3.16), (1.3.17) et (1.3.15) respectivement. Sous l'hypothèse (1.3.10) pour le champ de vitesse, le front de la flamme asymptotique est cerné entre les niveaux zéro  $\{\underline{u} = 0\}$  et  $\{\overline{\overline{u}} = 0\}$ , qui désignent la borne inférieure et la borne supérieure respectivement, voir la figure 1.4. Par conséquent, la vitesse de combustion,  $F(\mathbf{x}, t, \mathbf{n})$ , admet  $\overline{F}(\mathbf{x}, t, \mathbf{n})$  et  $\underline{F}(\mathbf{x}, t, \mathbf{n})$  comme bornes supérieure et inférieure respectivement.*

Si de plus le champ de vitesse à grande échelle est constant,  $\bar{\mathbf{v}} = \text{const}$ , le niveau zéro  $\{\bar{u} = 0\}$  est aussi une borne supérieure pour le front asymptotique, i.e., le front effectif obéit au principe géométrique d'Huygens et est donnée par  $\{\bar{u} = 0\}$ .

**Remarque 1.3.5.** Les auteurs de [46] montrent à l'aide d'exemples que les bornes sur le front définies ci-dessus sont optimales, i.e., il existe des vecteurs unitaires  $\mathbf{n}_1$  et  $\mathbf{n}_2$  tels que  $\bar{F}(\mathbf{n}_1) = F(\mathbf{n}_1)$  et  $\underline{F}(\mathbf{n}_2) = F(\mathbf{n}_2)$  respectivement. Par ailleurs, le calcul explicite de ces deux bornes est beaucoup moins complexe que celui du front de la flamme à grande échelle (voir Remarque 1.3.2), ce qui permettrait donc une estimation a priori pour ce dernier dans les cas les plus complexes. Ces bornes explicites sont aussi utiles pour la validation de code dans un calcul numérique.

**Remarque 1.3.6.** 1. Le théorème 1.3.2 nous garantit l'existence d'une borne inférieure pour le front de la flamme qui obéit au principe d'Huygens qui se déplace (normalement à lui-même) avec la même vitesse que ce dernier : la vitesse de combustion. Toujours d'après le même théorème, cette borne inférieure est confondue avec le front lui-même quand le champ de vitesse à grande échelle est constant.

2. Dans [46] on démontre à l'aide de contre exemple que ce principe d'Huygens est en général faux (i.e., la borne inférieure,  $\{u = 0\}$ , n'est pas toujours confondue avec la limite asymptotique de la flamme, c'est seulement le cas quand  $\bar{\mathbf{v}}$  est constant). Néanmoins, des exemples réalistes où le front donné par  $u$  est en bon accord avec le front de la flamme asymptotique sont connus [26]. Aussi, le cas test considéré dans le chapitre 5 est un cas où le front donné par  $u$  est en accord avec le front de la flamme asymptotique.

3. Le théorème 1.3.3 nous donne des bornes sur la vitesse de combustion  $F$  facile à quantifier du fait que les expressions pour  $\underline{H}$  et  $\bar{H}$  sont explicites.

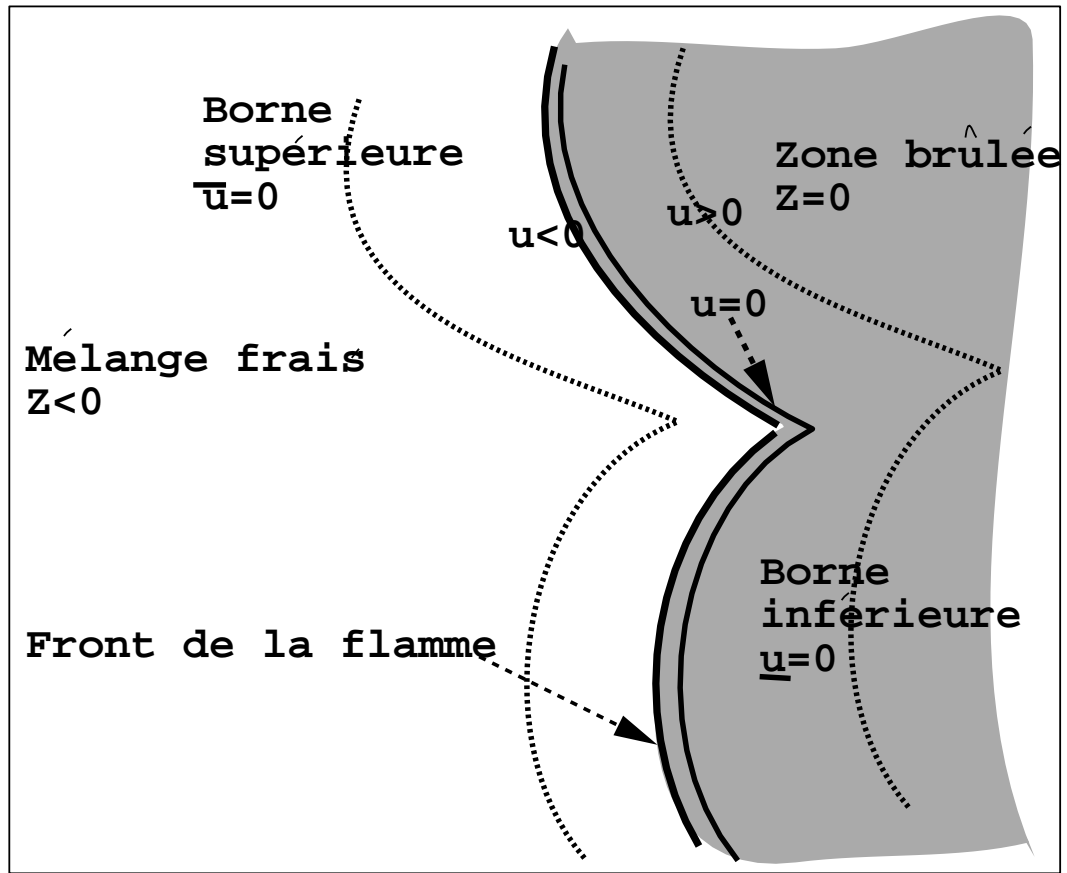


FIG. 1.4. Front de la flamme à grande échelle donnée par la théorie asymptotique et ses bornes géométriques.

4. Le calcul de la vitesse de combustion,  $F$ , nécessite la résolution du problème de minimisation (1.3.11) et du problème aux valeurs propres non linéaire (1.3.7).

#### 1.4. SCHÉMAS ENO D'ORDRE SUPÉRIEUR POUR LES ÉQUATIONS DE HAMILTON-JACOBI

Dans cette section, on présente une famille de méthodes numériques pour les équations de type Hamilton-Jacobi dont on se sert pour résoudre l'équation (1.2.1). La particularité de ce type d'équations aux dérivées partielles d'ordre un réside dans le fait qu'elles n'admettent pas toujours des solutions au sens classique

(i.e., de classe  $C^1$ ). Elles admettent des solutions de type viscosité [19, 18]. Ces solutions de viscosité sont des solutions au sens classique seulement en dehors d'un certain ensemble de points singuliers, typiquement, de mesure de Lebesgue nulle. Elles sont uniformément continues mais non partout dérivables (en général, elles sont dérivables presque partout (voir par exemple [19] et [18] pour les détails sur la théorie de ces solutions). Ainsi, la discrétisation par les schémas aux différences finies classiques (schémas centrés par exemple) n'est pas adéquate pour ce type de solutions car dans ce type de discrétisation on s'appuie sur les arguments de dérivabilité pour démontrer la compatibilité du schéma numérique avec l'équation aux dérivées partielles.

Comme alternative nous présentons ici, les schémas monotones pour les équations de Hamilton-Jacobi. Ce sont des schémas aux différences finies basés sur la technique de discrétisation amont (*upwind*) de telle sorte que la solution numérique converge vers la solution de viscosité de l'é.d.p. considérée. Les schémas monotones qui en résultent sont seulement d'ordre un, néanmoins, à l'aide de l'interpolation essentiellement non oscillatoires (ENO), on en construit une version d'ordre supérieur [53].

#### 1.4.1. Schémas monotones d'ordre un

On considère le problème de Cauchy donné par l'équation de type Hamilton-Jacobi d'ordre un en deux dimensions dans le cas particulier où le hamiltonien,  $H$ , est indépendant de  $(x, y, t)$  i.e

$$\begin{cases} u_t + H(u_x, u_y) = 0 & \text{dans } \mathbb{R}^2 \times (0, \infty) \\ u(x, y, 0) = u_0(x, y) & \text{dans } \mathbb{R}^2. \end{cases} \quad (1.4.1)$$

Ici, on admet l'existence et l'unicité d'une solution de viscosité,  $u$ , uniformément continue et bornée sur  $\mathbb{R}^2 \times (0, T]$ ,  $T > 0$  pour le problème (1.4.1) (voir [20] ou autre référence pour les théorèmes sur des questions telles que existence et unicité).

Soit une grille  $(\Delta x, \Delta y, \Delta t)$ . On note par  $u_{i,j}^n$  une approximation de la solution  $u(x_i, y_j, t_n) = u(i\Delta x, j\Delta y, n\Delta t)$  de (1.4.1), i.e.,

$$u_{i,j}^n \approx u(x_i, y_j, t_n) = u(i\Delta x, j\Delta y, n\Delta t)$$

On pose

$$\Delta^x u_{i,j} = u_{i+1,j} - u_{i,j} \text{ et } \Delta^y u_{i,j} = u_{i,j+1} - u_{i,j}$$

Un schéma monotone d'ordre un est un schéma aux différences finies de la forme

$$u_{i,j}^{n+1} = u_{i,j}^n - \Delta t \hat{H} \left( \frac{\Delta^x u_{i,j}}{\Delta x}, \frac{\Delta^x u_{i-1,j}}{\Delta x}, \frac{\Delta^y u_{i,j}}{\Delta x}, \frac{\Delta^y u_{i,j-1}}{\Delta x} \right) \quad (1.4.2)$$

tel que  $\hat{H}$ , appelé le hamiltonien numérique, est continu lipschitzien, consistant avec  $H$  (i.e.,  $\hat{H}(u, u, v, v) = H(u, v)$ ) et monotone, i.e., décroissant par rapport à la première et à la troisième variable et croissant par rapport aux deux autres. Symboliquement  $\hat{H}(\downarrow, \uparrow, \downarrow, \uparrow)$ .

Il est connu que les schémas monotones convergent vers la solution de viscosité du problème (1.4.1), [53] et [20]. Plus précisément, dans [20], on démontre qu'il existe une constante,  $c > 0$ , telle que

$$\max_{i,j, 0 \leq n \leq N} |u_{i,j}^n - u(x_i, y_j, t_n)| \leq c\sqrt{\Delta t} \quad (1.4.3)$$

**Exemples de schémas monotones** S. Osher et W-S Shu donnent quatre exemples de schémas monotones : le schéma de Lax-Friedrichs, le schéma de Godunov, le schéma de Lax-Friedrichs local qui est moins dissipatif que le premier et enfin, le schéma de Roe avec correction entropique qui est aussi peu dissipatif que le schéma de Godunov. On remarque que les noms donnés sont ceux des schémas amont connus dans le cadre des lois de conservation, ceci est dû au fait qu'ils sont dérivés de la même façon que ces derniers, i.e., par la technique de la discrétisation amont. En effet, en dimension un, on peut voir facilement que l'équation  $u_t + H(u_x) = 0$  est la primitive de  $u_{xt} + (H(u_x))_x = 0$ , i.e la dérivée de la solution d'une équation de Hamilton-Jacobi est une solution d'une loi de



conservation. Pour compléter, on donne le schéma de Roe avec correction entropique de Harten. Le choix de ce dernier est du au fait qu'il est peu dissipatif et est facile à mettre en œuvre.

### Flux de Roe avec correction entropique de Harten

Pour tout couple  $(a, b) \in \mathbb{R}$ , on désigne par  $I(a, b)$  l'intervalle  $[\min(a, b), \max(a, b)]$ . Soit  $H_1$  et  $H_2$  les dérivées partielles premières de  $H$  par rapport à la première et à la deuxième variable respectivement et  $A, B, C$  et  $D$  des réels fixés. On pose

$$\alpha^x(u^+, u^-) = \max_{\substack{u \in I(u^+, u^-) \\ C \leq v \leq D}} H_1(u, v) \alpha^y(v^+, v^-) = \max_{\substack{v \in I(v^+, v^-) \\ A \leq u \leq B}} H_1(u, v).$$

Le flux de Roe avec correction entropique de Harten est donné par

$$\hat{H}^R(u^+, u^-, v^+, v^-) = \begin{cases} H(u^*, v^*) & \text{si } H_1 \text{ et } H_2 \text{ ne changent pas de signe dans } I(u^+, u^-) \times I(v^+, v^-) \\ H\left(\frac{u^+ + u^-}{2}, v^*\right) - \frac{1}{2} \alpha^x(u^+, u^-)(u^+ - u^-) & \text{si } H_2 \text{ ne changent pas de signe dans } [A, B] \times I(v^+, v^-) \\ H\left(u^*, \frac{v^+ + v^-}{2}\right) - \frac{1}{2} \alpha^y(v^+, v^-)(v^+ - v^-) & \text{si } H_1 \text{ ne changent pas de signe dans } I(v^+, v^-) \times [C, D] \\ \hat{H}^{LLF}(u^+, u^-, v^+, v^-), & \text{sinon} \end{cases}$$

où

$$u^* = \begin{cases} u^+ & \text{si } H_1(u, v) \leq 0 \\ u^- & \text{si } H_1(u, v) \geq 0 \end{cases} \quad v^* = \begin{cases} v^+ & \text{si } H_2(u, v) \leq 0 \\ v^- & \text{si } H_2(u, v) \geq 0 \end{cases}$$

et  $\hat{H}^{LLF}$  est le flux local de Lax-Friedrichs donné par

$$\begin{aligned} \hat{H}^{LLF}(u^+, u^-, v^+, v^-) &= H\left(\frac{u^+ + u^-}{2}, \frac{v^+ + v^-}{2}\right) \\ &\quad - \frac{1}{2} \alpha^x(u^+, u^-)(u^+ - u^-) - \frac{1}{2} \alpha^y(v^+, v^-)(v^+ - v^-) \end{aligned}$$

### 1.4.2. Schémas ENO d'ordre supérieur

Les schémas monotones introduits ci-dessus utilisent une interpolation linéaire (deux points) pour approximer les dérivées partielles de la solution numérique  $(u_{ij}^n)$ , ils sont donc au plus d'ordre un. S. Osher et S-W. Shu ont utilisé l'idée de l'interpolation ENO afin de construire une version d'ordre supérieur dans l'espace. Comme le schéma donné en (1.4.2) utilise une discrétisation d'Euler dans le temps, l'ordre de précision dans le temps est au plus d'ordre un. Osher et Shu utilisent un schéma à variation totale décroissante (TVD) basée sur la méthode de Runge-Kutta pour passer à l'ordre supérieur dans le temps. Ci-dessous, on rappelle la notion d'interpolation ENO.

Étant donnée une fonction,  $f$ , connue sur une suite croissante de points équidistants,  $(x_i), i = 1, \dots, n, n \geq 1$ , par ses valeurs  $(f_i), i = 1, \dots, n$ . Admettant qu'on veut approximer la fonction  $f$  dans la cellule  $[x_i, x_{i+1}], i = 1, \dots, n$  fixé. Si on n'utilise que les points  $x_i$  et  $x_{i+1}$  l'approximation est d'ordre un seulement. Pour passer à une approximation d'ordre deux il faut rajouter un autre point. Ce troisième point peut être choisi à gauche ou à droite de la cellule ; parmi  $x_{i-1}$  et  $x_{i+2}$ . L'interpolation ENO consiste à choisir celui des polynômes d'interpolation relatifs aux points  $\{x_{i-1}, x_i, x_{i+1}\}$  ou  $\{x_i, x_{i+1}, x_{i+2}\}$  qui oscille le moins, i.e, qui présente la courbure la plus faible, ce qui est facilement vérifié par la comparaison des dérivées secondes. Pour passer de l'ordre deux à l'ordre trois, on rajoute aux trois points, déjà choisis, le point à gauche ou à droite qui réalise la plus petite dérivée troisième etc...En termes mathématiques la technique d'interpolation ENO se présente comme suit.

Soit  $P_i^{x,1}, i = 1, \dots, n$  le polynôme d'ordre un qui approxime la fonction  $f$  dans la cellule  $[x_i, x_{i+1}]$  tel que

$$P_i^{x,1}(x_i) = f_i, P_i^{x,1}(x_{i+1}) = f_{i+1}$$

Pour passer du polynôme  $P_i^{x,l}$  d'ordre  $l, 1 \leq l \leq r-1$ , au polynôme  $P_i^{x,l+1}$  d'ordre  $l+1$  on utilise l'algorithme suivant [37].

Étant donnés les  $l + 1$  points d'interpolation,  $x_{j(i)}, x_{j(i)+1}, \dots, x_{j(i)+l}$  relatifs au polynôme ENO d'ordre  $l$ ,  $P_i^{x,l}$ , qui approxime  $f$  dans la cellule  $[x_i, x_{i+1}]$ . Soient  $\mathcal{P}_-$  et  $\mathcal{P}_+$  les polynômes d'ordre  $l + 1$  qui interpolent  $f$  aux points  $x_{j(i)-1}, x_{j(i)}, \dots, x_{j(i)+1}$  et  $x_{j(i)}, x_{j(i)+1}, \dots, x_{j(i)+l+1}$  respectivement.

$$P_i^{x,l+1} = \begin{cases} \mathcal{P}_- & \text{si } \left| \frac{\partial^{l+1} \mathcal{P}_-}{\partial x} \right| \leq \left| \frac{\partial^{l+1} \mathcal{P}_+}{\partial x} \right| \\ \mathcal{P}_+ & \text{sinon.} \end{cases} \quad (1.4.4)$$

On revient au schéma monotone. Une fois que les polynômes ENO d'ordre  $r$ ,  $P_{i-k,j}^{x,r}$  et  $P_{i,j-k}^{y,r}$ , qui interpolent la solution  $u_{i,j}$  dans les cellules  $[x_{i-k}, x_{i-k+1}]$  et  $[y_{j-k}, y_{j-k+1}]$ ,  $k = 0, 1$ , dans les direction  $x$  et  $y$  sont construits selon l'algorithme en (1.4.4), on passe du schéma monotone d'ordre un au schéma ENO d'ordre  $r$  en remplaçant les dérivées dans (1.4.2) par

$$\begin{aligned} \frac{\Delta^x u_{i-k,j}}{\Delta x} &\approx \frac{d}{dx} P_{i-k,j}^{x,r}(x_i) \\ \frac{\Delta^y u_{i,j-k}}{\Delta x} &\approx \frac{d}{dy} P_{i,j-k}^{y,r}(y_j). \end{aligned} \quad (1.4.5)$$

La convergence des schémas ENO est garantie par l'utilisation de schémas TVD basés sur une intégration de type Runge-Kutta dans le temps, voir [53] pour les détails.

Dans [53], Osher et Shu montrent à l'aide de tests numériques que les schémas ENO, ainsi construits, sont de l'ordre voulu à l'intérieur des régions où la solution est régulière (de classe  $\mathcal{C}^r$  ou plus).

## Chapitre 2

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### PARAMÉTRISATION DE LA VITESSE D'UNE FLAMME TURBULENTE

Ce chapitre est constitué de l'article "Parametrizing the burning speed enhancement by small-scale periodic flows : I. unsteady shears, flame residence time and bending" par Boualem Khouider, Anne Bourlioux & Andrew Majda paru dans *Combustion Theory and Modeling* **5** (2001) 295-318.

Voici la liste des contributions principales de B.K. à cet article :

- élaborer et mettre en œuvre la méthode numérique qui a servi pour résoudre le problème cellulaire ;
- choisir les cas tests ;
- générer une base de données ;
- visualiser et analyser les données ;
- identifier explicitement les régimes (lent et rapide) qui décrivent le comportement de l'augmentation de vitesse de combustion ;
- analyser les statistiques des données pour proposer une paramétrisation qui a servi de base à l'analyse asymptotique ;
- comparer de façon détaillée la dynamique de la solution avec les prédictions asymptotiques.

# Parametrizing the burning speed enhancement by small-scale periodic flows :

## I. unsteady shears, flame residence time, and bending

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### ABSTRACT

*We document and explain the existence of two distinct scaling regimes for the burning speed enhancement of an idealized premixed flame as a result of its distortion by an unsteady periodic shear. The simplified model used in the present study allows for a rigorous, quantitative explanation of the bending in the scaling exponent, either linear or sublinear in the shear intensity, in terms of a non-dimensional flame residence time which compares the intrinsic time scale of the unsteady flow with the time it takes the corresponding steady shear to fully distort a flame. It is the nontrivial dependence of this latter flame wrinkling time with respect to the shear intensity that leads to the scaling behavior. A combination of asymptotic analysis and high resolution numerical simulations is used to validate the enhancement parameterization of both standing and traveling waves solutions for the perturbed front.*

## 2.1. INTRODUCTION

Turbulence in the flow always enhances the burning speed of a premixed flame with the burning speed enhancement strongly dependent on the turbulence intensity (for example see [17], [46] for rigorous lower bounds). Given the turbulence intensity  $u'$  (unit of velocity, typically defined as the square root of the turbulent kinetic energy), it has been observed that the burning speed enhancement depends linearly on  $u'$  for “large” values of  $u'$  but grows quadratically for “small” values. The change in scaling exponent from a linear dependence to a sublinear one is what is referred to in the literature as the *bending* of the turbulent burning speed (see for example [1], [64]). In this paper, we introduce a class of small scale unsteady shear flows for which bending can be linked very precisely to the transition between two enhancement regimes : in particular, we will show that for those idealized flows, the controlling parameter for bending is a non-dimensional time-scale that we refer to as the normalized flame residence time.

The results to be presented below confirm in a precise quantitative fashion some suggestions put forward recently by Denet [22] [23] and Ashurst [5] regarding the important role of time scales in premixed flame burning speed enhancement by turbulence. The novelty here is that we will pinpoint the transition in a very precise quantitative fashion by considering turbulent intensity and flow frequency as independent parameters and by introducing the appropriate non-dimensionalized time. The main result is presented in Section 2.2 with details provided in the following sections. The flame front behavior is modeled by the rigorous asymptotic model of Majda and Souganidis [46] - the use of this model for the present set-up is described in Section 2.3. The solution of the model for the steady case, with explicit predictions for maximal potential enhancement and for characteristic wrinkling time is in Section 2.4. A summary of the strategy to solve the unsteady problem numerically can be found in Section 2.5. The asymptotic/numerical description of the two scaling regimes, slow and fast, are in Section 2.6. While the

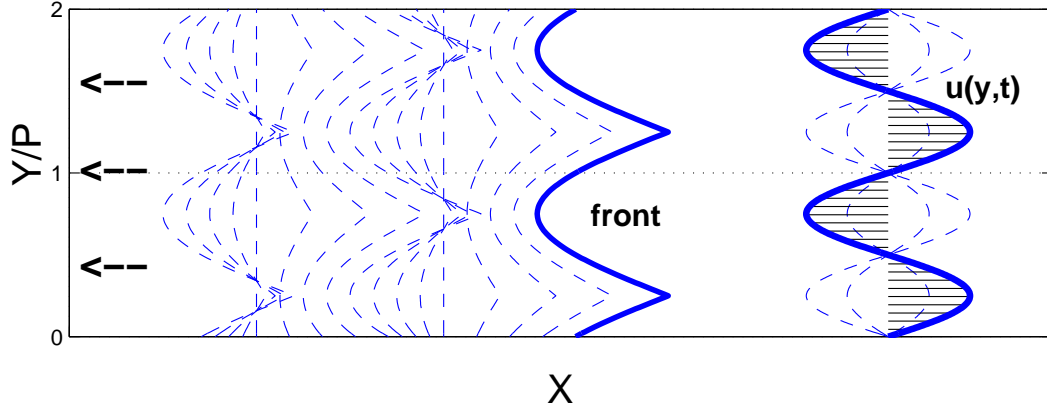


FIG. 2.1. Idealized set-up : distortion of a flame front by an unsteady horizontal shear.

time modulated shear in Eq.(2.2.1) below leads to a standing mode solution for the front, we will revisit in Section 2.7 a traveling mode solution previously studied by Embid et al [25] [24] and show that the same flame residence time considerations apply and allow one to parameterize very precisely the flame burning speed enhancement. A companion paper by the authors [11] describes the application of the basic concepts presented in this paper to the response of a flame front to small scale flows with more complex spatial structures such as jets and eddies : although flame patterns can become very complex for those new cases, one can still utilize the basic mechanisms identified here to explain qualitatively the trends observed in simulations.

## 2.2. MAIN RESULT : *bending* AS A SHARP TRANSITION BETWEEN TWO REGIMES - SLOW AND FAST

Since the normalized flame residence time involves in a rather unintuitive fashion the turbulence intensity as well as other factors, we state in this section the main result for one idealized set-up. All details as well as other examples will be provided in subsequent sections of the paper.

This basic set-up is shown in Fig.2.1 : an idealized thin flame front aligned with the  $y$ -axis and moving from right to left is subjected to a time modulated sine-shear in the direction normal to the front :

$$\mathbf{u}(\mathbf{x}, \mathbf{y}) = (\lambda \cos \omega t \sin(2\pi y/P), 0) \quad (2.2.1)$$

where  $\lambda > 0$  is the shear intensity and  $\omega$  the time-modulation frequency. If one were to try to imitate a turbulent spectrum, one could specify a spectral dependence  $\lambda = \lambda(\omega)$  [5] [22] [23] but in the present study,  $\lambda$  and  $\omega$  are varied independently so that their individual effect on the burning speed scaling can be identified in a systematic fashion. Periodic conditions are prescribed in the  $y$ -direction, with period  $P$ . This generic configuration is meant to mimic rough features of the small scales of a turbulent flow and their effects on a flame front.

As a result of the unsteady shear, the flame is distorted and its overall propagation speed  $S_T$  is greater than its laminar speed  $S_L$ . The overall propagation speed of the wrinkled flame is defined as the global fuel consumption rate divided by the channel width : it represents the speed of a planar flame that would burn instantaneously the same quantity of fuel as the wrinkled flame. Because of the time oscillations in the shear, the instantaneous burning speed also oscillates in time with the same period ; if one is interested in the long time, large scale behavior, a more useful diagnostic is to look at the overall burning speed averaged over one time period. Let  $Se = S_T - S_L$  represent the enhancement in this averaged overall burning speed compared to the laminar case. In the limit of low frequency  $\omega \rightarrow 0$ , an explicit expression is available for the burning speed enhancement (see Section 2.4 below) :

$$Se_0 = \lim_{\omega \rightarrow 0} Se = \frac{2\lambda}{\pi} \quad (2.2.2)$$

(hence, notice that for that case, the burning speed enhancement is always linear in the shear intensity). We use this zero-frequency limit value to define the



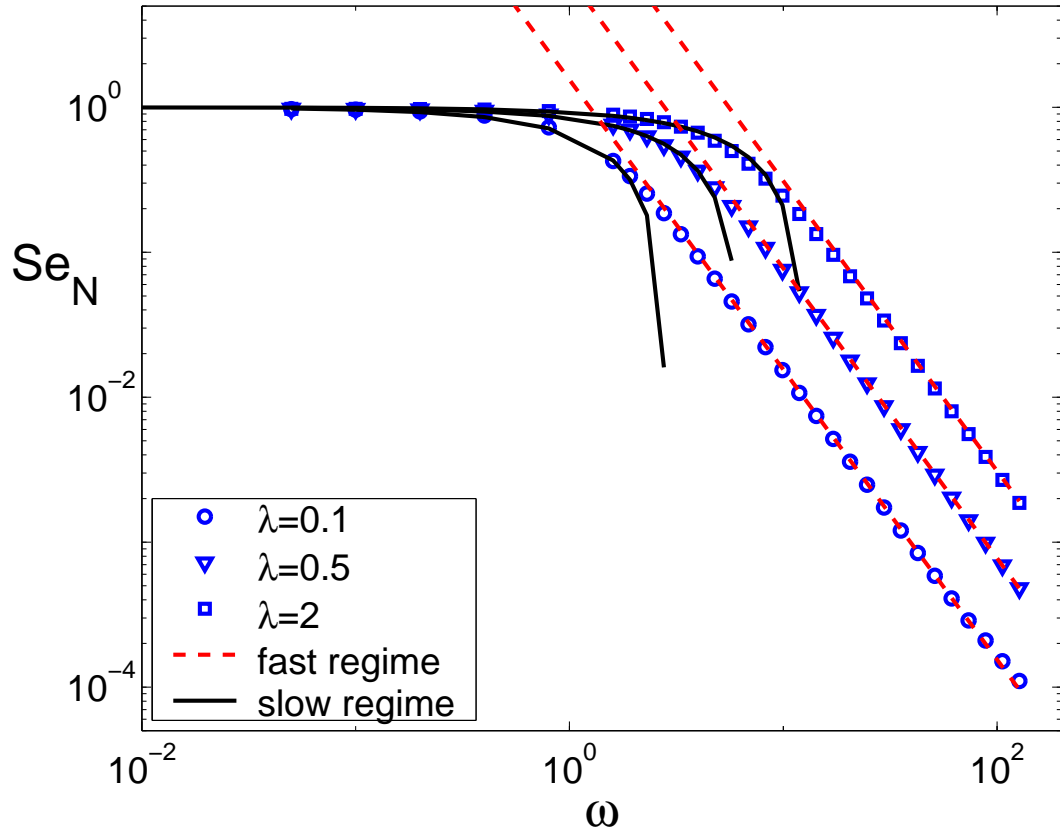


FIG. 2.2. Normalized burning speed enhancement  $Se_N$  as a function of  $\omega$  for shear intensity  $\lambda/S_L = 0.1, 0.5, 2$ . See text for the equations for the slow and fast regimes fitted curves.

normalized enhanced speed  $Se_N$  :

$$Se_N = \frac{Se}{Se_0} = \frac{S_T - S_L}{2\lambda/\pi} \quad (2.2.3)$$

The dependence of this normalized burning speed enhancement with respect to the forcing flow frequency  $\omega$  is illustrated in Fig. 2.2 with results for three shear intensities : small intensity  $\lambda/S_L = 0.1$ , intermediate intensity  $\lambda/S_L = 0.5$  and large intensity  $\lambda/S_L = 2$ . All the details on the numerical simulations will be provided later in the paper (Section 2.3 for the equations, Section 2.5 for their numerical solution.) The three curves display the same trend : for small frequencies ("slow" regime), the normalized enhancement is close to unity ( $Se_N =$

1 corresponds the reference  $\omega \rightarrow 0$  case). At large frequencies ("fast" regime) however, there is a marked reduction in enhancement. More quantitatively, for each value of  $\lambda$ , the slow and fast regimes are found to fit very closely with two distinct curves. The slow curve (solid line) is given by :

$$Se_{N,slow} = 1 - \frac{1}{\sqrt{2}} \frac{\omega/(2\pi) P}{\sqrt{\lambda/S_L} S_L} \quad (2.2.4)$$

In the slow regime,  $Se_N$  is therefore seen to be basically equal to one minus a small correction, and  $Se = 2\lambda Se_N/\pi$  is directly proportional to  $\lambda$  minus a small correction. For large frequencies, the fast curve (dash line) is given by :

$$Se_{N,fast} = \frac{\pi^3(\lambda/S_L) S_L^2}{2\omega^2 P^2} \quad (2.2.5)$$

Therefore, in the fast regime,  $Se_N$  is linear in  $\lambda$  and thus, from Eq.(2.2.3),  $Se$  depends quadratically on  $\lambda$ . The expressions are greatly simplified by introducing the following non-dimensional number

$$\tilde{t} = \pi \frac{S_L \sqrt{\lambda/S_L}}{P \omega/(2\pi)} \quad (2.2.6)$$

With that notation, we can rewrite :

$$Se_{N,slow} = 1 - \frac{\pi}{\sqrt{2\tilde{t}}} \quad (2.2.7)$$

valid for large values of  $\tilde{t}$  and

$$Se_{N,fast} = \frac{\tilde{t}^2}{8\pi} \quad (2.2.8)$$

valid for small values of  $\tilde{t}$ . The normalized burning speed enhancement  $Se_N$  is therefore a function exclusively of the parameter  $\tilde{t}$  and consequently the flame enhanced speed  $Se$  depends exclusively on the two parameters  $\lambda$  and  $\tilde{t}$  : the turbulence intensity  $\lambda$  dictates the maximum achievable enhancement and the non-dimensional number  $\tilde{t}$  (which depends on both  $\lambda$  and the flow frequency  $\omega$ ) controls whether this maximum enhancement will be actually observed in an unsteady simulation. This universal scaling is confirmed in Fig. 2.3 by replotting the results from Fig. 2.2 as  $Se_N(\tilde{t})$  (the plot also includes 100 additional data

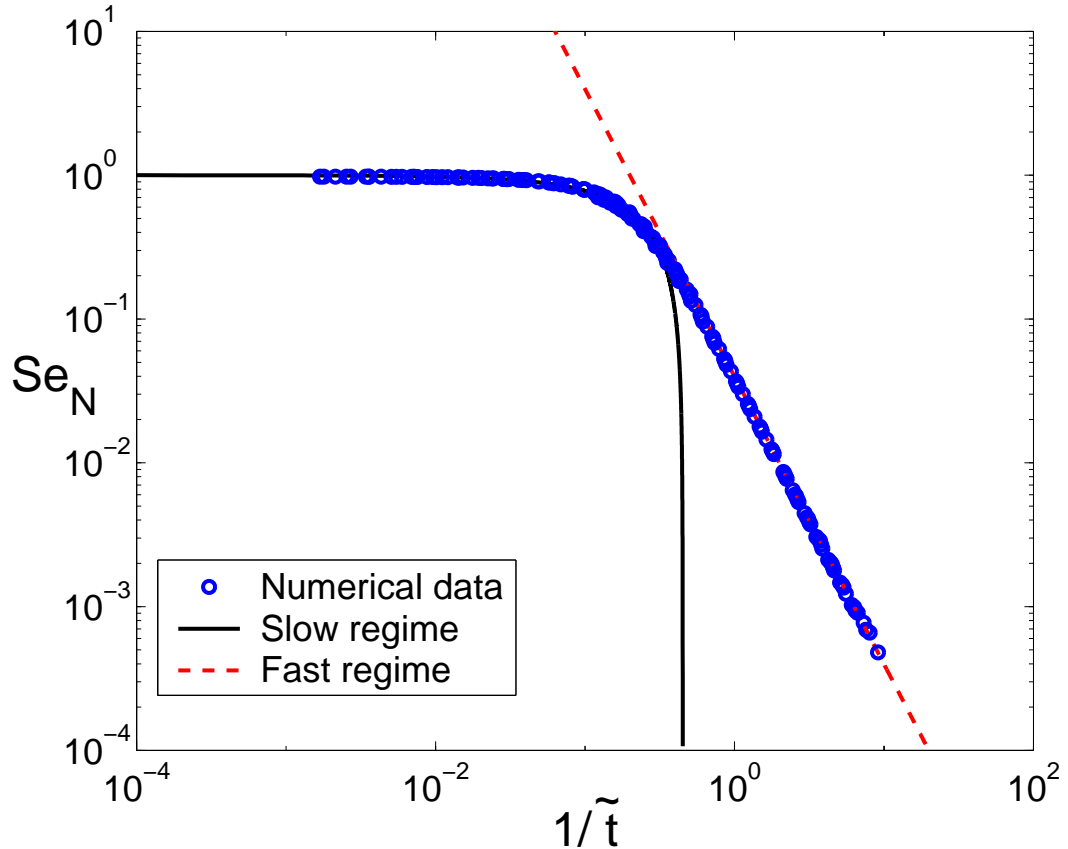


FIG. 2.3. Same as Fig. 2.2, except that the normalized burning speed enhancement  $Se_N$  is plotted now as a function of  $1/\tilde{t} = \frac{1}{\pi} \frac{P}{S_L} \frac{\omega/(2\pi)}{\sqrt{\lambda/S_L}}$ .

points covering a wide range of values for  $\lambda$  in  $[0.05, 128]$  and  $\omega$  in  $[5.2e^{-4}, 317]$ .) Indeed, all data appear to collapse on either the slow or the fast curve. A physical explanation of the scaling is possible by recognizing  $\tilde{t}$  as the ratio of two time-scales  $\tilde{t} = t_r/t_w$  with  $t_r$  and  $t_w$  defined as follows :

- $t_r = \frac{2\pi}{\omega}$  is the time-period of the shear amplitude modulation. It measures the time scale on which the unsteady flow is acting on the flame front, in other words, the flame “residence” time with respect to the unsteady distorting shear.

- $t_w$  is the flame wrinkling time and is given by :

$$t_w = \frac{1}{\pi} \frac{P}{S_L} \frac{1}{\sqrt{\lambda/S_L}} \quad (2.2.9)$$

We will demonstrate in Section 2.4 that  $t_w$  represents the time it would take a steady shear of intensity  $\lambda$  to wrinkle an initially planar flame to its maximum distortion and corresponding full burning speed enhancement  $\lambda$ .

Following this interpretation,  $\tilde{t}$  will be referred from now on as the **non-dimensional flame residence time**. It is not surprising that  $\tilde{t}$  involves the flow frequency ; however, the inverse square-root dependence with respect to the flow intensity is nontrivial (in particular not what is usually obtained using ad-hoc considerations for eddy turn-over times etc).

A physical explanation for the transition between the slow and fast curves observed in Fig. 2.3 is now obvious. If given an infinite time, the shear will distort the flame so that it achieves its maximal burning speed enhancement (recall that for the present set-up, this maximal enhancement is always linear in the shear intensity, regardless of the intensity, small or large, so that there can be effectively no bending in the limit of steady shears aligned with the front propagating direction). When the flow frequency is low, so that the non-dimensional flame residence time is large, the flame will have sufficient time to almost achieve full distortion and hence the steady maximal enhancement, so that again, the enhanced speed will be basically linear in the shear intensity if one ignores a small correction due to unsteady effects. On the other hand, when the non-dimensional flame residence time is small (at fixed  $\lambda$ , this corresponds to large frequencies), only a small fraction of the steady enhancement is possible because the flow oscillates too fast for the flame to follow it in detail and one observes a much reduced

enhancement with an overall quadratic dependence on the shear intensity (properly normalized).

Those intuitive considerations will guide the analysis of the numerical simulations and the asymptotic derivations in Section 2.6 : for the slow regime, a quasi-steady approximation will be used whereas the solution can be predicted to leading order by averaging the steady solutions corresponding to the successive shear modulated amplitudes  $\lambda|\cos\omega t|$  observed during one time-period. In the fast regime, fluctuations with respect to the mean are small and a linear perturbation analysis will be appropriate (note however that the mean solution around which perturbations are studied is far from trivial ; it has small amplitude but still contains cusps.)

### 2.3. BASIC EQUATIONS

The model for the flame front used in this study is the rigorous asymptotic model of Majda and Souganidis [46], Embid et al. [25]. It describes the propagation of an infinitely thin flame when the flame propagation is affected by a flow field that includes small scales intermediate between the flame thickness and the integral scale ; the asymptotic limit is the rigorous generalization of the laminar flamelet concept in the presence of turbulent flow. It has been shown to lead to predictions that can be significantly different from those using the G-equation formulation in the case of KPP-type chemistry in the paper by Embid et al. [24] although there are other regimes with strong agreement.

The model assumes that the heat release is weak and the Lewis number is equal to one so that the propagation of the flame front can be described by a single

reaction-diffusion advection equation for the temperature :

$$T_t + \mathbf{V} \cdot \nabla T = \epsilon \kappa \Delta T + \epsilon^{-1} f(T) \quad \mathbf{x} \in R^n, \quad 0 < t < \infty \quad (2.3.1)$$

Time and length in Eq.(2.3.1) are non-dimensionalized with respect to the integral scales. The flame thickness is of order  $\epsilon$ , as a result of the balance between the weak diffusion of order  $\epsilon$  and the fast reaction of order  $\epsilon^{-1}$ . The temperature is normalized so that  $T = 0$  on the unburnt side and  $T = 1$  on the burnt side. The reaction rate is assumed to be a single irreversible step of the KPP type, for example  $f(T) = KT(1 - T)$ . The nonlinear averaging theory of Majda and Souganidis provides the evolution of the effective flame front in Eq.(2.3.1) in the limit of  $\epsilon \rightarrow 0$  when the incompressible velocity field  $\mathbf{V}$  depends on two separate scales :

$$\mathbf{V} = \bar{\mathbf{V}}(\mathbf{x}, t) + \lambda \mathbf{v}(\mathbf{x}/\epsilon^\alpha, t/\epsilon^\alpha) \quad (2.3.2)$$

with  $0 < \alpha < 1$ . In that case, the velocity field has two components, a mean component  $\bar{\mathbf{V}}$  varying on the integral scale and a zero-mean fluctuation velocity  $\lambda \mathbf{v}$  involving the turbulent scale  $(\mathbf{x}/\epsilon^\alpha, t/\epsilon^\alpha)$ . In other words, the theory provides a rigorous framework to average out of the solution the details at the turbulent scale and below; this is precisely the type of result needed for our problem where the  $y$ -period  $P$  and time-period  $T = 2\pi/\omega$  in the time-modulated shear correspond to the intermediate  $\epsilon^\alpha$  scales in the asymptotic problem in (2.3.2). For the model velocity fields in 2.2.1,  $\mathbf{u} = \lambda \mathbf{v}$  in (2.3.2).

The asymptotic theory describes the evolution of the variable  $Z = \epsilon^{-1} \log T$  : this change of variable allows for a very detailed description of what goes on in the exponentially decaying pre-heat zone on the cold side of the flame. It is known that KPP chemistry flames are very sensitive to the cold side conditions near  $T = 0$ . For instance, for the laminar case (set  $\mathbf{V} = 0$ ), the laminar speed of propagation

of the flame is given by  $S_L = 2(\kappa f'(0))^{1/2}$ ; the theory in [46] rigorously generalizes this behavior under the action of turbulent mixing in the pre-heat zone. The asymptotic prediction is that, in the limit of  $\epsilon \rightarrow 0$ , the mean front will obey a variational inequality that involves the eigenvalue of a cell problem. We refer the interested reader to the references [46] [24] for the general formulation and give here only the version needed to address the special velocity field in (2.2.1).

When  $\mathbf{v} = (\lambda \sin(2\pi y/P) \cos(\omega t), 0)$ , the flame front in the idealized setup corresponding to Fig. 2.1 will always be the graph of a function of  $y$  so that at any time  $t > 0$ ,  $Z(x, y, t) = rz(x, y, t)$  with  $z(x, y, t) = x - \bar{x}(t) - \psi(y, t)$  and  $r$  a positive constant. A strategy to obtain  $r$ ,  $\bar{x}$  and  $\psi$  is given below; first we explain their physical interpretation in terms of the behavior of the flame. From the relationship between  $Z$  and  $T$ , one can see that the positive scalar  $r$  measures the rate of exponential decay of the temperature in the pre-heat zone. The special form for  $Z$  or  $z$  implies that the flame front location, which corresponds to the zero-level of  $Z$ , is given by  $x(y, t) = \bar{x}(t) + \psi(y, t)$  where  $\psi(y, t)$  is a bi-periodic, zero-mean function over the domain  $[0, P]X[0, T]$  and  $\bar{x}(t)$  is the flame mean  $x$ -location. The mean flame moves to the left at the turbulent burning speed  $-\frac{d\bar{x}}{dt} = S_T$ ; it is the prediction of  $S_T$  (or  $Se = S_T - S_L$ ) which is what one cares mostly about in this problem. According to the rigorous theory, this must be done using the following procedure :

- given  $r > 0$  and the fluctuating shear  $v(y, t)$  in (2.2.1), there exist an unique effective Hamiltonian  $H(r)$  and an unique corresponding eigenfunction  $\psi(y, t)$  of mean zero and bi-periodic over the space-time box  $[0, P]X[0, T]$  that satisfy the following cell-problem :

$$r\psi_t - \kappa r^2(1 + \psi_y^2) + rv(y, t) = -H(r) \quad (2.3.3)$$

The first step of the procedure is to compute  $H(r)$ .

- the enhanced burning speed can then be predicted by minimization :

$$S_T = \inf_{r>0} \frac{f'(0) + H(r)}{r} \quad (2.3.4)$$

For instance, for the laminar case (set  $v(y, t) = 0$ ), using the formula for  $S_T$  will give the expected formula for the laminar burning speed :

$$\psi_L(y, t) = 0 \quad H_L(r) = \kappa r^2 \quad S_L = 2(\kappa f'(0))^{1/2} \quad (2.3.5)$$

where the minimum for the burning speed is achieved for  $r = (f'(0)/\kappa)^{1/2} = r_L^*$ . In the next section, an explicit solution to the above cell-problem will be discussed for the case  $\omega = 0$  since it will be an useful reference for the discussions in the rest of the paper. When  $\omega > 0$ , there are no closed form solutions to the cell problem, so a numerical procedure is used instead, as described in Section 2.5.

#### 2.4. REFERENCE CASE : STEADY SHEAR NORMAL TO THE FRONT

In this section, we summarize basic results concerning the steady shear case ( $\omega = 0$  in Formula (2.2.1) for the shear) so that the small scale periodic flow is given by  $(\lambda \sin(2\pi y/P), 0)$ .

##### 2.4.1. long-time solution with the steady shear

If the front is distorted by a steady shear, it will asymptotically converge to a steady traveling wave solution whose speed as well as detailed spatial profile in  $y$  can be predicted explicitly using the steady version of the cell-problem. The problem is particularly simple because the eigenvalue is now a one-dimensional function  $\lim_{t \rightarrow \infty} \psi(y, t) = \psi_s(y)$ . It is easy to verify that the solution to the cell-problem in (2.3.3) is given as follows :

- the effective Hamiltonian is  $H = \kappa r^2 + r \lambda$ ;
- the turbulent burning speed is obtained using Eq.(2.3.4)  $S_T = S_L + \lambda$  and is achieved for the same exponential decay rate  $r = r_L^*$  as in the laminar case (Eq.(2.3.5)) ;



- the unique eigenfunction of period  $P$  corresponding to  $H$  at the infimum is :

$$\psi_s(y) = -\frac{2}{\pi}P\left(\frac{\lambda}{S_L}\right)^{1/2}(|\cos(\pi(y/P - 3/4))| - C_0) \quad (2.4.1)$$

with  $C_0$  a constant so that the mean of  $\psi_s(y)$  is zero.

In particular, the theoretical upper bound for  $Se$  is achieved here :  $Se = S_T - S_L = \lambda$ , i.e. the speed enhancement is equal to the maximum of the shear component in the flame mean propagating direction (see the theory in [46]).

#### 2.4.2. reference wrinkling time $t_w$

In Section 2.2, the so-called flame wrinkling time  $t_w$  was introduced as a convenient reference time by which to normalize unsteady time scales. We now justify the expression for  $t_w$  in Eq.(2.2.9) by studying the evolution of an initially undisturbed laminar front ( $\psi(y, t) = 0$  at  $t = 0$ ) until it reaches its asymptotic shape  $\psi_s(y)$  as described by Eq.(2.4.1). To obtain the transient evolution equation, we again assume that  $Z = rz(x, y, t)$  with  $z(x, y, t) = x - \psi(y, t)$  (in this case, we have not assumed that  $\psi(y, t)$  has zero mean). The initial conditions correspond to a laminar flame structure with  $\psi = 0$  and  $r = r_L^*$  from Eq.(2.3.5); the long time asymptotic solution will also have the same value for  $r = r_L^*$  so it is reasonable to study the evolution of  $Z$  assuming that  $r = r_L^*$  throughout the transient phase. Using formal asymptotic arguments inspired by the rigorous theory [46] summarized in Section 2.3, we derive an evolution equation for  $Z$  by substituting in Eq.(2.3.1)  $T = \exp(Z/\epsilon)$  with the special form of  $Z$  assumed here. For KPP chemistry,  $f(T)/T = f'(0)$  to leading order; using this result and neglecting higher order terms in  $\epsilon$ , one obtains the following equation :

$$\psi_t - \lambda \sin(2\pi y/P) + \kappa r_L^* \psi_y^2 = f'(0)/r_L^* \quad (2.4.2)$$

This equation looks somewhat similar to the cell-problem defined above, except for two major differences : in the present case, a steady traveling wave solution is

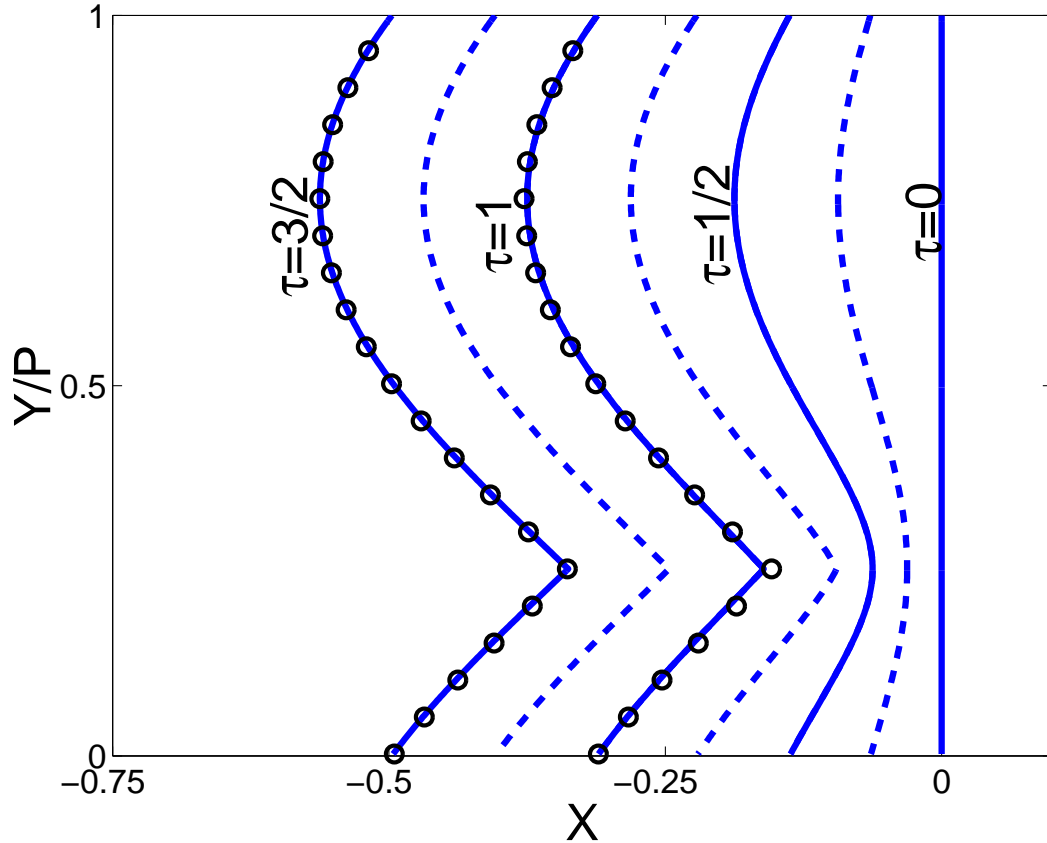


FIG. 2.4. Progressive front distortion starting from a planar front on the right. Solid and dash lines : snapshots of the front from the numerical solution of the evolution equation ; circles : steady-state solution  $\psi_s(y)$  from Eq.(2.4.1).

sought instead of a time periodic perturbation ; also Eq.(2.4.2) is not an eigenvalue problem, unlike the cell-problem, since its right-hand-side is known a priori. A convenient diagnostic to study the evolution of the front is to look at its distortion  $d(t)$ , defined as the maximum horizontal distance between two points on the front at any given time. For the present case, the distortion can be seen to simply correspond to the difference between the front  $x$ -location at the shear extrema :

$$d(t) = \max(\psi(y, t)) - \min(\psi(y, t)) = \psi(P/4, t) - \psi(3P/4, t) \quad (2.4.3)$$

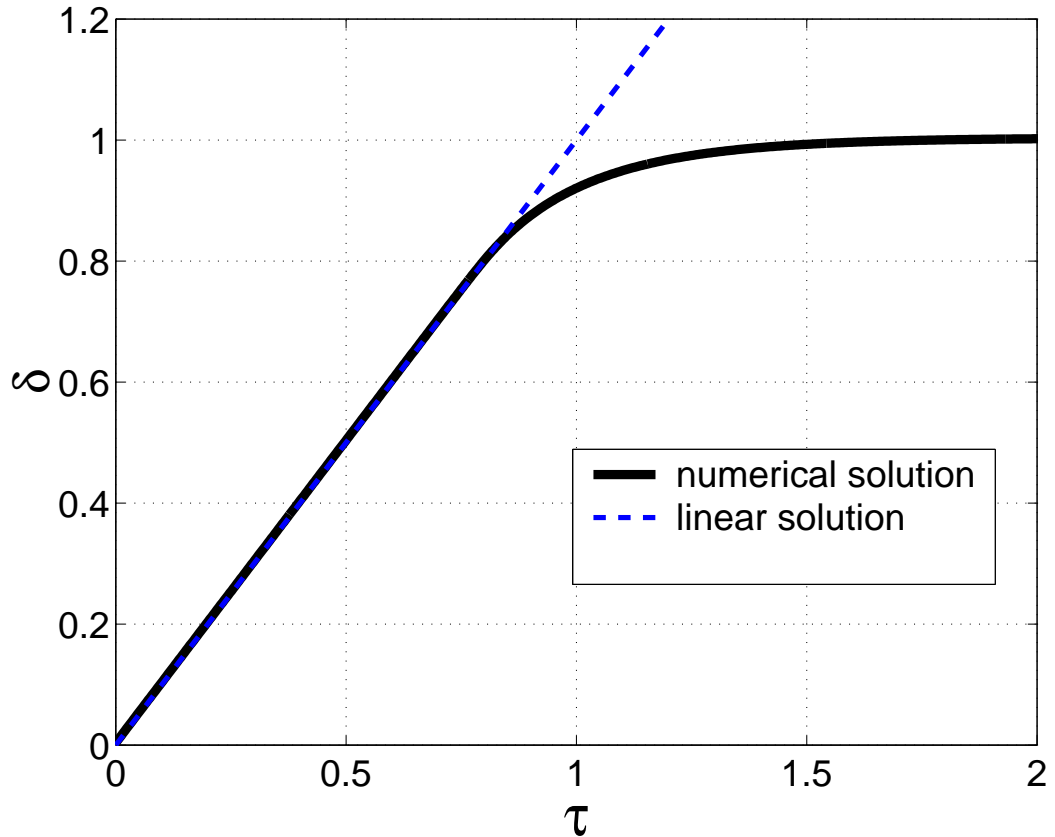


FIG. 2.5. Evolution of the normalized distortion amplitude  $\delta$  corresponding to the computation in Fig. 2.4; convergence to the full distortion  $\delta = 1$  for non-dimensional time  $\tau \approx 1$ .

Its initial value is  $d(t = 0) = 0$  and its final value, at steady state, can be obtained from Formula (2.4.1) as  $d_s = \frac{2}{\pi}P\sqrt{\lambda/S_L}$ . For a finite time, the solution  $\psi$  will be smooth (eventually a cusp will form at  $y = P/4$ ); as long as no cusp has formed, taking the difference between the evolution equation in (2.4.2) respectively at  $y = P/4$  and  $y = 3P/4$  will lead to a very simple linear equation for  $d(t)$  :

$$d_t = 2\lambda \quad (2.4.4)$$

Past the formation of the cusp, one needs to solve for  $\psi(y, t)$  numerically to obtain  $d(t)$ . Time and  $\psi$  can be rescaled as follows : the scale for  $\psi$  is taken to be the front distortion once the steady state has been reached  $d_s = \frac{2}{\pi}P\sqrt{\lambda/S_L}$ . A

time scale based on the linearized equation for  $d(t)$  (Eq.(2.4.4) above) is given by  $d_S/(2\lambda)$ . With the expression for  $d_S$  above, this time-scale turns out to be the wrinkling time  $t_w = \frac{1}{\pi} \frac{P}{S_L} (\lambda/S_L)^{-1/2}$  introduced in Section 2.2. Defining  $\tau = t/t_w$ ,  $\tilde{\psi}(y/P, \tau) = \psi/d_S$ , and  $\delta(\tau) = d(t)/d_S$ , one can easily verify that the evolution equation for  $\tilde{\psi}(y/P, \tau)$  (and hence for  $\delta(\tau)$ ) is independent of  $\lambda$ . Snapshots of the numerical results for the rescaled front are shown in Fig. 2.4 with the initial value on the right. A cusp is seen to form between  $\tau = 1/2$  and  $\tau = 1$ . By the time  $\tau = 1$ , the perturbation in the front with respect to the mean is in very good agreement with  $\psi_s(y)$ , the steady-state prediction from Formula (2.4.1), shown as black circles. Fig. 2.5 shows the normalized front distortion  $\delta(\tau) = d(\tau)/d_s$ : this plot confirms that  $\tau = 1$  is a good estimate for the time-scale for convergence to the asymptotic state  $\delta(\tau) = 1$ . The linear theory that was used to produce this estimate is also shown. There is excellent agreement between the nonlinear curve and the linear curve for most of the growth, which explains the merit of the linear estimate for the time-scale  $t_w$ .

An important observation is that, everything else being equal, a smaller intensity  $\lambda$  will lead to a longer wrinkling time scale ( $t_w$  is proportional to  $(\lambda/S_L)^{-1/2}$ .) For unsteady cases, this means that when  $\lambda$  is small, not only is the maximum possible enhancement small (proportional to  $\lambda$ ) but also it takes a much longer time to achieve it, so that in practice, at a finite time, the overall enhancement will be a small fraction of a small number, hence very small. (see the appendix of [8] for a qualitatively similar discussion for the case of a front obeying the G-equation).

### 2.4.3. reference case : prediction for the limit of $\omega \rightarrow 0$

In the introduction, the limit case of an infinitely slowly modulated shear ( $\lim \omega \rightarrow 0$  in Formula (2.2.1)) was used to define a reference burning speed enhancement. Notice that this limit is different from the enhancement obtained above simply

setting  $\omega = 0$  as done at the beginning of this section. The limit we are interested in corresponds to the average over the modulation period, which is infinitely long when  $\lim \omega \rightarrow 0$ ; over that period, the shear modulated amplitude will take on all possible values between 0 and  $\lambda$  and the reference enhancement  $Se_0$  used in the introduction is obtained by averaging over all such amplitudes across the period. Because the frequency is so small, unsteady effects are negligible and one can assume that at any time, the response of the flame corresponds to the asymptotic long-time solution corresponding to the instantaneous modulated amplitude, so that the average over one period is given by :

$$Se_0 = \lim_{\omega \rightarrow 0} \frac{\omega}{2\pi} \int_{t=0}^{t=\frac{2\pi}{\omega}} \lambda |\cos(\omega t)| dt = \frac{2\lambda}{\pi} \quad (2.4.5)$$

(for more details, see Section 2.6 below where formal asymptotics for both the fast and slow regimes are discussed.)

## 2.5. NUMERICAL SOLUTION OF THE UNSTEADY CELL-PROBLEM

The minimization step in Eq.(2.3.4) for the burning speed prediction is performed with the routine DUVMIF from the IMSLM library [13]. This routine finds the minimum point of a smooth function of a single variable using only function evaluations. This requires an efficient routine to compute the effective Hamiltonian  $H(r)$  since this routine will be called many times during the minimization process.

The effective Hamiltonian  $H(r)$  is computed via the cell-problem in Eq.(2.3.3); it is a nonlinear eigenvalue problem for  $H(r)$  and for the bi-periodic eigenfunction  $\psi(y, t)$  (with period  $[0, P] \times [0, T]$  and mean zero). Designing a numerical strategy to solve it is a challenge : the routine will be called by the minimization procedure for a range of values of  $r$ , so computing  $H(r)$  must be efficient and must not require any special a priori knowledge of the solution for the eigenvalue. One strategy would be to discretize Eq.(2.3.3) with finite differences and then solve

the resulting algebraic eigenvalue problem. This type of strategy would be neither efficient nor simple to use. Here are some of the difficulties that one would encounter. For accuracy reasons, the discretization steps would need to be small, resulting in a matrix problem that is both large and nonlinear, hence very costly numerically. Most likely, an iterative procedure would have to be used, requiring a good initial guess for the solution; some theoretical upper-bounds are known for the eigenvalue, but there are many cases for which those bounds turn out not to be practical for wild guesses for  $r$  during the early stages of the optimization. Another fundamental difficulty with the matrix approach is that the eigenfunction  $\psi(y, t)$  might develop cusps (as seen in Fig. 2.4 for the steady case). This means that upwinding or an explicit numerical viscosity must be used in the discretization, either which must be solution-dependent, hence further complicating the formulation as a matrix problem.

To circumvent those difficulties, we used an alternative strategy inspired by the procedure designed by Embid et al. in [24]. In that paper, the cell-problem was formulated for a steady shear, but with an arbitrary angle between the flame front and the shear direction and also with an arbitrary transverse mean flow (we will revisit that problem in Section 2.7 of this paper). In that case, the solution is steady so the eigenfunction is one-dimensional  $\psi(y)$  and there is actually a way of solving the eigenvalue problem utilizing only numerical quadrature and a root finder, as described in [24]. The problem is more complex for the unsteady case considered here and there is no such explicit procedure to compute the solution, but one key idea still works. The effective Hamiltonian  $H(r)$  does not actually require a solution for the eigenfunction  $\psi(y, t)$  itself, all that is needed is  $\psi_y(y, t)$ . Indeed, integrating Eq.(2.3.3) over the bi-periodic domain and taking into account the periodicity and zero-mean of  $v(y, t)$  and of  $\psi(y, t)$  results in an explicit formula

for  $H(r)$  in terms of  $\psi_y$  :

$$H(r) = \kappa r^2(1 + \langle \psi_y^2 \rangle_{P,T}) \quad (2.5.1)$$

where  $\langle \psi_y^2 \rangle_{P,T}$  represents the average of  $\psi_y^2(y, t)$  over the bi-periodic domain. Looking for a solution for  $\psi_y$  instead of  $\psi$  greatly simplifies the problem : the evolution equation for  $\psi_y$  is obtained by differentiating Eq.(2.3.3) with respect to  $y$ , hence effectively getting rid of the eigenvalue  $H(r)$ ! Introducing  $w(y, t) = r\psi_y(y, t)$ , the resulting nonlinear equation (no eigenvalue, though) for  $w$  is given by :

$$-w_t + (\kappa w^2 + rv(y, t))_y = 0 \quad (2.5.2)$$

with the following conditions :  $w(y, t)$  must be bi-periodic on  $[0, P] \times [0, T]$ ,  $w(y, t)$  must be of mean zero over the bi-periodic domain as was the case for  $\psi(y, t)$ ; additionally, because  $w(y, t)$  is the  $y$ -derivative of a periodic function, the average of  $w(y, t)$  with respect to  $y$  on  $[0, P]$  must be zero, for any fixed value of  $t \in [0, T]$ . The solution for  $w(y, t)$  is obtained by viewing Eq.(2.5.2) as the steady state for a pseudo time-marching conservation law :

$$u_s + \nabla_{\mathbf{z}} \cdot \mathbf{F}(u(s, \mathbf{z}), \mathbf{z}) = 0 \quad (2.5.3)$$

where the variables are  $s$ , the pseudo-time variable for marching, and the two original variables  $\mathbf{z} = (y, t)$ . The new unknown is  $u(s, \mathbf{z})$  and the flux  $\mathbf{F}$  is given by  $\mathbf{F}(u, \mathbf{z}) = [\kappa u^2 + rv(\mathbf{z}), u]$ . Eq.(2.5.3) is integrated numerically starting with the initial data  $u(0, \mathbf{z}) = 0$  at  $s = 0$ . A fourth order ENO scheme for conservation law [32] is used for the discretization. Using a conservative formulation and imposing periodic boundary conditions on  $u$  with respect to  $\mathbf{z} = (y, t)$  guarantees that the zero-mean conditions to be satisfied by  $w$  are always satisfied by  $u$  for any value  $s > 0$  because they were trivially satisfied at  $s = 0$ . Therefore, at steady-state, a solution for  $w(y, t)$  will have been obtained.

This approach has proved to be very robust for practical computations, it capitalizes on well-established numerical techniques for the solution of conservation

TAB. 2.1. Convergence of the effective Hamiltonian (relative error).

	ENO2	ENO3	ENO4
10 points	0.0509	0.0662	0.1122
20 points	0.0671	0.0629	0.0422
40 points	0.0318	0.0306	0.0205
80 points	0.0155	0.0151	0.0101

laws and it requires no a priori knowledge of the solution unlike what is usually the case for large eigenvalue problems, let alone nonlinear. Validation tests were performed by comparing the solution for the steady case with  $\lambda/S_L = 1$  obtained using this time-marching conservation law approach with the predictions from the explicit formulas in Section 2.4. The convergence of the effective Hamiltonian with respect to mesh refinement in  $y$  is reported in Tab. 2.1 for schemes of formal order 2, 3, 4 (the solution is steady so refinement in time is irrelevant). For the steady case, cusps play a dominant role in limiting the accuracy of the numerical solution so that globally, all schemes reduce to first order. Nevertheless, convergence is indeed achieved and the benefit of using higher order methods becomes more significant for flame fronts with more small scale spatial structures besides cusps.

A similar strategy for more complex cell-problems with two-spatial variables is described elsewhere [38] [11], including a detailed discussion of the conditions for effective convergence to a steady-state for the pseudo-time. The main result in [38] is that a critical condition for such convergence is that the computed solution be effectively the spatial gradient of a scalar function in some discrete sense. In the one space-dimension cases studied in this paper, this condition is always trivially satisfied for a one-dimensional function in space and the convergence result of [38] automatically applies.

## 2.6. ASYMPTOTIC ANALYSIS



### 2.6.1. nondimensionalized cell-problem

The cell-problem Eq.(2.3.3) is rescaled using the following :

- time scale  $T = 2\pi/\omega$ ; non-dimensional time  $\tau = t/T$
- length scale  $P$ ; non-dimensional  $y$ -coordinate  $\tilde{y} = y/P$
- non-dimensional eigenfunction  $\tilde{\psi}(\tilde{y}, \tau) = \psi/d_s = \psi(y, t)/(\frac{2}{\pi}\sqrt{\frac{\lambda}{S_L}}P)$  (see the expression for  $d_s$  as in Section 2.4.2)
- rescaled Hamiltonian  $\tilde{H} = (H - \kappa r^2)/(\lambda r)$  (hence in the steady case  $\tilde{H} = 1$ );
- non-dimensional exponential decay rate  $\rho = r/r_L^*$  (hence in the steady shear case,  $\rho = 1$ ).

The resulting non-dimensional equation is given by :

$$\frac{2}{\tilde{t}}\tilde{\psi}_\tau - \frac{2}{\pi^2}\rho\tilde{\psi}_y^2 + \sin(2\pi\tilde{y})\cos(2\pi\tau) = -\tilde{H} \quad (2.6.1)$$

where  $\tilde{t}$  is the non-dimensionalized flame residence time introduced in Eq.(2.2.6). Asymptotic behavior for small or large values of  $\tilde{t}$  are discussed next; in particular, it will be shown how the reference solution for the steady shear case in Section 2.4 plays a distinct role explaining the solution in each regime. A rigorous asymptotic analysis would entail the type of machinery used by Majda and Souganidis in [46] with tools such as test functions for viscosity solutions etc. Here we give only formal arguments that provide some insight on the behavior of the solution. Furthermore, our numerical results confirm the validity of the asymptotic expansions developed below.

### 2.6.2. Slow Regime : quasi-steady approximation

In the slow regime, the flame residence time  $\tilde{t}$  is large and we will seek an expansion in terms of  $\epsilon = 1/\tilde{t}$  (dropping the tilde) :

$$\psi = \frac{1}{\epsilon}\psi^{(-1)}(y, \tau) + \psi^{(0)}(y, \tau) + \epsilon\psi^{(1)}(y, \tau) + \dots$$

$$H = \frac{1}{\epsilon^2}H^{(-2)} + \frac{1}{\epsilon}H^{(-1)} + H^{(0)} + \epsilon H^{(1)} + \dots$$

Plugging those expressions in Eq.(2.6.1) and collecting terms of same order in  $\epsilon$  gives a sequence of equations :

**Order  $\epsilon^{-2}$  :**

$$-\frac{2\rho}{\pi^2}(\psi_y^{(-1)})^2 = -H^{(-2)}$$

The unique solution to this problem is trivial :  $H^{(-2)} = 0$  and  $\psi_y^{(-1)} = 0$  so that  $\psi^{(-1)}$  is a function of time only, arbitrary at this point.

**Order  $\epsilon^{-1}$  :**

One can easily verify that there are no order  $1/\epsilon$  terms on the left hand side and one obtains directly  $H^{(-1)} = 0$ .

**Order  $\epsilon^0$  :**

$$2\psi_\tau^{(-1)} - \frac{2\rho}{\pi^2}(\psi_y^{(0)})^2 + \sin(2\pi y) \cos(2\pi\tau) = -H^{(0)} \quad (2.6.2)$$

We will now show how one can construct explicitly a solution to this equation by building on the solution for the steady problem from Section 2.4. Because of the slow time modulation, we expect that at any time  $\tau$ , the flame front has adjusted instantaneously to the modulated shear of intensity  $\lambda \cos(2\pi\tau)$ . This implies that we expect that  $\psi^{(0)}(y, \tau)$  satisfies the following steady cell-problem, where  $\tau$  is viewed as a parameter :

$$-\frac{2\rho}{\pi^2}(\psi_y^{(0)})^2 + \sin(2\pi y) \cos(2\pi\tau) = -H^{(0)}(\tau)$$

The solution to that auxiliary problem is known : results in Section 2.4 give  $H^{(0)}(\tau) = |\cos(2\pi\tau)|$  and the rescaled perturbation  $\psi^{(0)}$  is given by

$$\psi^{(0)}(y, \tau) = \sqrt{|\cos(2\pi\tau)|} f(y)$$

where the detailed expression for  $f(y)$  will not be needed here. Plugging the expression for  $H^{(0)}(\tau)$  in Eq.(2.6.2) will impose the missing condition on  $\psi^{(-1)}$  and most importantly provide a way of computing  $H^{(0)}$  :

$$\pi\psi_\tau^{(-1)} - H^{(0)}(\tau) = -H^{(0)}$$

Recalling that  $\psi^{(-1)}$  is a periodic, zero-mean function over the time period, one can integrate this equation over a time period to obtain an expression for  $H^{(0)}$  :

$$H^{(0)} = \langle H^{(0)}(\tau) \rangle_T = 2/\pi$$

where  $\langle \cdot \rangle_T$  denotes the integration over the time period. At this point, one could easily integrate the equation for  $\psi^{(-1)}$  but this result is not needed here since all we really care about is the burning speed. The rescaled Hamiltonian  $H^{(0)}$  can be used to compute the leading order for the burning speed enhancement :

$$Se^{(0)} = \min_{r>0} \frac{f'(0) + r\lambda(H^{(0)}) + \kappa r^2}{r} - S_L = 2\lambda/\pi$$

which is the result that was announced in Section 2.2.

**Order  $\epsilon^1$  :**

$$2\psi_\tau^{(0)} - 4\rho\psi_y^{(0)}\psi_y^{(1)} = -H^{(1)}$$

At this order, the formal asymptotic strategy presented here breaks down because  $\psi_\tau^{(0)}$  is not sufficiently smooth. Regardless, it is plausible that this equation would lead to a correction of order  $\epsilon = 1/\tilde{t}$  in the rescaled Hamiltonian and hence explains the correction of the same form for  $Se_N$  that was observed in the numerical data for the enhanced speed. Further confirmation is provided in Fig. 2.6 which corresponds to a test case with  $\omega = 0.001$ ,  $\lambda = 2$ ,  $P = 1$ ,  $S_L = 1$  so that

$\tilde{t} = 2.8 \times 10^4$ , certainly large enough for the slow regime approximation. Pictured are the detailed spatial profile for the front perturbation with respect to the mean for various snapshots throughout the period along with their quasi-steady approximation  $\psi^{(0)}$  as computed above. For most snapshots, there is perfect agreement between the two; the only snapshot where one can actually see the difference between the computed profile and its quasi-steady approximation corresponds to the value  $\tau = 0.26$  near  $1/4$ :  $\tau = 1/4$  is the time at which the quasi-steady approximation breaks down at order  $\epsilon$  for lack of smoothness of the time derivative, so the differences between the two profiles around that particular time are to be expected. Nevertheless, the asymptotic prediction for the enhanced speed was reported in Section 2.2 to be very good overall.

### 2.6.3. Fast Regime : linear perturbation

When  $1/\tilde{t}$  is very large in Eq.(2.6.1), we seek an asymptotic expansion in terms of  $\tilde{t}$ :

$$\tilde{\psi}(\tilde{y}, \tau) = \psi^{(0)}(\tilde{y}, \tau) + \tilde{t}\tilde{\psi}^{(1)}(\tilde{y}, \tau) + \tilde{t}^2\tilde{\psi}^{(2)} + \tilde{t}^3\tilde{\psi}^{(3)} + \dots$$

$$\tilde{H} = \frac{1}{\tilde{t}}\tilde{H}^{(-1)} + \tilde{H}^{(0)} + \tilde{t}\tilde{H}^{(1)} + \tilde{t}^2\tilde{H}^{(2)} + \tilde{t}^3\tilde{H}^{(3)} + \dots$$

We plug these expressions in Eq.(2.6.1) and collect terms of same order in  $\tilde{t}$ :

**Order  $\tilde{t}^{-1}$  :**

$$2\tilde{\psi}_\tau^{(0)} = -\tilde{H}^{(-1)}$$

Taking into account that  $\tilde{\psi}$  is bi-periodic of mean zero (and hence, so are all the terms in the expansion  $\tilde{\psi}^{(i)}$ ), the only solution possible is  $\tilde{H}^{(-1)} = 0 = \tilde{\psi}^{(0)}$ .

**Order  $\tilde{t}^0$  :**

$$2\tilde{\psi}_\tau^{(1)} + \sin(2\pi\tilde{y}) \cos(2\pi\tau) = -\tilde{H}^{(0)}$$

Averaging with respect to  $\tilde{y}$  and  $\tau$  over the periodic box  $[0, 1] \times [0, 1]$ , one gets immediately that  $\tilde{H}^{(0)} = 0$ . One can then integrate the resulting linear equation

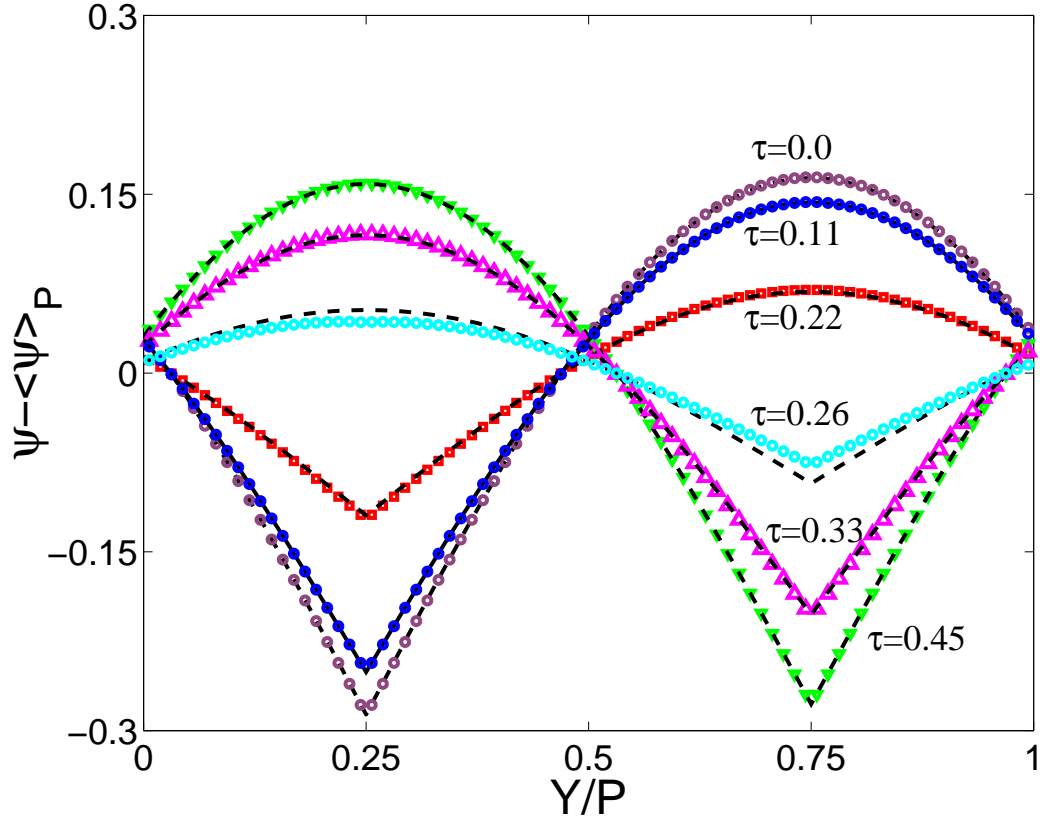


FIG. 2.6. Slow regime : successive snapshots of the front perturbation  $\psi$  with respect to its spatial mean  $\langle\psi\rangle_P$ . Comparison between the numerical solutions of the nonlinear cell-problem (symbols) and the quasi-steady approximation (dash line).  $\omega = 0.001$ ,  $\lambda = 2$ , corresponding to a very large non-dimensional flame residence time  $\tilde{t} = 2.8 \cdot 10^4$ .

for  $\psi^{(1)}$  :

$$\tilde{\psi}^{(1)}(\tilde{y}, \tau) = \frac{1}{4\pi^2} \sin(2\pi\tilde{y}) \sin(2\pi\tau) + \tilde{\psi}^{(1,A)}(\tilde{y}) = \tilde{\psi}^{(1,B)}(\tilde{y}, \tau) + \tilde{\psi}^{(1,A)}(\tilde{y}) \quad (2.6.3)$$

where  $\tilde{\psi}^{(1,A)}$  is at this point an arbitrary function which can depend on  $\tilde{y}$  only.

**Order  $\tilde{t}^1$  :**

$$2\tilde{\psi}_\tau^{(2)} = -\tilde{H}^{(1)}$$

The same arguments used for the order  $1/\epsilon$  terms lead to  $H^{(1)} = 0 = \tilde{\psi}^{(2)}$ .

**Order  $\tilde{t}^2$  :**

$$2\tilde{\psi}_\tau^{(3)} - \frac{2\rho}{\pi^2}(\tilde{\psi}_y^{(1)})^2 = -\tilde{H}^{(2)}$$

Averaging this expression over time leads to :

$$\frac{2\rho}{\pi^2}\langle(\tilde{\psi}_y^{(1)})^2\rangle_T = H^{(2)}$$

Taking into account the expression for  $\tilde{\psi}^{(1)}$  in Eq.(2.6.3) gives :

$$\langle(\tilde{\psi}_y^{(1,A)})^2\rangle + \langle(\tilde{\psi}_y^{(1,B)})^2\rangle_T = \pi^2 H^{(2)} / (2\rho)$$

Manipulating the trigonometric expression results in :

$$(\psi_y^{(1,A)})^2 + (1 + \cos(4\pi\tilde{y})) / 16 = \pi^2 \tilde{H}^{(2)} / (2\rho)$$

The solvability condition at order  $\tilde{t}^2$  is therefore similar to a cell-problem for a steady shear  $\frac{\cos(4\pi\tilde{y})}{16}$  plus a mean  $\frac{1}{16}$  ! Predictions for a steady shear are known from Section 2.4 and it is trivial to add a steady horizontal mean. As a result of this forcing, the  $\tilde{y}$ -period of the time-average component  $\tilde{\psi}^{(1,A)}$  is now  $1/2$  (so the period for the mean has been halved compared to the period of the original forcing shear.) Using the prediction for  $\tilde{H} = \tilde{t}^2 \tilde{H}^{(2)}$  in the minimization step to predict the enhanced speed in Formula (2.3.4) leads to the result that :

$$Se = S_L \left( \sqrt{1 + \frac{\lambda \tilde{t}^2}{2S_L \pi^2}} - 1 \right)$$

For  $\tilde{t}$  small, this can be approximated by :

$$Se = \frac{\lambda \tilde{t}^2}{4\pi^2}$$

Hence, we recover the following expression for the normalized enhanced speed in the fast regime :

$$Se_{N,fast} = \frac{\tilde{t}^2}{8\pi}$$

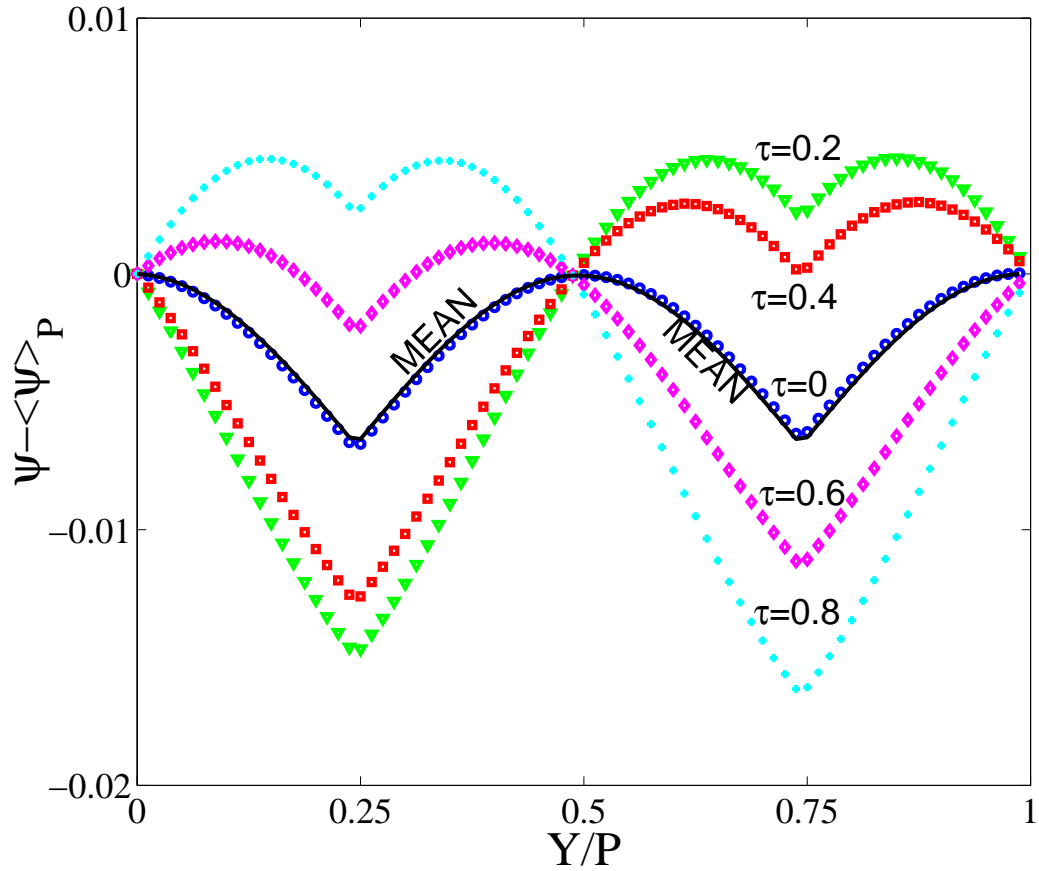


FIG. 2.7. Fast regime : successive snapshots of the front perturbation  $\psi$  with respect to its spatial mean  $\langle\psi\rangle_P$  from the numerical solution of the nonlinear cell-problem (symbols). The solid line corresponds to the time-average of those snapshots over one time period (it coincides pretty much with the  $\tau = 0$  snapshot.)  $\omega = 106$ ,  $\lambda = 2$ , corresponding to a small non-dimensional flame residence time  $\tilde{t} = 0.2634$ .

This speed is exactly what was obtained by fitting the data as presented in Section 2.2.

Through numerical simulations, we examine the spatial structure of the front in more details, in particular of its time-averaged behavior. Fig. 2.7 displays the

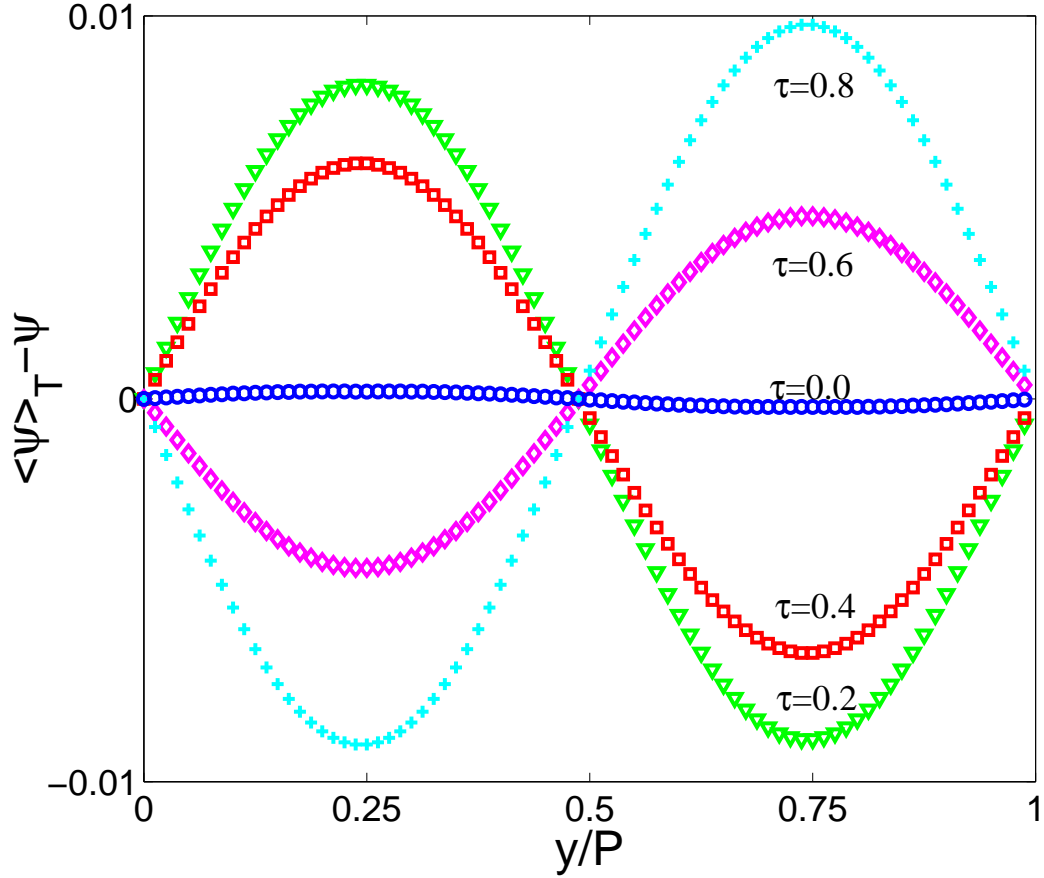


FIG. 2.8. Same data as in Fig. 2.7, but with the temporal mean  $\langle \psi \rangle_T$  subtracted from each profile.

eigenfunction at various non-dimensional times  $\tau = t/T$  throughout the time-period as well as the mean component. The time fluctuations are shown in the plot in Fig. 2.8; they are obtained by subtracting from the eigenfunction the time-averaged component. As predicted by the asymptotic analysis, the unsteady part of the eigenfunction (Fig. 2.8) is a smooth Fourier mode while the time-averaged profile (solid curve in Fig. 2.7) is a double-cusp solution as would be obtained with a steady shear of period  $P/2$ . The capturing of such small amplitude cusps is possible in the present computation because no excessive numerical viscosity was used in the computation, instead high order ENO schemes for Hamilton-Jacobi equations are used to deal with the nonlinearity. A physical explanation for the



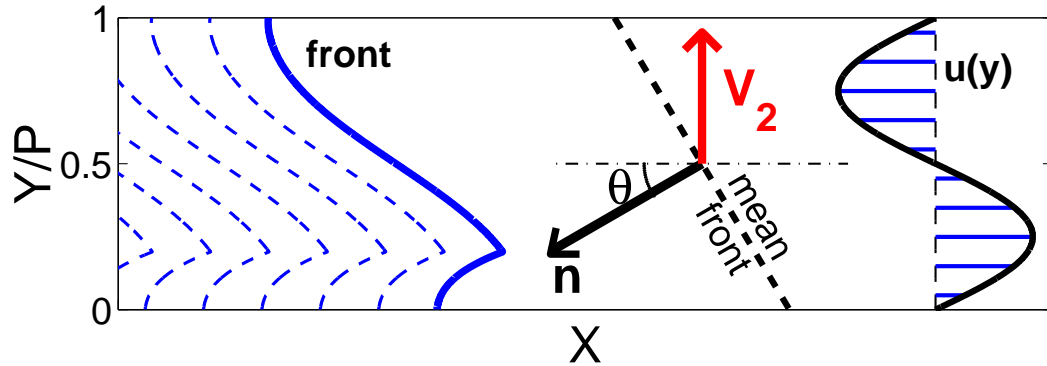


FIG. 2.9. Set-up for the traveling mode case : normal  $\mathbf{n}$  to the mean front tilted at angle  $\theta$  with respect to the steady horizontal shear  $\mathbf{u}(y)$  direction ; mean flow  $V_2$  transverse to the shear direction.

coexistence of the cusps at the local extrema of the shear is easy to understand : in the quasi-steady case, there is alternatively a cusp at  $y = 1/4$  (when the modulated amplitude  $\lambda \cos \omega t$  is positive) and at  $y = 3/4$  (which is the front minimum when the modulated amplitude is negative). The solution evolves on a sufficiently slow time scale that the cusp at one extremum has time to disappear before another cusp reappears at the other extremum. In the fast regime we are presently looking at, it is not the case, the flame has no time to adjust beyond the linear fluctuations ; amplitudes are small and both cusps coexist at all times.

## 2.7. TRAVELING WAVE MODE

We now illustrate the use of the flame residence time concept for another simple test case. The new set-up in this section corresponds to a test-case studied extensively by Embid et al. [25] [24] for the purpose of contrasting predictions obtained with the rigorous averaging procedure (as outlined in Section 2.3) with those obtained based on ad-hoc averaging via the G-equation limit. The flame is now subjected to a horizontal shear which, unlike in the previous case, is now steady and to which we have also added a constant mean flow of intensity  $V_2$

orthogonal to the shear direction :

$$\mathbf{u}(\mathbf{x}, \mathbf{y}, \mathbf{t}) = (\lambda \sin(2\pi \frac{y}{P}), V_2)$$

(one can easily verify that, with the present set-up, a mean flow  $V_1$  along the shear direction will just result in a Galilean change of frame of reference and hence will not affect the burning speed turbulent enhancement). Moreover, the mean front is no longer assumed to be normal to the shearing direction, but is allowed to be tilted with an arbitrary angle  $\theta$  between the front normal  $\mathbf{n}$  and the shear direction. This configuration is particularly amenable to extensive study because the cell problem entails now a one-dimensional function  $\psi(y)$  :

$$-\kappa r^2(\cos^2 \theta + (\sin \theta - \psi_y)^2) + \lambda r \sin(2\pi y/P) \cos \theta + V_2 r (\sin \theta - \psi_y) = -H \quad (2.7.1)$$

(indeed it is easy to verify that with  $\mathbf{u}$  defined above, the front perturbation with respect to the mean is steady and is the graph of a function of  $y$ .)

Solving this problem can be done numerically using only simple quadratures and root solvers [25] [24]. The burning speed enhancement was shown to be particularly sensitive to the ratio  $V_2/S_L$ , with either a quadratic or a linear dependence on the shear intensity  $\lambda$  depending on the ratio being very large or very small. Here, we apply the concepts developed in this paper to understand those results. Even though the solution is steady, we will show next that a non-dimensional flame residence time argument still applies and is sufficient to explain this sensitive dependence.

First, we rewrite the cell-problem from Eq.(2.7.1)

$$-\kappa r^2(1 + \psi_y^2) + \lambda r \sin(2\pi y/P) \cos \theta + V_2 r (\sin \theta - \psi_y) + 2\kappa r^2 \sin \theta \psi_y = -H$$

One recovers an equation very similar to the cell-problem for the standing-wave case by introducing the following change of variables :

$$\xi = y - (V_2 - \rho S_L \sin \theta)t \quad \tau = t$$

with  $\rho = r/r_L^*$  (as introduced in Section 2.6) and  $S_L = 2\kappa r_L^*$  (see Formula (2.3.5)). In the new frame of reference, the cell problem becomes :

$$r\phi_\tau - \kappa r^2(1 + \psi_\xi^2) + r\tilde{\lambda} \sin(2\pi\xi/P - \omega\tau) = -\tilde{H} \quad (2.7.2)$$

with the reduced shear intensity  $\tilde{\lambda} = \lambda \cos \theta$ , the equivalent flow frequency  $\omega = 2\pi(V_2 - \rho S_L \sin \theta)/P$  and  $\tilde{H} = H + rV_2 \sin \theta$ . This equation is very similar to the cell-problem Eq.(2.3.3) studied in the previous sections (except that the shear now corresponds to a traveling sine, instead of a pulsating sine and that the shear frequency  $\omega$  is now a function of  $r$ , the minimization variable.) Accordingly, this suggests that the following time scales will play an important role in the scaling for the burning speed enhancement :

- $t_r = 2\pi/\omega = P/|V_2 - \rho S_L \sin \theta|$  as the relevant flow characteristic time, the so-called "flame residence time". Its physical interpretation is clear if one considers a marker on the mean front that is advected by the mean flow and also moves normal to the front with a speed  $\rho S_L$ .  $t_r$  represents the time period for such a marker to loop once through the shear  $y$ -period, hence the reference to the flame residence time.
- $t_w = \frac{1}{\pi} \frac{P}{S_L} \frac{1}{\sqrt{\tilde{\lambda}/S_L}}$  as the flame intrinsic wrinkling time. It is identical to the expression used before, except that it takes into account the fact that the component of the shear normal to the front is now reduced to  $\tilde{\lambda} = \lambda \cos \theta$ .

As for the standing mode, we define the nondimensional flame residence time  $\tilde{t}$  as the ratio of the two time scales above :

$$\tilde{t} = \frac{t_r}{t_w} = \pi \frac{\sqrt{\lambda |\cos \theta|}}{|V_2/S_L - \rho \sin \theta|} \quad (2.7.3)$$

One expects as before that large values of  $\tilde{t}$  will correspond to large enhancements, linear in the shear intensity (or more precisely linear in  $\tilde{\lambda}$ , the shear's component normal to the mean front) while small values of  $\tilde{t}$  will correspond to much smaller enhancements. This is confirmed next by asymptotic analysis and numerical simulations. Of course, now that the issues of identifying relevant "time-scales" for this steady problem have been addressed, we return to the original formulation in Eq.(2.7.1) which leads to much simpler analysis as the cell-problem in that frame of reference corresponds to a steady, one-dimensional eigenfunction.

As we did in Section 2.4 for the standing mode case, we first look at the limit case  $\omega \rightarrow 0$ . In the present case, one can easily check that it is obtained by simply setting  $\omega = 0$  in Eq.(2.7.2) so that one can use directly the predictions in Section 2.4 for a steady shear of intensity  $\tilde{\lambda} = \lambda |\cos(\theta)|$ . In particular, the burning speed enhancement  $Se_0 = \tilde{\lambda}$  and this value will be used to normalize the results to be discussed next for non-zero values of  $\omega$ .

### 2.7.1. slow regime

When  $\omega = 0$ , the effect of the transverse mean flow and that of the self-propagation of the front normal to itself cancel each other exactly. We are now interested in small departures from this balance, with  $\omega$  very small so that the flame residence time is large. One way to approach it is to do a small parameter expansion in terms of  $1/\tilde{t}$  as was done in Section 2.6 for the standing mode problem. We present here an alternative approach. One feature of the steady case is that the cell-problem eigenvalue is achieved at its lower bound as explained next. Indeed, in Eq.(2.3.3) for the steady case, it is clear that

$$H = \kappa r^2(1 + \psi_y^2) - rv(y) \geq H_{min} = \kappa r^2 - r \min_y(v(y)) = \kappa r^2 + r\lambda$$

This lower bound  $H_{min}$  is precisely the effective Hamiltonian reported in Section 2.4. We will now formulate the problem in Eq.(2.7.1) so that again we can easily obtain a lower bound for the eigenvalue and we will make the assumption that the

eigenvalue is still well approximated by its lower bound, as it is exactly the case when  $\omega = 0$ . First we define  $U = \sin \theta - V_2/(2\kappa r)$  and use it to rewrite equation 2.7.1 as :

$$-\kappa r^2(1 + (\psi_y - U)^2) + r\tilde{\lambda} \sin(2\pi y/P) = -\tilde{H} \quad (2.7.4)$$

where we have redefined  $\tilde{H} = H + V_2 r \sin \theta + \kappa r^2 U^2$ . Clearly, a lower bound for  $\tilde{H}$  is  $\tilde{H}_{min} = \kappa r^2 + r\tilde{\lambda}$  and hence, a lower bound for  $H$  is given by  $H_{min} = \kappa r^2(1 - U^2) + r\tilde{\lambda} - V_2 r \sin \theta$ . Assuming that  $H$  indeed takes on its lower bound, we plug  $H_{min}$  in the minimization problem in Eq.(2.3.4) to obtain :

$$\begin{aligned} Se &= \inf_{r>0} \frac{f'(0) + H(r)}{r} - S_L + V_2 \sin \theta \\ &= \lambda |\cos(\theta)| + S_L(\sqrt{(\cos \theta)^2(1 - (V_2/S_L)^2)} - 1) + V_2 \sin \theta \end{aligned}$$

where the minimum is achieved for  $r = \rho r_L^*$  with  $\rho = \sqrt{1 - (V_2/S_L)^2}/|\cos \theta|$ . This expression is of course valid only if  $V_2/S_L$  is sufficiently small. A more familiar expression is obtained by doing a Taylor expansion if both  $V_2/S_L$  and  $\sin \theta$  are small; in that case, one can verify that to leading order, the expression for  $Se$  above is equivalent to :

$$Se_N = Se/(\lambda |\cos \theta|) = 1 - \frac{\pi^2}{2\tilde{t}^2}$$

where the non-dimensional residence time is defined as

$$\tilde{t} = \pi \frac{\sqrt{\lambda |\cos \theta|/S_L}}{|\rho \sin \theta - (V_2/S_L)|}$$

with  $\rho = 1$  to first order.

In conclusion, the asymptotic prediction for the slow regime is that to leading order, the burning speed enhancement will again be linear in  $\tilde{\lambda} = \lambda |\cos \theta|$ , i.e. the intensity of the shear in the direction normal to the mean front. While in the standing mode case, the next order correction was linear in  $1/\tilde{t}$ , in the present case, the correction is even smaller, quadratic in  $1/\tilde{t}$ .

### 2.7.2. fast regime

In the fast regime, the strategy is very similar to the one used for the standing wave case and details are omitted. The relevant small parameter for the present case is  $\epsilon = \frac{\lambda |\cos \theta|}{\rho S_L \sin \theta - V_2}$ . An expansion in terms of  $\epsilon$  is carried on and the leading term for the correction of the effective Hamiltonian compared to the laminar case is a second order term in  $\epsilon$ .

$$H = \kappa r^2(1 + \epsilon^2/2) - V_2 r \sin \theta$$

The enhanced turbulent burning speed is then given by :

$$Se = \inf_{r>0} \frac{f'(0) + H(r)}{r} - S_L + V_2 \sin \theta$$

Rigorously, the minimization above must take into account the  $r$ -dependence of  $\epsilon$  (recall that  $\rho S_L = 2\kappa r$ ). The result that is stated next is valid only if one assumes that  $\rho = 1$  to leading order in the expression for  $\epsilon$ . (It turns out that the result below is also exact for the two special cases when either  $V_2 = 0, \theta \neq 0$  or  $V_2 \neq 0, \theta = 0$ .)

$$Se_{N,fast} = \frac{\sqrt{1 + \frac{\epsilon^2}{2}} - 1}{\lambda |\cos \theta| / S_L}$$

with the minimum achieved at  $\rho = \sqrt{1 + \frac{\epsilon^2}{2}}$  which validates the assumption that  $\rho = 1$  to leading order in this regime. Again, a more recognizable expression is obtained as a Taylor series expansion in terms of  $\epsilon$ . To leading order, the normalized burning speed enhancement is therefore obtained as :

$$Se_{N,fast} = \frac{\tilde{t}^2}{4\pi^2}$$

Hence, in the fast regime, the (unnormalized) burning speed enhancement  $Se$  has exactly the same form in both the traveling and standing modes.

### 2.7.3. numerical results

In all three test cases to be described next, the enhanced speed was predicted numerically via the solution of the cell problem using the procedure described in [24]. In the first test case, we investigate the effect of  $V_2$  by computing the burning speed enhancement for the case  $\lambda = S_L$ ,  $V_2/S_L$  varying between 0 and 4 and  $\theta = 0$ . When  $\theta = 0$ , increasing  $V_2$  will always lead to a decrease in flame residence time so that it is expected that the burning speed enhancement will decrease also. This is indeed observed in Fig. 2.10. The circles are the data obtained by solving the complete cell-problem along with the minimization step. The solid and dash curves correspond respectively to the slow and fast asymptotic regimes. When  $V_2$  is closed to zero so that  $\tilde{t}$  is large, one expects the slow regime scaling to apply. As  $V_2$  is increased, a marker on the front would sweep increasingly fast through the shear period, the flame residence time goes down and the burning enhancement is therefore expected to decrease. This is indeed what is observed in Fig. 2.10 : agreement with the simulation is excellent with a clear transition between the two regimes for  $1/\tilde{t} \approx 0.3$ ,  $\tilde{t} \approx 3$ .

The second test case corresponds to  $V_2 = 0$ ,  $\lambda = S_L$  and  $\theta$  varying between 0 and  $\pi$  (symmetric results are expected between  $-\pi$  and 0). Results are displayed in Fig. 2.11. Here we show un-normalized values  $Se(\theta)$ ; normalized values imply dividing by  $|\cos \theta|$  which is not convenient as the denominator goes to zero. While in the previous test case, modifying  $V_2$  had a straightforward effect on the flame residence time and hence on the burning speed enhancement, the effect of a variation of  $\theta$  is more complex : at a non-zero angle  $\theta$ , the front will have a self-propagation component transverse to the shear direction which will reduce the flame residence time compared to the aligned case (formally, this corresponds to the effect of the factor  $\rho S_L \sin \theta$  in the expression for  $\tilde{t}$  in Eq.(2.7.3). Also, because of the tilting, the component of the shear normal to the front will be smaller, so

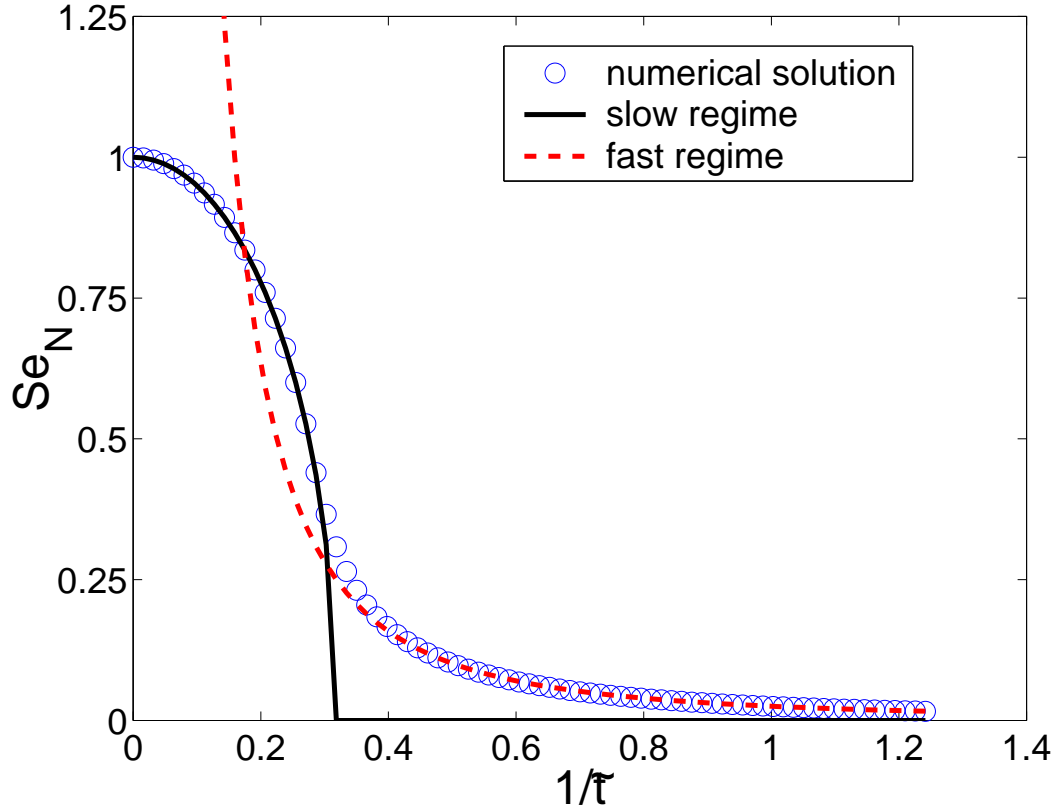


FIG. 2.10. Traveling wave problem : normalized enhanced speed as a function of flame residence time when  $V_2$  is varied while  $\theta = 0$ .

that the maximum achievable enhancement is smaller (this corresponds to the formula  $Se_0 = \lambda |\cos \theta|$ ). Finally, the corresponding wrinkling time is longer, further reducing the normalized flame residence time (this corresponds to the factor  $\lambda |\cos \theta|$  in the expression for  $\tilde{t}$ .) So overall, tilting the front (in the absence of a transverse mean) is also expected to reduce the burning speed enhancement, but this time through a combination of factors. This reduction is indeed observed in Fig. 2.11. For angles  $\theta$  close to 0 or  $\pi$ , the front is hardly tilted and relatively large enhancements are observed, with excellent agreement with the curve corresponding to the slow asymptotic regime. At  $\theta = \pi/2$  on the other hand, the front is parallel to the shear, so that there is actually zero enhancement. For angles close to that value, the flame residence time is very short and very little enhancement



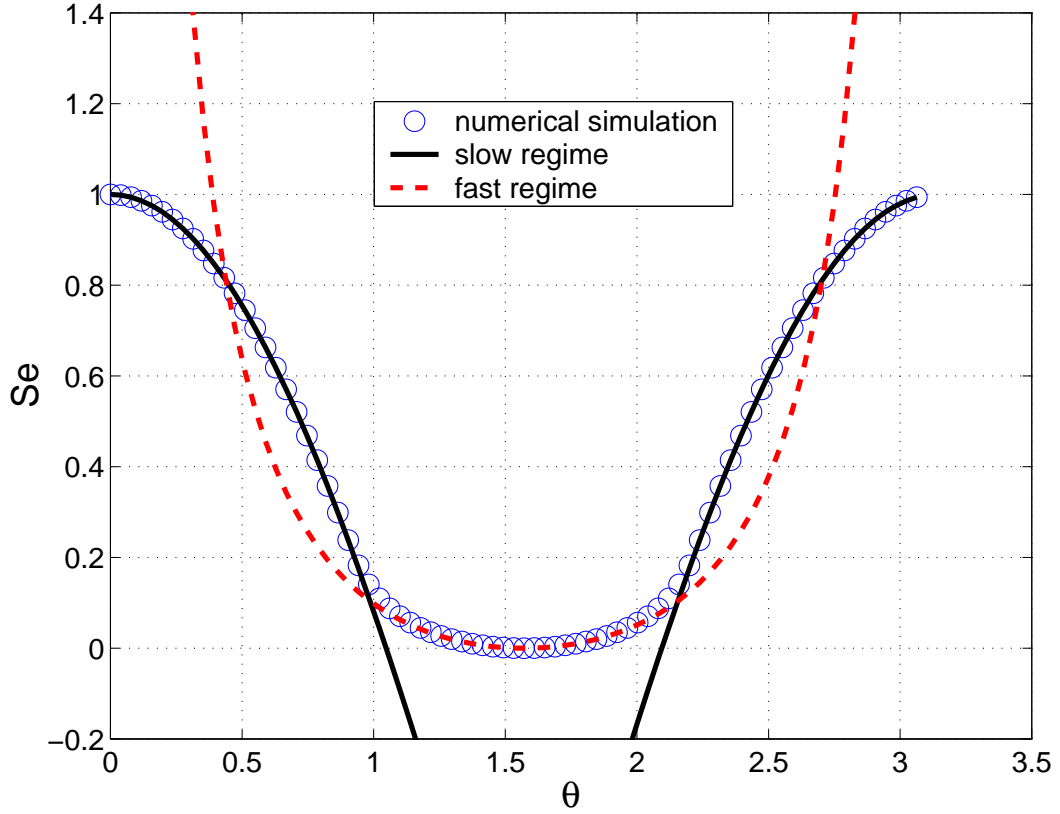


FIG. 2.11. Traveling wave problem : normalized enhanced speed as a function of flame residence time when  $\theta$  is varied while  $V_2 = 0$ .

is observed, with excellent agreement with the fast asymptotic regime predictions.

The final test-case combines the effect of tilting the front and adding a mean velocity  $V_2$  transverse to the shear direction.

In Fig. 2.12, we display the (dimensional) burning speed enhancement  $Se(\theta)$  when  $V_2 = 0.5$ ,  $\lambda = S_L$ , and  $\theta$  varies in  $[-\pi, \pi]$ . The flame residence time is small if the transverse mean component  $V_2$  and the front self-propagating component  $\rho S_L \sin \theta$  nearly balance each other. Assuming that  $\rho$  is equal to one to leading order, as it is the case in either asymptotic regime, there can be a range of angles  $\theta$  for which this balance will be approximately achieved only if  $|V_2|/S_L < 1$ . When this condition is satisfied, there is indeed a solution  $\theta = \theta^*$  such that  $\sin \theta^* - V_2/S_L = 0$

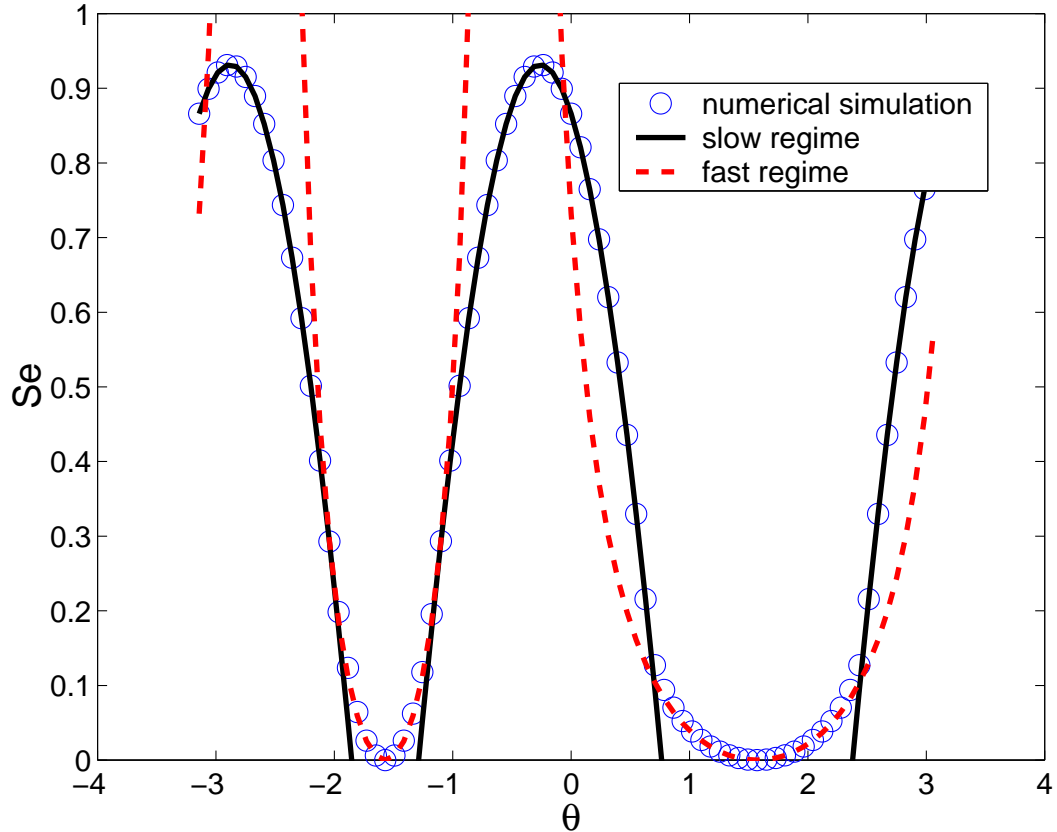


FIG. 2.12. Traveling wave problem : normalized enhanced speed as a function of flame residence time when  $\theta$  is varied and  $V_2 = 0.5$ .

with the corresponding flame residence time infinitely long ; in the neighborhood of  $\theta^*$ , the residence time is finite but still fairly long, so that a linear scaling of the enhancement can be expected.

Of course, for angles close to  $\theta = \pm\pi/2$ , the front is once again parallel to the shear, the flame wrinkling time is infinite, and a fast regime approximation must apply, with very small enhancements quadratic in the shear intensity component normal to the mean front. This is indeed what is observed in Fig. 2.12, with again excellent agreement between the simulation data and the asymptotic predictions. If  $|V_2|$  had been larger than  $S_L$  however, there could have been no angle  $\theta^*$  for which the flame residence time could have been infinitely long, so that in such cases, the fast regime would have applied to all angles and the dependence

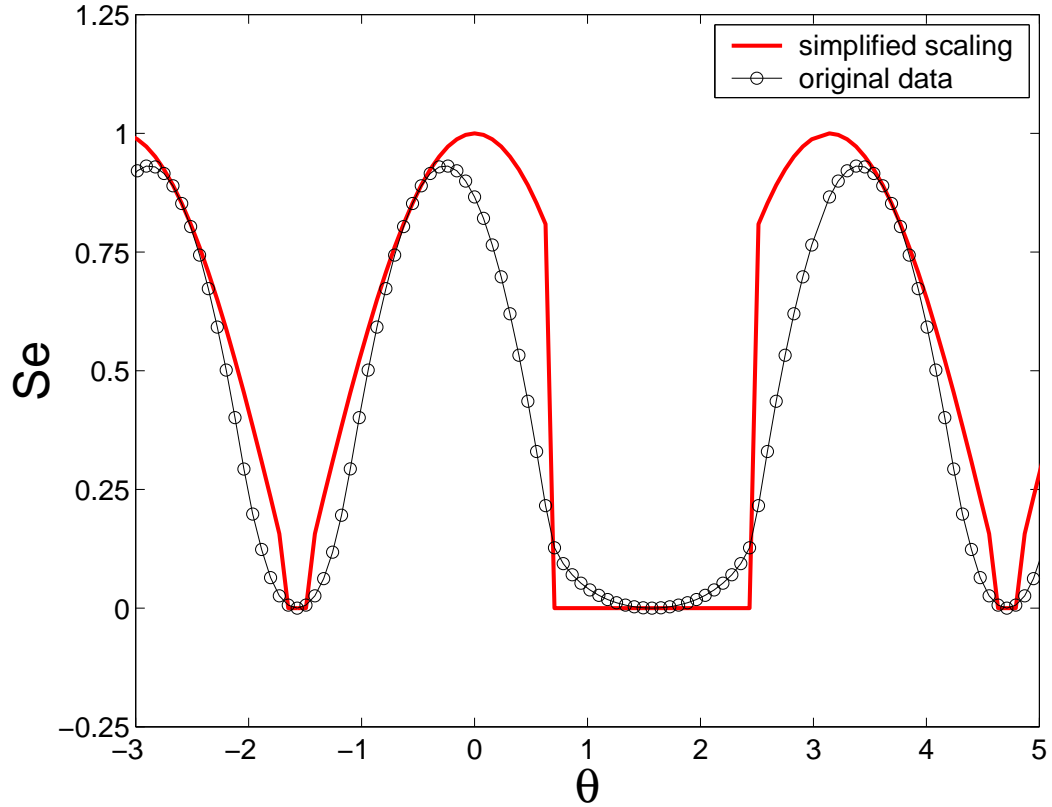


FIG. 2.13. Traveling mode : simplified approximations in both scaling regimes.

with respect to the shear intensity would have been quadratic everywhere. The flame residence time argument therefore offers a quantitative explanation for the sensitive dependence of the enhancement scaling with respect to  $V_2/S_L$  that was reported in [25] [24].

#### 2.7.4. practical approximation

The expressions in both regimes might seem complicated. In particular, the precise correction to the leading order in the slow regime is different in the standing and the traveling mode cases. For practical purposes, such details are unimportant, only the leading terms are relevant, as illustrated for the last example in Fig.

2.13. Numerical results are shown as circles again, while the solid line represents the crudest approximations in either regime :

- if  $\tilde{t} > \tilde{t}_{crit}$  : slow regime, take  $Se = \lambda |\cos \theta|$ ;
- if  $\tilde{t} < \tilde{t}_{crit}$  : fast regime, take  $Se = 0$ ;

where we picked  $\tilde{t}_{crit} = 3$  based on Fig. 2.10. In practice, one could therefore come up with a reasonable estimate for the speed enhancement based only on the intensity of the normal shear and a crude estimate for its relevant time scale.

## 2.8. CONCLUSIONS

In this study, we have proved that the enhanced burning speed of an idealized premixed flame subjected to a small scale time-dependent periodic shear undergoes a scaling transition controlled by a non-dimensional flame residence time. When the residence time is large (which tends to be the case if the turbulence intensity is large) the burning speed enhancement scales linearly with the turbulent speed, while when the residence time is small (this will likely be the case at small intensities or at very small scales) the enhancement is sublinear (here quadratic) with respect to the intensity. This transition bears a lot of resemblance with the well-known bending effect in the burning speed observed in experiments.

This work was done in the rigorous asymptotic context developed in [46] for *KPP*-type flames. A more popular contemporary model to describe the propagation of a flame front is the G-equation approach (used for example in [5] [22]). While the Majda-Souganidis asymptotic model and the G-equation can lead to significantly different predictions in some regimes, they agree qualitatively in others [24]. Regarding the scaling issues discussed in this paper, ongoing work seems to indicate excellent agreement, with both models displaying a qualitative similar transition between a slow (linear) and fast (sublinear) regime [8] [62].

The robustness of the transition mechanism to such variations in the model as well as the similarity with experimental observations are encouraging indications regarding the potential relevance of the main results of this paper to real turbulent

flames. While rather drastic simplifying conditions were needed to derive a model amenable to a systematic asymptotic analysis as well as to affordable, reliable computations, it is hoped that the results will be in some sense relevant to a much wider class of realistic configurations. One objective of the parameterization is to provide subgrid models for large eddy simulations of turbulent premixed flames - for that purpose, one needs to extend the parameterization to more realistic small scale turbulent flows and a step in that direction is taken in the sequel to this paper [11] that will discuss the enhanced speed for idealized small scale flows with more complex spatial structures. Ultimately, studies of the type presented here could be used as guides to select relevant generic configurations for direct numerical simulations of the full reactive Navier-Stokes equations with realistic chemistry. This would allow one to address explicitly questions beyond the scope of the idealized model used here - examples of such issues are the effects on the burning speed of non-unit Lewis number, complex chemistry, heat release/compressibility, realistic turbulent flow with randomness and a wide range of length and time scales etc. Computations with such realistic models are extremely costly - hopefully, the intuition gained from the idealized model studied here will be of some use in that context.

#### ACKNOWLEDGMENTS

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## Chapitre 3

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### SCHÉMA NUMÉRIQUE POUR LE HAMILTONIEN EFFECTIF

Ce chapitre est constitué de l'article "Computing the effective Hamiltonian in the Majda-Souganidis model of turbulent premixed flames" par Boualem Khouider & Anne Bourlioux qui a été accepté pour publication en 2002 dans *SIAM Journal on Numerical Analysis*.

Voici la liste des contributions principales de B.K. à cet article :

- reformuler le problème cellulaire en un problème qui consiste à chercher l'état stationnaire pour un système de lois de conservation ;
- fournir les outils mathématiques nécessaires pour l'analyse du schéma proposé (par exemple, la stabilité linéaire) ;
- élaborer le schéma mixte d'ordre deux dans l'espace et ordre un dans le temps qui converge rapidement vers l'état stationnaire ;
- mettre en œuvre numériquement ;
- choisir les cas tests pour
  - comparer le schéma proposé ici avec les approches classiques ;
  - comparer l'efficacité du schéma mixte (d'ordre deux dans l'espace et ordre un dans le temps) avec la version d'ordre deux globalement.

L'idée essentielle de formuler le problème comme un problème pour le gradient est de B.K. ; la suggestion de *préserver le gradient* pour surmonter le problème de la non-hyperbolicité est due à Andrew Majda tandis que l'idée de construire un tel schéma en utilisant *les grilles décalées* revient à Anne Bourlioux.

# Computing the effective Hamiltonian in the Majda-Souganidis model of turbulent premixed flames

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## ABSTRACT

*Turbulence enhances the speed of propagation of a premixed flame front. According to the Majda-Souganidis model, the procedure to predict this enhancement involves computing the effective Hamiltonian in a small-scale nonlinear cell-problem. We first discuss how to transform this problem into computing the steady-state solution of a system of conservation laws whose vector solution represents the gradient of the eigenfunction associated with the effective Hamiltonian. Theoretical arguments as well as numerical evidence are presented to emphasize the importance of enforcing the constraint that the vector solution must effectively be the gradient of a scalar function. We introduce a scheme that satisfies this constraint exactly by relying on staggered grids for the gradient components. Also discussed is the issue of selecting a time-integrator to achieve fast convergence to steady state. Validation is performed by examining convergence under grid refinement and by comparison with analytical results when available.*

**Keywords.** gradient-preserving scheme, ENO, staggered grid, Hamilton-Jacobi equation, conservation laws, steady state

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**AMS subject classifications.** 65M06, 65M12, 65M25

### 3.1. INTRODUCTION

The flamelet regime in premixed combustion is characterized by a very thin reaction zone that separates burnt and fresh gas, so that for all practical matters, it can be viewed as an infinitely thin flame front, propagating normal to itself due to burning and advection. The speed of propagation of that interface can be easily predicted in the laminar case, where advection plays a trivial role. It is however much more difficult to predict its enhancement due to turbulence, when the front is wrinkled by a multiple scale advecting flow field. A rigorous asymptotic strategy to predict this enhancement has been developed by Majda and Souganidis [46] for a flow field with separate scales. According to the theory, the procedure to compute the enhanced burning speed involves minimizing a function of the effective Hamiltonian for the flame; the effective Hamiltonian must be computed as the eigenvalue of a nonlinear cell-problem. In [25], this procedure was implemented for the simple case of a one-dimensional shear layer; for that case, the solution can be expressed mostly through explicit formulas. The method presented in this paper extends the procedure for more general small scale turbulent-like flows such as steady arrays of eddies, or combinations of eddies and shears; for such cases, explicit formulas are no longer available and the problem must be solved numerically. Solving the cell-problem is the hardest part: it requires computing the eigenvalue of a Hamilton-Jacobi equation. Numerical methods for Hamilton-Jacobi equations (without eigenvalues) are well known [20, 53], and so are iterative methods to compute the eigenvalues for large linear systems. The present case combines both problems and the challenge from a numerical point-of-view is to provide a scheme capable of a robust handling of the nonlinearity of Hamilton-Jacobi equations and of an efficient search for the eigenvalue of the resulting discretized equations (hence, a large nonlinear system). The method presented in this paper tackles this challenge by reformulating the problem so



that the eigenvalue is effectively eliminated from the preliminary phase of the computation by differentiation of the eigenvalue problem. This strategy leads to a very robust and practical scheme for two main reasons : the entire eigenvalue search is replaced by a simple algebraic post-processing of the results instead of the typical iterative process ; the system obtained by differentiation leads to a system of conservation laws which is a class of problems for which a well established numerical machinery is available. The paper is organized as follows. In Section 2, the Majda-Souganidis asymptotic model equations are stated as well as the reformulation of the eigenvalue problem as one of finding a pseudo-time steady state solution for the eigenfunction gradient. In Section 3 and Section 4, some key theoretical properties of the equations are discussed to motivate the strategy to design the scheme. In Section 3, the lack of strong hyperbolicity of the gradient equation is established. Yet, In Section 4, convergence results for the equivalent time-marching problem for the eigenfunction itself are exploited to formulate the principal constraint to guarantee that a discrete solution of the gradient problem will also converge to steady state. This constraint is that the discrete vector solution be in some sense the discrete gradient of a scalar function. In Section 5, we describe a novel *gradient-preserving* scheme i.e. a scheme that explicitly preserves the gradient structure of the initial data throughout the computation, in some appropriate discrete sense. The fact that the gradient-preserving property is essential for convergence is further demonstrated by numerical experiments in Section 6, where the performance of the gradient-preserving scheme is contrasted with that of other schemes which do not quite satisfy that constraint. A second order spatially accurate version of the scheme is presented in Section 7, along with a discussion on how to select the time integrator to accelerate convergence to steady state. In Section 8, the performance of the method is validated systematically by comparison with the reference solutions for the case of a simple shear layer [25, 24].

## 3.2. HOMOGENIZATION THEORY FORMULATION

### 3.2.1. The Majda-Souganidis asymptotic model

Here we simply state the model equations to be solved numerically ; details regarding the derivation of the model can be found in [25, 46]. Assuming that the heat release due to combustion is weak and that temperature and all the relevant chemical species diffuse at the same rate (Lewis number unity), the flame propagation can be described using a single advection-diffusion-reaction equation for temperature. The homogenization theory that leads to the model equations Eq.3.2.1 and Eq.3.2.2 below applies under the following additional assumptions :

- the reaction zone is thin, as a result of the balance between very weak diffusion and very fast reaction ;
- the incompressible advecting velocity field includes two separate scales : one large scale and a scale intermediate between the large scale and the flame thickness ;
- the reaction rate is of the KPP-type. A typical example of such reaction rate is given by  $f(T) = \bar{K} T(1 - T)$  where the temperature  $T$  has been normalized between  $T = 0$  on the cold (unburnt) side and  $T = 1$  on the hot (burnt) side and  $\bar{K} > 0$  is the reaction rate constant.

The intermediate scale velocity field causes the flame front to wrinkle : qualitatively, the increase in flame area due to this wrinkling leads to an overall burning speed enhancement. The objective of the homogenization theory is to predict this enhanced speed of propagation of the flame. The equations in the form stated below describe how to do this assuming that, at large scales, the advecting velocity field is constant and the flame front is planar.

Given the flame front unit normal  $\mathbf{n} = (\cos \theta, \sin \theta)$ , the flame speed  $F(\mathbf{n})$  in that direction must be computed as :

$$F(\mathbf{n}) = \min_{r>0} \frac{H(r\mathbf{n}) + \bar{K}}{r} \quad (3.2.1)$$

where  $\bar{K} = f'(0)$  is the positive constant used to define the reaction rate above and  $H$  is the effective Hamiltonian of the flame, computed as the unique eigenvalue of the following so-called *cell-problem* :

$$-|\mathbf{p} + \mathbf{D}w|^2 + \mathbf{V}(\mathbf{y}) \cdot (\mathbf{p} + \mathbf{D}w) = -H(\mathbf{p}). \quad (3.2.2)$$

(At least for steady flows, it is trivial from a numerical point of view to deal with the unsteady terms - they are linear - so we will not discuss this issue in this paper - see [39] for examples with unsteady flows). The eigenfunction  $w(\mathbf{y})$  must be of zero-mean and bi-periodic with respect to the spatial variables  $\mathbf{y} = (x, y)$  (one can always assume that the bi-periodic domain has been rescaled to an unit square).  $\mathbf{D}w$  represents the spatial gradient of the eigenfunction. The velocity field  $\mathbf{V}(\mathbf{y})$  is assumed to combine a large scale constant flow and the smaller scale "turbulent" flow :

$$\mathbf{V} = \bar{\mathbf{v}} + \lambda \mathbf{v} = \bar{\lambda}(\cos \bar{\theta}, \sin \bar{\theta}) + \lambda \mathbf{v}(\mathbf{y})$$

Here,  $\bar{\lambda}$  and  $\lambda$  represent the magnitude of the velocity field respectively at large and intermediate scales while  $\mathbf{v}(\mathbf{y})$  is the intermediate scale velocity field defined over the unit periodic box. It is also assumed to have a zero mean and to be bi-periodic as well as to be incompressible. For example, in Section 8 below and elsewhere [11, 40], we use our procedure on velocity fields obtained from the Childress-Soward stream function  $\psi(\mathbf{y})$  :

$$\psi(\mathbf{y}) = \psi(x, y) = \sin(2\pi x) \sin(2\pi y) + \delta \cos(2\pi x) \cos(2\pi y) \quad 0 \leq \delta \leq 1. \quad (3.2.3)$$

Streamlines for  $\delta = 0, 0.5, 1$  are shown in Fig. 3.1.

In summary, the input data are :

- the front angle  $\theta$  ;
- $\delta, \lambda$  : the parameters that define the "turbulent" velocity field responsible for the burning speed enhancement ;
- $\bar{\lambda}, \bar{\theta}$  : the parameters that define the large scale (constant) velocity field.

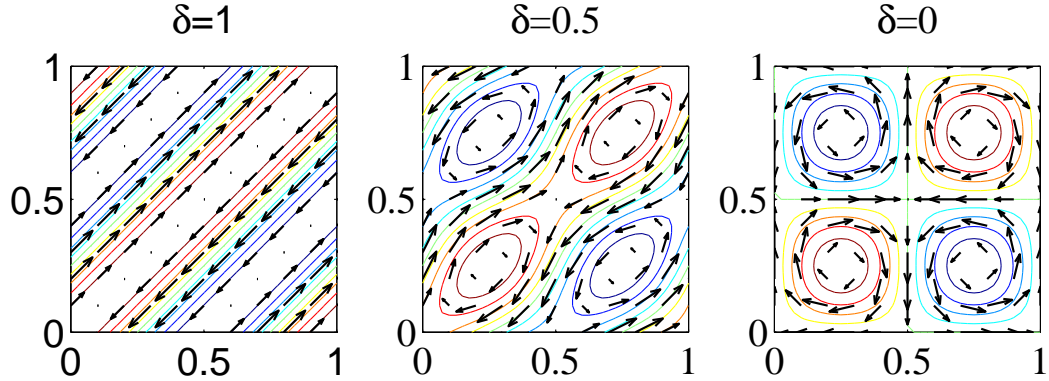


FIG. 3.1. Streamlines for the Childress-Soward flow :  $\delta = 1$  : simple shear tilted at 45 degrees,  $\delta = 0.5$  : combination of eddies and shear layers and  $\delta = 0$  : periodic array of eddies.

Results are typically presented in terms of the flame speed enhancement  $F_e$  defined as :

$$F_e = F + \bar{\mathbf{v}} \cdot \mathbf{n} - S_L \quad (3.2.4)$$

with  $S_L = 2/\sqrt{K}$  the laminar burning speed of the flame - in the rest of the paper, the problem is rescaled so that  $S_L = 1$ ;  $F_e$  represents the increase in burning speed of the flame compared to the laminar case. A qualitative understanding of the wrinkling of the front can be achieved by looking at the isolevels of the eigenfunction  $w$  : they can be related to successive realizations of the wrinkled flame front as it moves across the periodic cell due to burning and advection.

The main challenge in performing the optimization over the variable  $r$  in Equation 3.2.1 is to provide the effective Hamiltonian  $H(r\mathbf{n})$ , which must be computed as the eigenvalue in Equation 3.2.2. The ultimate objective here is to design a method sufficiently efficient to allow for the extensive tabulation of  $F_e$  as a function of all the input data. Each entry in such a table requires iterating numerically over many values of  $r$  to perform the minimization in Equation 3.2.1, hence requiring multiple evaluations of  $H$ ; the main issue is therefore to design an efficient, robust,

fully automated algorithm to compute this effective Hamiltonian for a wide range of parameters.

Equation 3.2.2 is both nonlinear and contains an eigenvalue (the effective Hamiltonian  $H$ ) : it is very challenging numerically to deal simultaneously with both difficulties and it is therefore very tempting to try to avoid to deal directly with at least one of them. One possible strategy along that line would be to linearize the problem, hence eliminating the nonlinearity aspect and retaining the eigenvalue ; this could be done by adding a small viscous term of order  $\epsilon$  and do the following transformation  $T^\epsilon(x, y) = \exp(Z(x, y)/\epsilon)$  with  $Z(x, y) = \mathbf{p} \cdot (x, y) + w(x, y)$  ; formulating the problem in terms of  $T^\epsilon$  instead of  $w$  basically undoes one of the steps in the homogenization procedure in [46]. The main difficulty with this approach is that the amount of viscosity  $\epsilon$  needed to lead to a system of equations that can be safely discretized by a centered scheme is not known a priori but is solution-dependent. Another difficulty is that the discretized equations would lead to a very large linear eigenvalue problem, requiring a costly iterative procedure for its numerical solution along with the need of generating an adequate initial guess for the eigenvalue.

In that sense, the strategy to be discussed in the rest of the paper is much more robust. It is the eigenvalue aspect that is eliminated from the formulation by differentiating the cell-problem, resulting in a system of equations for the eigenfunction gradient that is still nonlinear, but that no longer contains the eigenvalue explicitly. This strategy is described next.

### 3.2.2. Reformulation as a gradient problem

By differentiating (3.2.2) with respect to  $\mathbf{y}$ , we eliminate the eigenvalue and obtain the following nonlinear equation for the eigenfunction gradient  $\mathbf{D}w$  :

$$\mathbf{D}\{-|\mathbf{D}w|^2 - 2\mathbf{p} \cdot \mathbf{D}w + (\bar{\mathbf{v}} + \lambda \mathbf{v}(\mathbf{y})) \cdot \mathbf{D}w + \lambda \mathbf{v}(\mathbf{y}) \cdot \mathbf{p}\} = 0 \quad (3.2.5)$$

Integrating (3.2.2) over one periodic cell and using the divergence theorem, one obtains a formula that relates algebraically  $H$  and  $\mathbf{D}w$  :

$$H(\mathbf{p}) = |\mathbf{p}|^2 + \langle |\mathbf{D}w|^2 \rangle - \bar{\mathbf{v}} \cdot \mathbf{p} \quad (3.2.6)$$

where  $\langle \cdot \rangle$  represents the average over the periodic cell. Therefore, assuming that indeed one is able to solve Equation 3.2.2, the effective Hamiltonian  $H$  can be computed very economically a posteriori by simple post-processing of the solution for  $\mathbf{D}w$ , hence avoiding entirely any eigenvalue iterative procedure.

A practical approach to compute the solution of Equation 3.2.5 is to view it as the steady-state of the following system

$$\begin{cases} \partial_s u + \partial_x K(u, v, x, y) = 0 \\ \partial_s v + \partial_y K(u, v, x, y) = 0 \end{cases} \quad (3.2.7)$$

where  $K$  is given by

$$K(\mathbf{u}, x, y) = -|\mathbf{u}|^2 - 2\mathbf{p} \cdot \mathbf{u} + (\bar{\mathbf{v}} + \lambda \mathbf{v}(x, y)) \cdot \mathbf{u} + \lambda \mathbf{v}(x, y) \cdot \mathbf{p} \quad (3.2.8)$$

and  $\mathbf{u} = (u, v) = \mathbf{D}w$  is the eigenfunction gradient.

The pseudo-time marching method to solve Equation 3.2.7 to steady-state is described in details in Section 5 below. Before describing the numerical method however, some results regarding the equation before discretization are reported in Section 3 (lack of strong hyperbolicity) and Section 4 (effective convergence to a steady-state); those results provide with essential insight on the type of constraints to be taken into account in order to design a successful numerical method, with a particular concern for the convergence property of the algorithm toward a steady-state solution.

### 3.3. LACK OF STRONG HYPERBOLICITY

Here we prove that (3.2.7) is not strongly hyperbolic. Set  $F = (F_1, F_2)$  with

$$F_1(\mathbf{u}, x, y) = \begin{pmatrix} K(\mathbf{u}, x, y) \\ 0 \end{pmatrix} \text{ and } F_2(\mathbf{u}, x, y) = \begin{pmatrix} 0 \\ K(\mathbf{u}, x, y) \end{pmatrix}.$$

The associated system is strongly hyperbolic if for all reals  $\alpha$  and  $\beta$  the matrix

$$A = \alpha \frac{\partial F_1}{\partial \mathbf{u}} + \beta \frac{\partial F_2}{\partial \mathbf{u}},$$

where

$$\frac{\partial F_1}{\partial \mathbf{u}} = \begin{bmatrix} \frac{\partial K}{\partial u} & \frac{\partial K}{\partial v} \\ 0 & 0 \end{bmatrix}$$

and

$$\frac{\partial F_2}{\partial \mathbf{u}} = \begin{bmatrix} 0 & 0 \\ \frac{\partial K}{\partial u} & \frac{\partial K}{\partial v} \end{bmatrix},$$

has two real eigenvalues and two linearly independent eigenvectors [30].

The eigenvalues of the matrix  $A$  are  $\nu = \alpha \frac{\partial K}{\partial u} + \beta \frac{\partial K}{\partial v}$  and 0. Clearly, if  $\frac{\partial K}{\partial v} \neq 0$  or  $\frac{\partial K}{\partial u} \neq 0$  one can choose the constants  $\alpha$  and  $\beta$  such that  $\nu$  is zero and the matrix  $A$  is not identically zero. This is equivalent to setting

$$\begin{cases} \frac{\partial K}{\partial u} \neq 0 \text{ or } \frac{\partial K}{\partial v} \neq 0 \\ \alpha \frac{\partial K}{\partial u} + \beta \frac{\partial K}{\partial v} = 0 \end{cases}$$

In this case, the matrix  $A$  has only one free eigenvector associated with the double eigenvalue 0, i.e.,  $A$  is equivalent to a Jordan block. Thus, (3.2.7) is not strongly hyperbolic. The lack of strong hyperbolicity for the pseudo-time marching equation has important consequences regarding the possibility of reaching numerically a steady state by long time marching :

1. without taking into account other specific properties of the system studied here (as will be done in Section 3.4 below), the lack of strong hyperbolicity

means that there is no guarantee that the solution will converge to a steady-state [29];

2. standard numerical methods for conservation laws might not work, as most rely on the strong hyperbolic nature of the equations.

**Remark 3.3.1.** *The vector solution to be computed here is actually a gradient, a property which was not taken into account in the discussion above. It is interesting to notice that imposing this additional constraint on the solution is per se not sufficient to recover strong hyperbolicity.*

Take  $\mathbf{u} = \mathbf{D}\phi$  and  $\mathbf{V} = \bar{\mathbf{v}} + (\psi_y, -\psi_x)$  for some periodic functions  $\phi$  and  $\psi$ , a mean flow  $\bar{\mathbf{v}} = (\bar{v}_1, \bar{v}_2)$  and a mean flame gradient  $\mathbf{p} = (p_1, p_2)$ . The conditions of non-hyperbolicity (3.3) are equivalent to

$$\begin{cases} 2\phi_x + 2p_1 - \bar{v}_1 - \psi_y \neq 0 \text{ or } 2\phi_y + 2p_2 - \bar{v}_2 + \psi_x \neq 0 \\ \alpha(2\phi_x + 2p_1 - \bar{v}_1 - \psi_y) + \beta(2\phi_y + 2p_2 - \bar{v}_2 + \psi_x) = 0. \end{cases}$$

It is easy to construct examples that would satisfy those non-hyperbolicity conditions. Let

$$\phi(x, y) = \frac{1}{2}\psi(y, -x)$$

and choose the constant parameters such that

$$2p_1 - \bar{v}_1 \neq 0 \text{ or } 2p_2 - \bar{v}_2 \neq 0$$

and

$$\alpha(2p_1 - \bar{v}_1) + \beta(2p_2 - \bar{v}_2) = 0.$$

### 3.4. CONVERGENCE TO STEADY STATE

The main conclusion from Section 3.3 is that if one views the system of equations in 3.2.7 as a system of conservation laws for a vector solution, there is no guaranty that, starting from general initial data, convergence to steady state can be



achieved by pseudo-time marching because of the lack of strong hyperbolicity of the system of equations 3.2.7.

Such a convergence result however can be recovered by considering first the convergence of the following pseudo-time marching equation for the eigenfunction itself :

$$w_s - |\mathbf{p} + \mathbf{D}w|^2 + \mathbf{V}(\mathbf{y}) \cdot (\mathbf{p} + \mathbf{D}w) = -H(\mathbf{p}). \quad (3.4.1)$$

with  $H$  the eigenvalue of the cell-problem in Equation 3.2.2. Convergence of  $w + Hs$  to a steady solution was proved by Barles and Souganidis [6], for general initial data. This long-time convergence property automatically implies convergence, in the weak sense, of the gradient  $\mathbf{D}w$ , therefore establishing that the pseudo-time iterations on Equations 3.2.7 should converge, at least theoretically (i.e. before numerical discretization). The key implication of this remark relevant to the design of a scheme to solve those equations numerically is that one way to recover convergence for the gradient system is to insure that the vector solution of Equation 3.2.7 is effectively the gradient, in some appropriate discrete sense, of a scalar function.

For smooth functions, a vector function is a gradient if it is curl-free. We state next an equivalent definition to the curl-free condition which does not involve derivatives and hence constitute an useful generalization to weak derivatives - this equivalent definition will also turn out to be very useful in dealing with discrete data, as done in the next section. Let  $(u, v)$  be an integrable vector function :

- $(u, v)$  is the gradient of a function  $w$  if and only if, given a reference point  $(a, b)$ , we have the double equality

$$w(x, y) = \int_a^x u(\xi, y) d\xi + w(a, y) = \int_b^y v(x, \xi) d\xi + w(x, b)$$

for a.e. each point  $(x, y)$ . But, similarly,

$$w(a, y) = \int_b^y v(a, \xi) d\xi + w(a, b)$$

and

$$w(x, b) = \int_a^x u(\xi, b) d\xi + w(a, b),$$

hence, without referring to any primitive, we can state that  $(u(x, y), v(x, y))$  is a gradient in the weak sense if and only if for a.e.  $(x, y)$  we have

$$\int_b^y v(a, \xi) d\xi + \int_a^x u(\xi, y) d\xi = \int_a^x u(\xi, b) d\xi + \int_b^y v(x, \xi) d\xi \quad (3.4.2)$$

- in addition, the primitive function is bi-periodic of period  $T$  if and only if for a.e.  $(x, y)$

$$\int_a^{a+T} u(\xi, y) d\xi = 0 \quad (3.4.3)$$

$$\int_b^{b+T} v(x, \xi) d\xi = 0 \quad (3.4.4)$$

### 3.5. GRADIENT-PRESERVING SCHEME

Brute force attempts at numerically solving Equation (3.2.5) to steady-state with standard numerical schemes for conservation laws failed to converge, and this comes as no surprise given the considerations in Sections 3 and 4 above. Instead, the results in Section 4 suggest that convergence could be guaranteed only if the discrete vector solution is actually a gradient. The method we propose here has precisely this property : the scheme is **gradient-preserving** in the discrete sense of Formula 3.4.2 inasmuch as, given initial vector data which are a discrete gradient, the solution will remain a discrete gradient at all later discrete times (in practice, the simplest such initial data are identically zero). The scheme is actually based on a fairly standard conservative formulation except for the staggered discretization grids to be described first.

### 3.5.1. Staggered grids

Let  $h = 1/n$  define the mesh discretization of the interval  $[0, 1]$  with  $x_i = ih$ ,  $x_{i+1/2} = x_i + h/2$ ,  $y_j = jh$  and  $y_{j+1/2} = y_j + h/2$ , for any integers  $0 \leq i, j \leq n$ . We consider the staggered grid obtained by the superposition of the two grids  $(x_i, y_j)$  and  $(x_{i+1/2}, y_{j+1/2})$  (see Fig. 3.2).

The first component,  $u$ , of the gradient solution is defined at the nodes  $(x_i, y_j)$  while the second component,  $v$ , is defined at the nodes  $(x_{i+1/2}, y_{j+1/2})$ . The scalar primitive (the eigenfunction)  $w$  itself is defined at the hybrid nodes  $(x_{i+1/2}, y_j)$ .

### 3.5.2. Conservative formulation

Using the notation  $\mathbf{V} = (V_1, V_2)$  and  $\mathbf{p} = (p_1, p_2)$ , the starting point of the strategy is to notice the symmetry in the flux function  $K$  in Equation 3.2.8, which can be split into two independent parts  $K(u, v, x, y) = f(u, x, y) + g(v, x, y)$ , with

$$f = f(u, x, y) = -u^2 - 2p_1u + V_1(x, y)u + V_1(x, y)p_1$$

and

$$g = g(v, x, y) = -v^2 - 2p_2v + V_2(x, y)v + V_2(x, y)p_2$$

The conservative formulation is obtained by integrating the conservation laws over each  $u$ - and  $v$ -control volume. Taking the integral of

$$\partial_s u + \partial_x f(u, x, y) + \partial_x g(v, x, y) = 0$$

over the cell  $[x_{i-1/2}, x_{i+1/2}] \times [y_{j-1/2}, y_{j+1/2}] \times [s_n, s_{n+1}]$  and the integral of

$$\partial_s v + \partial_y f(u, x, y) + \partial_y g(v, x, y) = 0,$$

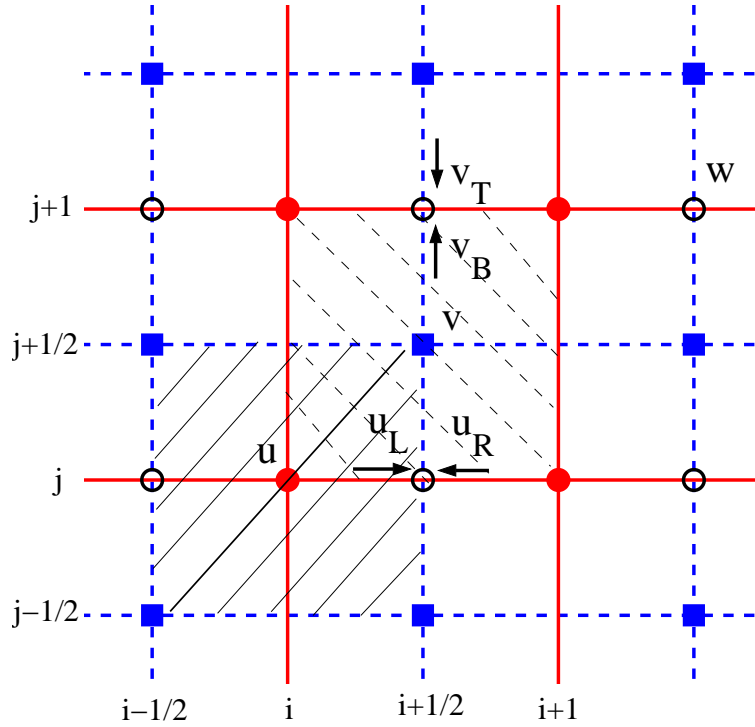


FIG. 3.2. Staggered grid for a gradient preserving scheme :  $u$  is defined on the vertices  $(i, j)$  by its cell averages on  $[i-1/2, i+1/2] \times [j-1/2, j+1/2]$  (filled circles),  $v$  on the vertices  $(i+1/2, j+1/2)$  by its cell averages on  $[i, i+1] \times [j, j+1]$  (filled squares), and the primitive  $w$  is obtained on  $(i+1/2, j)$  (empty circles). The shaded squares show the control volumes for  $u$  and  $v$  respectively, and the arrows point out to the associated Riemann problems.

over  $[x_{i-1}, x_i] \times [y_{j-1}, y_j] \times [s_n, s_{n+1}]$  and then dividing by the control volume area  $h^2$ , one obtains the following equations in conservative form :

$$\begin{aligned} \bar{u}_{i,j}^{n+1} = \bar{u}_{i,j}^n - \frac{1}{h^2} \int_{s_n}^{s_{n+1}} \int_{y_{j-1/2}}^{y_{j+1/2}} \{f(u, x_{i+1/2}, y) + g(v, x_{i+1/2}, y)\} dy ds \quad (3.5.1) \\ + \frac{1}{h^2} \int_{s_n}^{s_{n+1}} \int_{y_{j-1/2}}^{y_{j+1/2}} \{f(u, x_{i-1/2}, y) + g(v, x_{i-1/2}, y)\} dy ds \end{aligned}$$

and

$$\begin{aligned} \bar{v}_{i-1/2,j-1/2}^{n+1} &= \bar{v}_{i-1/2,j-1/2}^n - \frac{1}{h^2} \int_{s_n}^{s_{n+1}} \int_{x_{i-1}}^{x_i} \{f(u, x, y_j) + g(v, x, y_{j-1})\} dx ds \\ &\quad + \frac{1}{h^2} \int_{s_n}^{s_{n+1}} \int_{x_{i-1}}^{x_i} \{f(u, x, y_{j-1}) + g(v, x, y_{j-1})\} dx ds \end{aligned} \quad (3.5.2)$$

where

$$\bar{u}_{i,j}^k = \frac{1}{h^2} \int_{x_{i-1}}^{x_i} \int_{y_{j-1/2}}^{y_{j+1/2}} u(x, y, s_k) dx dy$$

is the cell average of  $u$  with the obvious corresponding considerations for  $v$ . This can be expressed simply as :

$$\bar{u}_{i,j}^{n+1} = \bar{u}_{i,j}^n - \frac{\Delta s}{h} \left( F_{i+1/2,j}^{n,1} - F_{i-1/2,j}^{n,1} \right) \quad (3.5.3)$$

and

$$\bar{v}_{i-1/2,j-1/2}^{n+1} = \bar{v}_{i-1/2,j-1/2}^n - \frac{\Delta s}{h} \left( F_{i-1/2,j+1}^{n,2} - F_{i-1/2,j}^{n,2} \right) \quad (3.5.4)$$

where the flux  $F_{i-1/2,j}^{n,1}$  corresponds to the double space-time integral in Equation 3.5.1 over one time-step and over the vertical edge (of a  $u$ -cell) with the edge center located at  $(x_{i-1/2}, y_j)$  :

$$F_{i-1/2,j}^{n,1} = \frac{1}{h \Delta s} \int_{s_n}^{s_{n+1}} \int_{y_{j-1/2}}^{y_{j+1/2}} \{f(u, x_{i+1/2}, y) + g(v, x_{i+1/2}, y)\} dy ds \quad (3.5.5)$$

while the flux  $F_{i-1/2,j}^{n,2}$  corresponds to the double space-time integral in Equation 3.5.2 over one time-step and over the horizontal edge (of a  $v$ -cell) with the edge center also located at  $(x_{i-1/2}, y_j)$  :

$$F_{i-1/2,j}^{n,2} = \frac{1}{h \Delta s} \int_{s_n}^{s_{n+1}} \int_{x_{i-1}}^{x_i} \{f(u, x, y_{j-1}) + g(v, x, y_{j-1})\} dx ds \quad (3.5.6)$$

As will be shown in Prop.5.1 below, the key in designing a gradient-preserving scheme is to use the same numerical value for  $F_{i-1/2,j}^{n,1}$  and  $F_{i-1/2,j}^{n,2}$ . This can be justified as follows. In evaluating  $F_{i-1/2,j}^{n,1}$  for instance, it is clear that the  $f$ -component of the flux (corresponding to the integration of  $f(u, x, y)$ ) should be

estimated using a standard Riemann solver, with left and right states corresponding to  $\bar{u}_{i-1,j}^n$  and  $\bar{u}_{i,j}^n$  respectively (for a first order method at least). The  $g$ -component of the flux however can be specified somewhat more arbitrarily because it only depends on  $v$  and is independent of  $u$ . A second order accurate choice is to estimate that portion of the integral by its value at the mid-point of the edge  $(x_{i-1/2}, y_j)$ , in which case this contribution can be shown to be equal to second order to the  $g$ -component of the  $F_{i-1/2,j}^{n,2}$  flux, to be estimated by resorting again to a Riemann solver, this time with top and bottom states given by  $\bar{v}_{i-1/2,j}^n$  and  $\bar{v}_{i-1/2,j-1}^n$  respectively. Specifically :

$$F_{i-1/2,j}^{n,1} = F_{i-1/2,j}^{n,2} = F_{i-1/2,j}^n = f(\mathfrak{R}_{i-1/2,j}^1, x_{i-1/2}, y_j) + g(\mathfrak{R}_{i-1/2,j}^2, x_{i-1/2}, y_j) \quad (3.5.7)$$

where  $\mathfrak{R}_{i-1/2,j}^1$  is the solution of the Riemann problem for the flux  $f$  associated with the vertical edge  $(i-1/2, j)$  and the left and right states  $u_L$  and  $u_R$  ( $\bar{u}_{i-1,j}$  and  $\bar{u}_{i,j}$  for the first order scheme) and  $\mathfrak{R}_{i-1/2,j}^2$  is the solution for the Riemann problem for the flux  $g$  at the horizontal edge  $(i-1/2, j)$  for the bottom and top states  $v_B$  and  $v_T$  ( $\bar{v}_{i-1/2,j-1/2}$  and  $\bar{v}_{i-1/2,j+1/2}$  for the first order scheme) - see Fig. 3.2.

The scheme can be rewritten as :

$$\begin{aligned} \bar{u}_{i,j}^{n+1} &= \bar{u}_{i,j}^n - \frac{\Delta s}{h} \{F_{i+1/2,j}^n - F_{i-1/2,j}^n\} \\ \bar{v}_{i-1/2,j-1/2}^{n+1} &= \bar{v}_{i-1/2,j-1/2}^n - \frac{\Delta s}{h} \{F_{i-1/2,j}^n - F_{i-1/2,j-1}^n\} \end{aligned} \quad (3.5.8)$$

**Proposition 3.5.1.** *The scheme in (3.5.8) is gradient preserving in the sense that if the numerical vector solution satisfies the condition (3.4.2) at some given initial time,  $s_0$ , then this condition will be satisfied at any latter time,  $s_n > s_0$ . Furthermore, if the primitive function is periodic at the initial time then it remains periodic, i.e., (3.4.3) and (3.4.4) are also satisfied at time,  $s_n$ , if they were satisfied at time  $s_0$ .*

**Proof.** It is straightforward to verify the second part of the proposition by exploiting the conservative formulation. To prove the first claim, recall that the discrete values representing the numerical solution for  $(u, v)$  are cell averages, so, given these values at any time,  $s_n$ , we can get the solution primitive at the hybrid vertices  $((i - 1/2), j)$ , without any further approximation. Taking  $(a, b) = (x_{1/2}, y_0)$  and  $(x, y) = (x_{i-1/2}, y_j)$  in Equation 3.4.2 leads to :

$$\sum_{k=1}^{i-1} \bar{u}_{k,0} + \sum_{k=1}^j \bar{v}_{i-1/2,k-1/2} = \sum_{k=1}^j \bar{v}_{1/2,k-1/2} + \sum_{k=1}^{i-1} \bar{u}_{k,j}. \quad (3.5.9)$$

To show that the scheme is gradient-preserving, we must show that if the discrete solution at time  $s_n$  verifies (3.5.9), then so does the solution at time  $s_{n+1} = s_n + \Delta s$ , which is equivalent to show that the same condition is satisfied by the difference of the two vector solutions in (3.5.8), i.e.,

$$\begin{aligned} & \sum_{k=1}^{i-1} F_{k+1/2,0}^n - F_{k-1/2,0}^n + \sum_{k=1}^j F_{i-1/2,k}^n - F_{i-1/2,k-1}^n \\ &= \sum_{k=1}^j F_{1/2,k}^n - F_{1/2,k-1}^n + \sum_{k=1}^{i-1} F_{k+1/2,j}^n - F_{k-1/2,j}^n \end{aligned}$$

and the two sides of the equality collapse to their common value

$$F_{i-1/2,j}^n - F_{1/2,0}^n$$

thus, (3.5.8) is gradient preserving.

### 3.5.3. Linear stability analysis for the first order scheme

Here we show that the gradient preserving scheme (3.5.8) is linearly stable under a CFL condition. We consider the linear version of our problem

$$\begin{cases} u_s + au_x + bv_x = 0 \\ v_s + av_y + bv_y = 0 \end{cases} \quad (3.5.10)$$

where  $a$  and  $b$  are two non-negative constants, for simplicity. The scheme in (3.5.8) applied to (3.5.10) gives

$$\begin{aligned} u_{i,j}^{n+1} &= u_{i,j}^n - \frac{\Delta s}{h} \{a(u_{i,j}^n - u_{i-1,j}^n) + b(v_{i+1/2,j-1/2}^n - v_{i-1/2,j-1/2}^n)\} \\ v_{i+1/2,j+1/2}^{n+1} &= v_{i+1/2,j+1/2}^n - \frac{\Delta s}{h} \{a(u_{i,j+1}^n - u_{i,j}^n) + b(v_{i+1/2,j+1/2}^n - v_{i+1/2,j-1/2}^n)\} \end{aligned} \quad (3.5.11)$$

where the over bars are dropped for simplicity.

**Proposition 3.5.2.** *Let  $\lambda_1 = a \frac{\Delta s}{h}$  and  $\lambda_2 = b \frac{\Delta s}{h}$ . The linearized version of the gradient preserving scheme given in (3.5.11) is stable under the CFL condition*

$$\lambda_1 + \lambda_2 \leq 1$$

**Proof.** We perform a Von Neumann analysis by considering the following expansion in Fourier series :

$$\begin{aligned} u_{i,j}^n &= \sum_{k_1=-\infty}^{+\infty} \sum_{k_2=-\infty}^{+\infty} \rho_{k_1,k_2}^{1,n} \exp(2\pi(k_1 i + k_2 j)Ih) \\ v_{i+1/2,j+1/2}^n &= \sum_{k_1=-\infty}^{+\infty} \sum_{k_2=-\infty}^{+\infty} \rho_{k_1,k_2}^{2,n} \exp(2\pi(k_1(i+1/2) + k_2(j+1/2))Ih) \end{aligned}$$

where  $I$  is the complex square root of unity. To simplify we set  $\phi_k = 2\pi kh$ , then replacing  $u_{i,j}^n$  and  $v_{i+1/2,j+1/2}^n$  in the linear scheme by their respective Fourier series leads to

$$\begin{aligned} \sum_{k_1,k_2} \rho_{k_1,k_2}^{1,n+1} \exp(i\phi_{k_1} I + j\phi_{k_2} I) &= \sum_{k_1,k_2} \exp(i\phi_{k_1} I + j\phi_{k_2} I) \times \\ &\left\{ (1 - \lambda_1(1 - \exp(-I\phi_{k_1})))\rho_{k_1,k_2}^{1,n} - \lambda_2 \exp(-\frac{\phi_{k_1} + \phi_{k_2}}{2} I) (\exp(I\phi_{k_1}) - 1)\rho_{k_1,k_2}^{2,n} \right\} \end{aligned}$$

and

$$\begin{aligned} \sum_{k_1,k_2} \rho_{k_1,k_2}^{2,n+1} \exp((i+1/2)\phi_{k_1} I + (j+1/2)\phi_{k_2} I) &= \sum_{k_1,k_2} \exp((i+1/2)\phi_{k_1} I + (j+1/2)\phi_{k_2} I) \times \\ &\left\{ (1 - \lambda_2(1 - \exp(-I\phi_{k_2})))\rho_{k_1,k_2}^{2,n} - \lambda_1 \exp(-\frac{\phi_{k_1} + \phi_{k_2}}{2} I) (\exp(I\phi_{k_2}) - 1)\rho_{k_1,k_2}^{1,n} \right\} \end{aligned}$$



Set  $X = 1 - e^{-I\phi_{k_1}}$  and  $Y = 1 - e^{-I\phi_{k_2}}$ , then by uniqueness of the Fourier expansion we have, for fixed wave numbers  $k_1$  and  $k_2$ ,

$$\begin{pmatrix} \rho_{k_1, k_2}^{1, n+1} \\ \rho_{k_1, k_2}^{2, n+1} \end{pmatrix} = G \begin{pmatrix} \rho_{k_1, k_2}^{1, n} \\ \rho_{k_1, k_2}^{2, n} \end{pmatrix}$$

where the amplification matrix  $G$  is given by

$$G = \begin{bmatrix} 1 - \lambda_1 X & -\lambda_2 \exp\left(-\frac{\phi_{k_1} + \phi_{k_2}}{2} I\right) (\exp(I\phi_{k_1}) - 1) \\ -\lambda_1 \exp\left(-\frac{\phi_{k_1} + \phi_{k_2}}{2} I\right) (\exp(I\phi_{k_2}) - 1) & 1 - \lambda_2 Y \end{bmatrix},$$

whose characteristic polynomial is

$$P(\mu) = (1 - \lambda_1 X - \mu)(1 - \lambda_2 Y - \mu) - \lambda_1 \lambda_2 XY.$$

The roots of  $P$  are  $\mu_1 = 1$  and  $\mu_2 = 1 - \lambda_1 X - \lambda_2 Y$ . So (3.5.11) is stable if and only if the modulus of  $\mu_2$  is less or equal to one.

$$\begin{aligned} |\mu_2|^2 &= |1 - \lambda_1(1 - e^{-I\phi_{k_1}}) - \lambda_2(1 - e^{-I\phi_{k_2}})|^2 \\ &= \{1 - \lambda_1(1 - \cos(\phi_{k_1})) - \lambda_2(1 - \cos(\phi_{k_2}))\}^2 + \{\lambda_1 \sin(\phi_{k_1}) + \lambda_2 \sin(\phi_{k_2})\}^2 \\ &= 1 - 4\lambda_1(1 - \lambda_1) \sin^2\left(\frac{\phi_{k_1}}{2}\right) - 4\lambda_2(1 - \lambda_2) \sin^2\left(\frac{\phi_{k_2}}{2}\right) \\ &\quad + 2\lambda_1 \lambda_2 \{1 + \cos(\phi_{k_1} - \phi_{k_2}) - \cos(\phi_{k_1}) - \cos(\phi_{k_2})\} \\ &= 1 - 4\lambda_1 \{1 - (\lambda_1 + \lambda_2)\} \sin^2\left(\frac{\phi_{k_1}}{2}\right) \\ &\quad - 4\lambda_2 \{1 - (\lambda_1 + \lambda_2)\} \sin^2\left(\frac{\phi_{k_2}}{2}\right) - 2\lambda_1 \lambda_2 \{1 - \cos(\phi_{k_1} - \phi_{k_2})\} \end{aligned}$$

thus,  $|\mu_2|$  is less or equal to one provided  $\lambda_1 + \lambda_2$  is less or equal to one.

### 3.6. FAILURE OF NON GRADIENT-PRESERVING SCHEMES

The constraint of formulating a gradient-preserving scheme was motivated theoretically in Sections 3 and 4. Here, we provide with more practical motivations by reporting the results from failed numerical experiments with three schemes that

do not quite satisfy that constraint.

### 3.6.1. Roe's scheme (GNPS1)

The first scheme is the standard Roe's Riemann solver approximation scheme for hyperbolic systems [43]. The scheme relies heavily on hyperbolic features so it obviously may not work for our system because of the lack of strong hyperbolicity.

### 3.6.2. Direction-splitting on a single uniform grid (GNPS2)

The second scheme is obtained by giving up the staggered grid, instead using the same uniform grid for the two components  $(u, v)$ . The direction-splitting leads to the following expressions for the edge fluxes :

$$\begin{aligned} F_{i-1/2,j}^{n,1} &= f(\mathfrak{R}_{i-1/2,j}^1, x_{i-1/2}, y_j) + g(v_{i-1/2,j}^n, x_{i-1/2}, y_j) \\ F_{i,j-1/2}^{n,2} &= f(u_{i,j-1/2}^n, x_i, y_{j-1/2}) + g(\mathfrak{R}_{i,j-1/2}^2, x_i, y_{j-1/2}) \end{aligned}$$

where one can simply estimate

$$v_{i-1/2,j}^n = (v_{i-1,j}^n + v_{i,j}^n)/2$$

and a similar expression for  $u_{i,j-1/2}^n$ . Those centered approximations are adequate here because of the directional splitting.

### 3.6.3. Staggered grid without flux approximation (GNPS3)

For the third scheme, we retain the staggered grid in Fig. 3.2 and the conservative formulation in (3.5.1) and (3.5.2) but give up the centered quadrature approximation for the integrals, using instead the exact integration in space-time of the corresponding Riemann problem. For instance :

$$F_{i-1/2,j}^{n,1} = f(\mathfrak{R}_{i-1/2,j}^1, x_{i-1/2}, y_j) + \frac{1}{h \Delta s} \int_{s_n}^{s_{n+1}} \int_{y_{j-1/2}}^{y_{j+1/2}} g(v_{\mathfrak{R}^2}(y, s), x_{i-1/2}, y) dy ds$$

where  $v_{\mathbb{R}^2}(y, s)$  represents the detailed solution in space-time of the Riemann problem with initial states  $(v_B, v_T)$ . The gradient preserving scheme simply replaces the detailed expression for  $v(y, s)$  in the integral by the constant value  $v(y = y_j, s) = \mathfrak{R}_{i-1/2, j}^2$ .

Except for the fact that they do not automatically preserve gradients, the last two test schemes are actually very similar to the gradient-preserving scheme (3.5.8), and one could expect them to perform similarly. In Fig. 3.3, however, the difference in performance is striking. The eigenvalue is seen to grow indefinitely with time for each one of the three alternative test-schemes, and converges to a steady state only in the case of the gradient-preserving scheme. This confirms the theoretical intuition that, to achieve convergence, the gradient-preserving property is essential to compensate for the lack of strong hyperbolicity in the system of conservation laws for the gradient.

### 3.7. EFFICIENT SECOND ORDER SCHEME

A second order version of the scheme is designed by resorting to the essentially non oscillatory (ENO) interpolation strategy in space, coupled with a Runge-Kutta time-integrator [34, 43].

Increasing the spatial order of accuracy to second order will be shown in Section 8 to improve significantly the efficiency of the method, as much less resolution is required to achieve a given accuracy with the higher order method than with the first order scheme. However, pseudo-time accuracy is not needed here : the main consideration for an efficient scheme is that a converged state be reached in as few pseudo-time steps as possible, so as to minimize the overall cost of the calculation.

Numerical experiments such as the one reported in Fig. 3.4 a) and c), reveal that the ENO second order scheme coupled with a standard Runge-Kutta method of the same order does not converge to steady state as rapidly as the first order scheme previously discussed. This is a serious drawback if the scheme is to be used

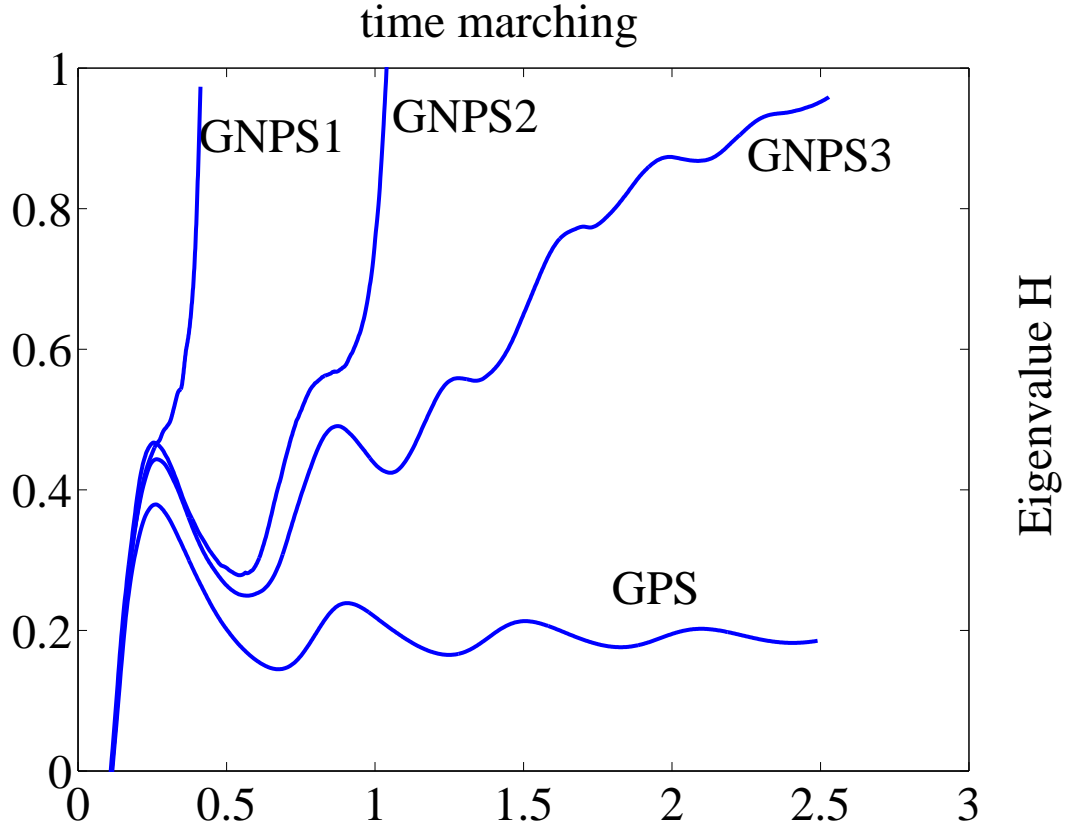


FIG. 3.3. Effective Hamiltonian  $H(r)$  as a function of pseudo-time; comparison of the performance of the gradient preserving scheme (GPS) with the three non gradient-preserving schemes (GNPS) described in Section 3.6. Spatial resolution  $40 \times 40$ , 800 pseudo-time iterations with CFL=0.45;  $\lambda = 1$ ,  $\bar{\lambda} = 2$ ,  $\theta = \bar{\theta} = \delta = 0$ .

repeatedly for tabulation. In the rest of this section, we gain some insight on the time-convergence properties of various two-step Runge-Kutta time-integrators by studying their linear stability for two limit versions of the ENO scheme : the two limit schemes are obtained by artificially freezing the discretization stencils and correspond respectively to the best (upwind) and worst (downwind) case scenario. We use this insight to identify constraints on the coefficients of the Runge-Kutta

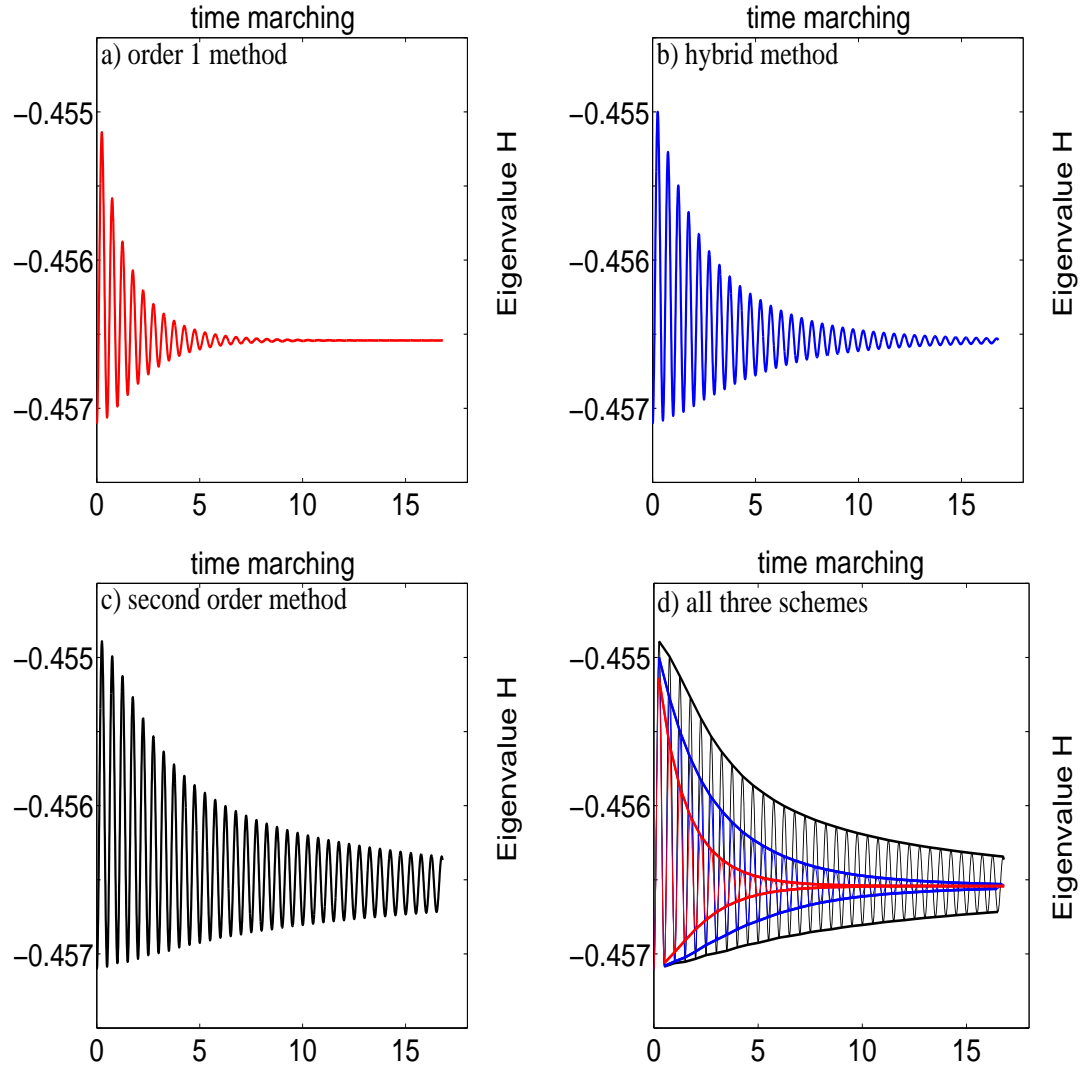


FIG. 3.4. Effective Hamiltonian  $H$  as a function of pseudo-time, comparing the performance of the hybrid scheme (second-order in space, first-order in time ENO2+RKM) compared with the overall second-order scheme (ENO2+RK2) and with the first-order scheme (O1). Spatial resolution  $40 \times 40$ , 3200 time iterations with  $CFL = 0.45$ ;  $\bar{\lambda} = 2$ ,  $\theta = \pi/4$ ,  $\delta = 0.5$  and  $\lambda = 0.1$ .

integrator likely to lead to good damping properties and fast convergence to steady-state.

### 3.7.1. Order of accuracy

To analyze the stability and accuracy properties of a generic explicit two-step Runge-Kutta scheme for our set of equations, we introduce first the difference operator  $\mathcal{A}$  associated with the original first-order scheme (3.5.8), i.e.,

$$\mathcal{A} \begin{pmatrix} \bar{u}_{i,j} \\ \bar{v}_{i-1/2,j-1/2} \end{pmatrix} = \frac{1}{h} \begin{pmatrix} F_{i+1/2,j} - F_{i-1/2,j} \\ F_{i-1/2,j} - F_{i-1/2,j-1} \end{pmatrix}$$

for which the left and right states in the Riemann problems are reconstructed by the primitive functions according to the ENO second order interpolation. Set

$$U^n = \begin{pmatrix} \bar{u}_{i,j}^n \\ \bar{v}_{i-1/2,j-1/2}^n \end{pmatrix}$$

so the Euler version of our scheme can be written

$$U^{n+1} = U^n - \Delta s \mathcal{A}(U^n).$$

We consider the Runge-Kutta two-step method

$$\begin{aligned} U^{n+1/2} &= U^n - \beta_0 \Delta s \mathcal{A}(U^n) \\ U^{n+1} &= \alpha_1 U^n + \alpha_2 U^{n+1/2} - \Delta s \beta_1 \mathcal{A}(U^n) - \Delta s \beta_2 \mathcal{A}(U^{n+1/2}) \end{aligned}$$

or

$$U^{n+1} = (\alpha_1 + \alpha_2) U^n - (\alpha_2 \beta_0 + \beta_1) \Delta s \mathcal{A}(U^n) - \beta_2 \Delta s \mathcal{A}(U^n - \beta_0 \Delta s \mathcal{A}(U^n)).$$

A standard accuracy analysis by matching terms in the Taylor expansion of the exact solution leads to the usual **conditions for first order accuracy**

$$\alpha_1 + \alpha_2 = 1 \tag{3.7.1}$$

$$\alpha_2 \beta_0 + \beta_1 + \beta_2 = 1 \tag{3.7.2}$$

and the usual **additional condition for second order accuracy**

$$\beta_2 \beta_0 = \frac{1}{2} \tag{3.7.3}$$

If the coefficients of the time-integrator satisfy those constraints, the complete scheme coupling this integrator with the second order ENO scheme in space will lead to an overall convergent scheme with second order accuracy in smooth regions, as long as the time-step is subjected to the appropriate CFL condition [43].

### 3.7.2. Linear stability of frozen-stencil schemes

Taking into account the constraint for a first order accuracy in Equation 3.7.1, the scheme can be written as :

$$U^{n+1} = U^n - (1 - \beta_2)\Delta s\mathcal{A}(U^n) - \Delta s\beta_2\mathcal{A}(U^n - \Delta s\beta_0\mathcal{A}(U^n)) \quad (3.7.4)$$

With the same notation as in Section 3.5 the associated scheme with the operator  $I_d - \beta_0\Delta s\mathcal{A}$  is given by

$$\begin{aligned} u_{i,j}^{n+1} &= u_{i,j}^n - \frac{\beta_0\Delta s}{h} \{a(u_{i,j}^n + S_{i,j}^n - u_{i-1,j}^n - S_{i-1,j}^n) + b(v_{i+1/2,j-1/2}^n \\ &\quad + T_{i+1/2,j-1/2}^n - v_{i-1/2,j-1/2}^n - T_{i-1/2,j-1/2}^n)\} \\ v_{i+1/2,j+1/2}^{n+1} &= v_{i+1/2,j+1/2}^n - \frac{\beta_0\Delta s}{h} \{a(u_{i,j+1}^n + S_{i,j+1}^n - u_{i,j}^n - S_{i,j}^n) \\ &\quad + b(v_{i+1/2,j+1/2}^n + T_{i+1/2,j+1/2}^n - v_{i+1/2,j-1/2}^n - T_{i+1/2,j-1/2}^n)\} \end{aligned} \quad (3.7.5)$$

where  $S_{i,j}$  and  $T_{i+1/2,j+1/2}$  are the corrections associated with the second order ENO reconstruction :

$$S_{i,j} = \begin{cases} \frac{u_{i+1,j} - u_{i,j}}{2} & \text{if } |u_{i+1,j} - u_{i,j}| \leq |u_{i,j} - u_{i-1,j}| \\ \frac{u_{i,j} - u_{i-1,j}}{2} & \text{otherwise} \end{cases}$$

$$T_{i+1/2,j+1/2} = \begin{cases} \frac{v_{i+1/2,j+3/2} - v_{i+1/2,j+1/2}}{2} & \text{if } |v_{i+1/2,j+3/2} - v_{i+1/2,j+1/2}| \\ & \leq |v_{i+1/2,j+1/2} - v_{i+1/2,j-1/2}| \\ \frac{v_{i+1/2,j+1/2} - v_{i+1/2,j-1/2}}{2} & \text{otherwise} \end{cases}$$

The expressions for the corrections  $S_{i,j}$  and  $T_{i+1/2,j+1/2}$  involve discretization stencils which are solution-dependent so that the discretization operator  $\mathcal{A}$  corresponding to an ENO scheme has non-constant coefficients. To gain insight in the behavior of the time-integrator, "frozen-stencil" variations will be studied next. For such schemes, one of the two choices for the corrections  $S$  and  $T$  is systematically used for the entire domain, for all time-iterations, regardless of the computed solution. As a result, the corresponding operator  $\mathcal{A}$  is linear with constant coefficients and a standard Fourier analysis is feasible. It is clear that such frozen-stencil schemes would not converge numerically for a general nonlinear problem, unlike the original ENO-scheme; the motivation for studying such unpractical scheme is given at the end of the section. When the stencil is frozen, the discrete operator  $\mathcal{A}$  is constant and Equation 3.7.4 can be rewritten as :

$$U^{n+1} = U^n - \Delta s \mathcal{A}(U^n) + (\Delta s)^2 \beta_2 \beta_0 \mathcal{A}^2(U^n) \quad (3.7.6)$$

Let  $G_2$  be the amplification matrix associated with the operator  $-\Delta s \mathcal{A}$  and  $I_d$  the identity matrix, then the amplification matrix,  $\mathcal{G}$ , associated with (3.7.6) is given by

$$\mathcal{G} = I_d + G_2 + \beta_0 \beta_2 G_2 \circ G_2. \quad (3.7.7)$$

Note that  $\mu$  is an eigenvalue for  $G_2$  if and only if  $1 + \mu + \beta_0 \beta_2 \mu^2$  is an eigenvalue for  $\mathcal{G}$ . So one needs only to compute  $G_2$  and its eigenvalues. Next, we analyze the spectral radius of  $G_2$  for two particular choices of frozen stencils.

### 1. Worst case scenario with frozen stencil : downwind scheme

Intuitively, the worst case scenario as far as stability is concerned corresponds to the case where the stencil in both directions includes systematically downwind information. With the advecting velocities  $a, b > 0$ , this corresponds to the choices :

$$S_{i,j} = \frac{u_{i+1,j} - u_{i,j}}{2} \quad \text{and} \quad T_{i+1/2,j+1/2} = \frac{v_{i+1/2,j+3/2} - v_{i+1/2,j+1/2}}{2}.$$



Replacing  $(u_{i,j}, v_{i+1/2,j+1/2})$ , in (3.7.5) by a single Fourier harmonic leads to the amplification matrix

$$G_2 = \begin{bmatrix} -\lambda_1 I \sin(\phi_{k_1}) & -\lambda_2 I \left( \sin\left(\frac{\phi_{k_1} + \phi_{k_2}}{2}\right) + \sin\left(\frac{\phi_{k_1} - \phi_{k_2}}{2}\right) \right) \\ -\lambda_1 I \left( \sin\left(\frac{\phi_{k_1} + \phi_{k_2}}{2}\right) - \sin\left(\frac{\phi_{k_1} - \phi_{k_2}}{2}\right) \right) & -\lambda_2 I \sin(\phi_{k_2}) \end{bmatrix}$$

whose eigenvalues are  $\mu_1 = 0$  and  $\mu_2 = -(\lambda_1 \sin(\phi_{k_1}) + \lambda_2 \sin(\phi_{k_2}))I = -\Phi I$ . The spectral radius of the matrix  $\mathcal{G}$ , given in (3.7.7), is less or equal to one if and only if

$$|1 - \Phi I - \beta_0 \beta_2 \Phi^2| \leq 1 \quad (3.7.8)$$

$$\sqrt{1 + (\beta_0 \beta_2 \Phi^2)^2 - (2\beta_0 \beta_2 - 1)\Phi^2} \leq 1 \quad (3.7.9)$$

$$\implies (2\beta_0 \beta_2 - 1) > 0. \quad (3.7.10)$$

Taking into account that  $|\phi| \leq \lambda_1 + \lambda_2$ , if this last inequality is verified, then the stability condition for this case is given by the following CFL condition :

$$\lambda_1 + \lambda_2 \leq \frac{\sqrt{2\beta_0 \beta_2 - 1}}{\beta_0 \beta_2}. \quad (3.7.11)$$

## 2. Best case scenario with frozen stencil : upwind scheme.

$$S_{i,j} = \frac{u_{i,j} - u_{i-1,j}}{2} \quad \text{and} \quad T_{i+1/2,j+1/2} = \frac{v_{i+1/2,j+1/2} - v_{i+1/2,j-1/2}}{2}.$$

This case corresponds to a standard second order upwind scheme. A sufficient condition for stability is that each sub-step satisfies a classical CFL condition :

$$|\beta_0|(\lambda_1 + \lambda_2) \leq 1, \quad (3.7.12)$$

$$(|\beta_1 \alpha_2| + |\beta_2|)(\lambda_1 + \lambda_2) \leq 1.$$

A detailed analysis would lead to similar CFL conditions with less restrictive constants ; however the exact expressions will not be needed here. An interesting

observation at this stage is that, as to be expected, the stability condition for the downwind scheme 3.7.10 and the CFL stability conditions 3.7.11 3.7.12 show opposite trends. For instance, one way to stabilize the downwind scheme is to pick  $\beta_0, \beta_2$  large, which implies taking an intermediate time-step which is actually larger than the final time-step. Such a choice however would lead to a very severe final time-step restriction because of the CFL conditions, in particular those of the upwind scheme.

The motivation to study the frozen-stencil schemes is to get some insight on how to achieve steady-state as efficiently as possible. The heuristic in selecting coefficients for an efficient Runge-Kutta integrator is that a scheme that satisfies all the stability constraints from the two frozen-stencil limit schemes (in addition to at least the first order accuracy conditions 3.7.1, 3.7.2) must have excellent damping properties as it stabilizes even the particularly unstable downwind scheme. Therefore, it is expected that such integrator would lead to an efficient pseudo-time marching scheme to steady-state by damping numerically the oscillations faster than a time-accurate scheme would.

A first observation is that the condition in Equation 3.7.10 for stability of the downwind frozen-stencil scheme is incompatible with the condition in Equation 3.7.3 for second-order accuracy in pseudo-time. It is also trivial to verify that, as one should expect, the standard one-step forward Euler scheme (with  $\beta_0 = 0$ ) cannot possibly satisfy the frozen-stencil stability condition for the downwind scheme.

Good damping per time-step is expected to be achieved by selecting a time-integrator with coefficients that minimize the spectral radius in Equation 3.7.9 (with a similar expression for the upwind scheme). One could attempt to find an optimal set of coefficients to minimize the spectral radii in a systematic search. However, such a procedure would be costly and probably not very useful because the results might not be relevant to the actual ENO scheme with variable stencil as used for the nonlinear cell-problem. Instead, we limited the search to sampling

a small number of combinations for the time-integrator coefficients and compared their performance (in conjunction with the second-order variable-stencil ENO scheme), in numerical experiments for the actual cell-problem. Among the combinations we tested were the standard explicit Runge-Kutta integrators of order one and two mentioned earlier - that they were outperformed is consistent with the heuristic analysis above.

The best performance observed in our limited search was achieved by the following combination, whose coefficients satisfy all the frozen-stencil stability constraints :

$$\alpha_1 = \frac{1}{3} \quad \alpha_2 = \frac{2}{3} \quad \beta_0 = \frac{3}{2} \quad \beta_1 = -\frac{1}{2} \quad \beta_2 = \frac{1}{2}$$

with the following CFL condition

$$\lambda_1 + \lambda_2 \leq \frac{2}{3} \tag{3.7.13}$$

Even though this linearly stable scheme (in the frozen-stencil sense) is only first order accurate with respect to the pseudo-time variable, numerical experiments such as the one reported in Fig. 3.4 demonstrate that it improves significantly the convergence to steady state compare to the second-order time-integrator. In that example, the eigenvalue oscillates rapidly in the pseudo-time with the oscillation amplitude decaying to zero when the pseudo-time grows, as predicted theoretically. The oscillations are rapidly damped with the first order scheme, a), and with the hybrid second-order in space and first-order in time scheme, but are much less so with the overall second-order scheme, c). Because we are not interested in an accurate prediction of the time-evolution but only in the steady-state, the new scheme has the advantage of converging to steady state almost as efficiently as the first-order scheme while at the same time, achieving second-order accuracy in space (at least in cases with smooth eigenfunctions) as

will be demonstrated in the next section by analyzing the convergence of the results under systematic mesh refinement.

### 3.8. VALIDATION

#### 3.8.1. Small scale shears

To validate the method, we first consider the response of the flame to velocity fields generated with the Childress-Soward flow (see stream function in Equation 3.2.3) with  $\delta = 1$ . Then, the velocity field is given by

$$v_1(x, y) = v_2(x, y) = \frac{\lambda}{\sqrt{2}} (-\sin(2\pi x) \cos(2\pi y) + \cos(2\pi x) \sin(2\pi y)).$$

This flow field actually represents a simple sine shear tilted at 45 degrees. The problem can be reduced to a one-dimensional problem by aligning the coordinate system with the shearing direction, and the results in [25] and [46] can be applied directly to provide us with reference data. (Here, the stream function is scaled so that  $\lambda$  represents the maximum shear intensity.) We solve the problem numerically in the original coordinate system as a two-dimensional case using the gradient-preserving scheme. The combustion speed enhancement is then compared with the reference value.

The numerical procedure consists in minimizing  $F(r)$  in Equation 3.2.1 as a function of  $r$ , which requires solving the cell-problem corresponding to each trial value for  $r$ . The minimization is performed using a standard routine [13] to a specified tolerance; all our numerical experiments showed that there were no numerical difficulty associated with the minimization routine itself, the key numerical issue being to be able to provide a sufficiently accurate value for the effective Hamiltonian  $H(r)$ .

The test-cases reported below correspond to the front angle  $\theta = \pi/4$  (i.e. the front normal is aligned with the shearing direction) and no mean flow  $\bar{\lambda} = \bar{\theta} = 0$ . With those parameters, it is particularly straightforward to predict analytically the

TAB. 3.1. Convergence of speed enhancement with  $\delta = 1$ ,  $\theta = \pi/4$ ,  $\bar{\lambda} = 0$ .

$\lambda$	reference $F_e$	Grid	$F_e$ order 1	(Error)	$F_e$ order 2	(Error)
0.4	0.4	16X16	0.24902	0.15098	0.39540	0.00460
		32X32	0.31928	0.08072	0.39939	0.00060
		64X64	0.35815	0.04184	0.39989	0.00011
1.6	1.6	16X16	1.06888	0.53112	1.58045	0.01955
		32X32	1.30876	0.29124	1.59761	0.00239
		64X64	1.44679	0.15320	1.59959	0.00040
6.4	6.4	16X16	3.39313	3.00687	6.27134	0.12866
		32X32	4.69028	1.70972	6.38566	0.01434
		64X64	5.50819	0.89182	6.39792	0.00208

burning speed enhancement as those set-ups are known theoretically to achieve the upper bound  $F_e = \lambda$ . Tab. 3.1 reports the computed values of  $F_e$  for three values of  $\lambda$  : small turbulence intensity  $\lambda = 0.4$ , medium intensity  $\lambda = 1.6$ , large turbulence intensity  $\lambda = 6.4$  (recall that in all the test cases here, velocities are normalized with the laminar burning speed  $S_L = 1$ ). Fig. 3.5 shows sequences of the corresponding wrinkled fronts : they represent a flame propagating from the right upper corner towards the left lower corner of the domain. Both the order 1 and the order 2 methods are seen in Tab. 3.1 to converge under mesh refinement, with the expected order of convergence : in particular, the gain in accuracy going from a first order to a second order method is significant at low resolutions - for practical purposes, it is possible, with the hybrid second order scheme, to predict  $F_e$  within one or two percent with the very coarse resolution of 16X16! Notice that the eigenfunctions computed here are not smooth (for instance, see the cusps in the flame fronts in Fig. 3.5, corresponding to shocks in the gradients.) As a consequence, one would expect a detailed numerical convergence study of the eigenfunction to show a reduction to first order convergence, even with the

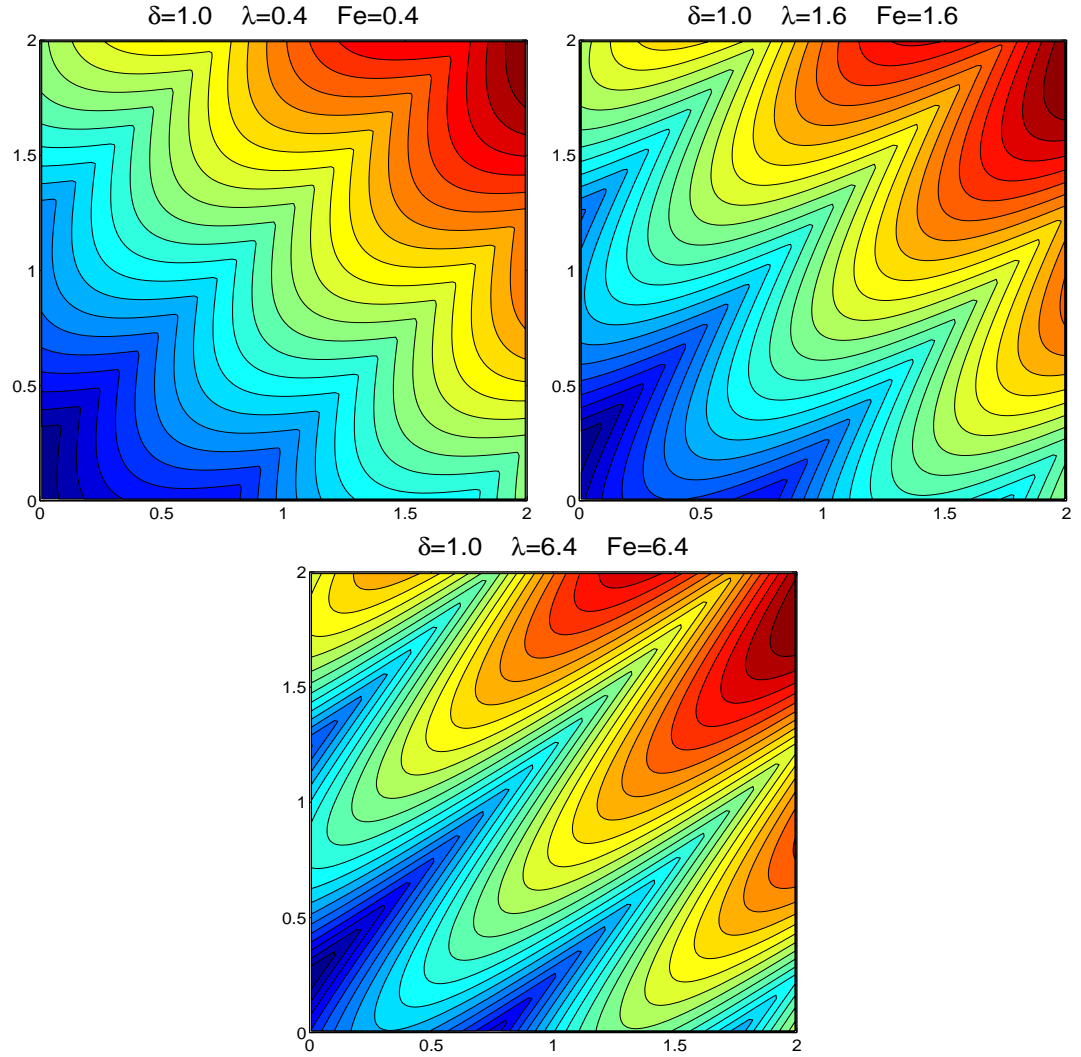


FIG. 3.5. Instantaneous flame fronts with  $\delta = 1$  - same data as in Tab. 3.1 (Hybrid) second order method, resolution  $64 \times 64$  (an array of  $2 \times 2$  cells is shown).

second order method. However, we are interested here only in the enhanced speed, obtained by processing the effective Hamiltonian, which itself is obtained by integration of the square of the norm of the eigenfunction gradient over the domain : this processing is sufficient to recover second order accuracy (see the last column of Tab. 3.1) even if the eigenfunction is locally first order accurate in the vicinity of the cusps.

### 3.8.2. Other flows

TAB. 3.2. Convergence of speed enhancement with  $\delta = 0.5$ ,  $\theta = \pi/4$ ,  $\bar{\lambda} = 0$ .

$\lambda$	reference $F_e$	Grid	$F_e$ order 1 (Error)	$F_e$ order 2 (Error)
1.6	1.50539	16X16	1.00988 0.49551	1.45519 0.05019
		32X32	1.23407 0.27132	1.49656 0.00882
		64X64	1.36283 0.14255	1.50331 0.00208
		128X128	1.43227 0.07311	1.50494 0.00044

TAB. 3.3. Convergence of speed enhancement with  $\delta = 0.0$ ,  $\theta = \pi/4$ ,  $\bar{\lambda} = 0$ .

$\lambda$	reference $F_e$	Grid	$F_e$ order 1 (Error)	$F_e$ order 2 (Error)
1.6	1.06534	16X16	0.77352 0.33186	0.99950 0.06588
		32X32	0.88433 0.18106	1.04836 0.01702
		64X64	0.97049 0.09485	1.06186 0.00347
		128X128	1.01676 0.04858	1.06485 0.00048

In the test-cases with  $\delta = 1$  just described, the small scale flow is a simple shear aligned with the normal to the large scale front so that the wrinkled flame front has a very simple topology, traveling without changing shape from the upper right corner into the unburnt mixture in the lower left corner, at a constant velocity. Such a simple flame pattern could have been computed using explicit formulas [25] and it was considered here only for the sake of validation. However, the gradient-preserving scheme is very robust and is designed to handle much more complex flame fronts behaviors. For instance, selecting  $\delta < 1$  in (3.2.3) leads to more interesting turbulent-like flows. For  $\delta = 0$  the flow corresponds to an array of eddies and for  $\delta = 0.5$  we have a combination of eddies and shears,

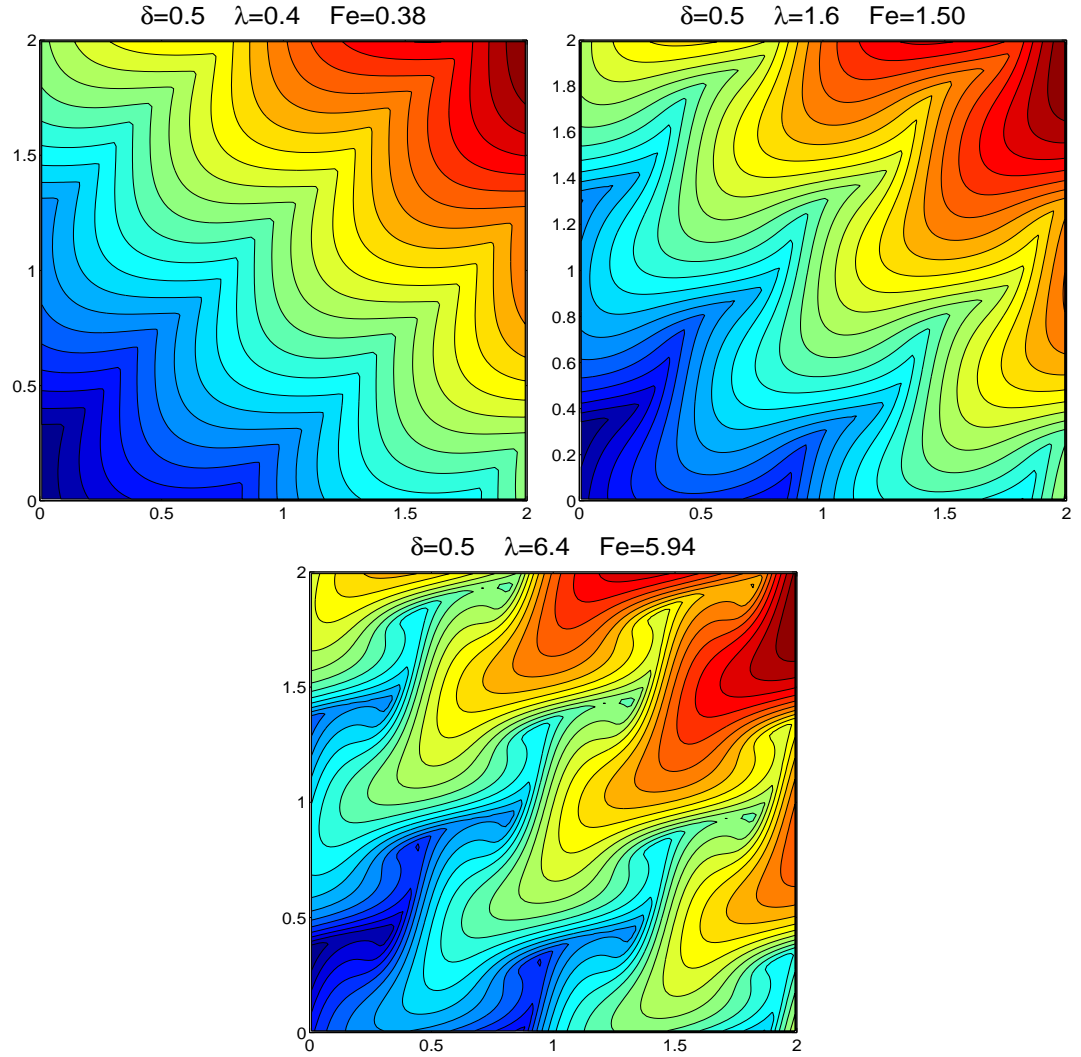


FIG. 3.6. Same as Fig. 3.5, with  $\delta = 0.5$ .

Fig. 3.1. Results for those two cases are reported in Tab. 3.2 and Tab. 3.3 as well as in Fig. 3.6 and Fig. 3.7. Again, the data are  $\theta = \pi/4$ ,  $\bar{\lambda} = \bar{\theta} = 0$ . The results of the mesh refinement reported in the two tables for the intermediate turbulence intensity  $\lambda = 1.6$  confirm the predicted order of accuracy and the significant gain in accuracy with the second order method. When  $\delta \neq 1$ , there are no analytical predictions available for  $F_e$  : instead, a reference value is obtained here by extrapolation of the data with the second order method - this should



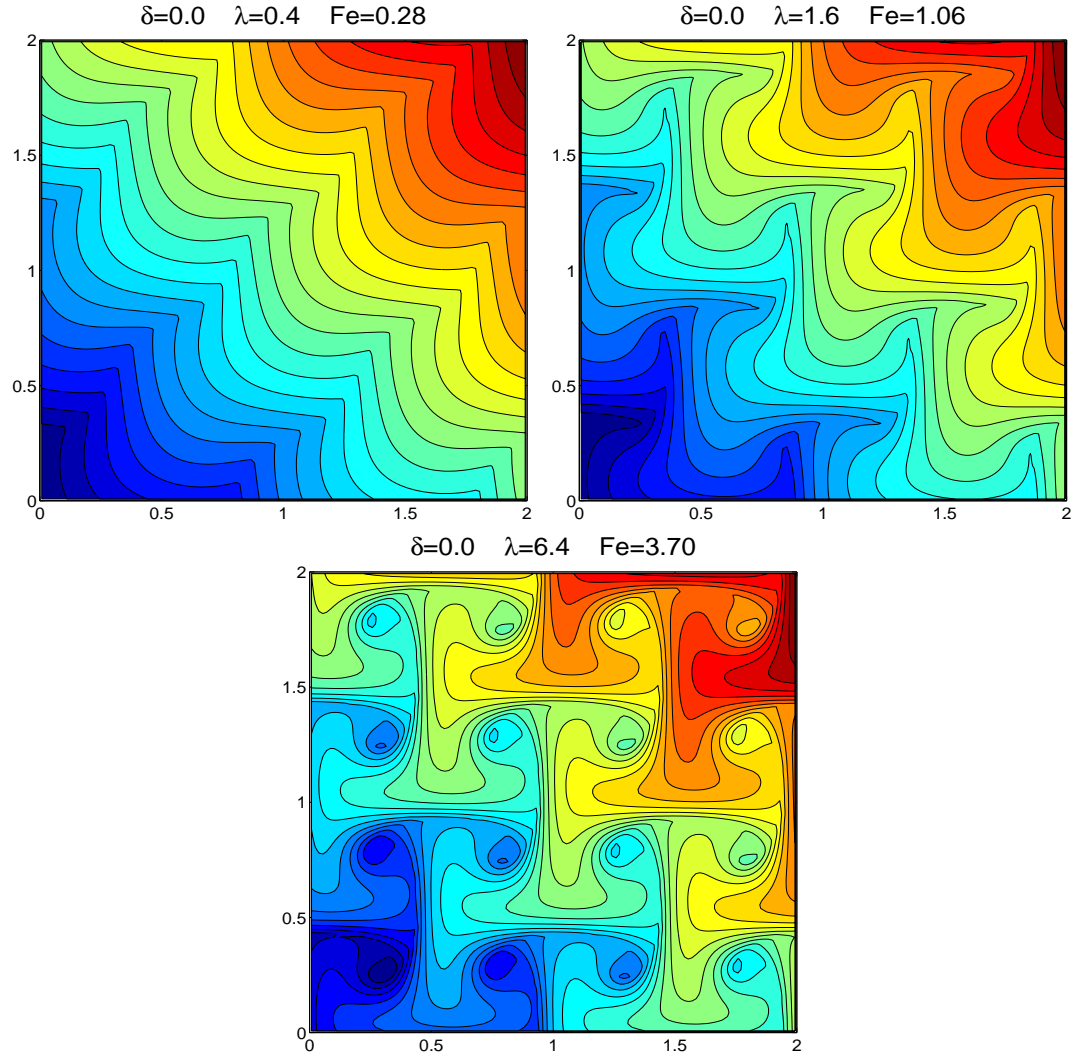


FIG. 3.7. Same as Fig. 3.5, with  $\delta = 0.0$ .

not affect the error analysis, except maybe for the estimation of the error on the finest grid. At low turbulence intensity  $\lambda = 0.4$ , the flame patterns at the top of Fig. 3.6 and Fig. 3.7 appear to be very similar to the simple shear case from Fig. 3.5 (notice however that  $F_e$  decreases with  $\delta$ .) At larger intensities however, in particular when  $\lambda = 6.4$ , the flame patterns become much more complex, some portions of the front overlap other portions, and there are even topological changes associated with pockets of unburnt gas lagging behind the leading front. Many

more computations of this type can be found in [39], [11], along with a more detailed analysis of the parameterization of  $F_e$  as a function of the characteristics of the flow.

**Remark 3.8.1.** *The gradient-preserving scheme derived here can be used in general for computing the solutions of Hamilton-Jacobi equations of the type [6, 51, 52, 57, etc]*

$$\tilde{Z}_s - K(\nabla \tilde{Z}, x, y) = 0, \quad \tilde{Z}(x, y, 0) = \tilde{Z}_0(x, y) \quad (3.8.1)$$

such that

$$\tilde{Z}(x, y, s) \approx w(x, y) + c_0 s, \quad \text{for large } s \quad (3.8.2)$$

or equivalently for PDE systems of the form

$$\begin{aligned} \frac{\partial u}{\partial s} &= \frac{\partial}{\partial x} K(u, v, x, y) \\ \frac{\partial v}{\partial s} &= \frac{\partial}{\partial y} K(u, v, x, y) \\ u(x, y, 0) &= u_0(x, y), \quad v(x, y, 0) = v_0(x, y) \end{aligned} \quad (3.8.3)$$

such that

$$(u, v)(x, y, s) \approx \nabla w(x, y), \quad \text{for large } s \quad (3.8.4)$$

Notice that, in this case of using the gradient-preserving scheme, the constant  $c_0$  in (3.8.2) (which might represent the effective speed of the moving front; for example, in the case of the  $G$  equation known in combustion) has to be computed by postprocessing like in (3.2.6).

Indeed, it is clear how to pass from the Hamilton-Jacobi equation for  $\tilde{Z}$  in (3.8.1) to the PDE system for its gradient  $\nabla \tilde{Z} = (u, v)$  in (3.8.3). Hence, consider the PDE system in (3.8.3).

From our derivation of the conservative formulation on the staggered grids, we obtain the following numerical scheme

$$\bar{u}_{i,j}^{n+1} = \bar{u}_{i,j}^n + \frac{\Delta s}{\Delta x} [K(R_1 u^{i+1/2,j}, R_2 v^{i+1/2,j}) - K(R_1 u^{i-1/2,j}, R_2 v^{i-1/2,j})]$$

$$\bar{v}_{i+1/2,j+1/2}^{n+1} = \bar{v}_{i+1/2,j+1/2}^n + \frac{\Delta s}{\Delta y} [K(R_1 u^{i+1/2,j+1}, R_2 v^{i+1/2,j+1}) - K(R_1 u^{i+1/2,j}, R_2 v^{i+1/2,j})]$$

which, clearly, has the general form in (3.5.8) so that it is easy to check that it conserves the gradient in the weak sense (even with  $\Delta x \neq \Delta y$ ).

The values  $R_1 u^{i-1/2,j}, R_2 v^{i-1/2,j}$  are (to be) obtained at each time step by solving the following (somehow complicated but solvable!) “2 D Riemann problem” at the respective interfaces.

$$\frac{\partial u}{\partial s} = \frac{\partial}{\partial x} K(u, v, x, y)$$

$$\frac{\partial v}{\partial s} = \frac{\partial}{\partial y} K(u, v, x, y)$$

$$u(x, y, 0) = u_0(x, y), \quad v(x, y, 0) = v_0(x, y)$$

with

$$u_0(x, y) = \begin{cases} u^R & \text{if } x > 0 \\ u^L & \text{if } x < 0 \end{cases}; \quad v_0(x, y) = \begin{cases} v^R & \text{if } y > 0 \\ v^L & \text{if } y < 0 \end{cases}$$

Notice that the fact that the flux,  $K$ , in (3.2.8) emanating from the cell problem of M-S theory splits into  $K(u, v) = f(u) + g(v)$  simplifies the above “2d Riemann problem” into two uncoupled simple (1d) Riemann problems.

### 3.9. CONCLUSION

A numerical method has been introduced to solve the nonlinear eigenvalue cell-problem arising in the homogenization theory of turbulent premixed flame fronts [46]. The scheme allows for the efficient second-order accurate computation of both the effective Hamiltonian (i.e. the eigenvalue) and the eigenfunction (related to successive realizations of the wrinkled flame front). The eigenvalue problem is solved using pseudo-time marching to steady-state of a system of conservation

laws for the eigenfunction gradient. Theoretical arguments are presented regarding the importance of satisfying the constraint that the steady-state vector solution be effectively the gradient of a scalar function. Exploiting the symmetry of the problem, a novel staggered grid formulation is shown to automatically satisfy the gradient-structure constraint in some appropriate discrete sense if the initial data did. Numerical experiments with variations of the scheme confirm the theoretical predictions by demonstrating that (i) the gradient-preserving property is necessary to guarantee convergence to steady state - Fig. 3.3 - (ii) time-integrators with good damping properties can be achieved by studying their behavior for frozen-stencil variations of the scheme - Fig. 3.4 - (iii) the scheme does achieve the predicted second-order accuracy, with a significant gain compared to the first order scheme at low resolution - Tabs. 3.1, 3.2 and 3.3.

The idea of converting a multi-dimensional Hamilton-Jacobi equation into a system of conservation laws for the gradient of the solution  $w$  was also used by Jin and Xin [35]. Their scheme also enforces to some extent the gradient condition in a formulation that has many advantages for general cases. The scheme presented here is different in several respects : it exploits the specific structure of the Hamiltonian to enforce the gradient condition exactly, not in a relaxation sense as in [35]; the two components of the discrete vector solution are represented on staggered grids, in [35] they are collocated, only  $w$  is staggered; the scheme presented here is geared toward the efficient computation of a steady-state solution for the effective Hamiltonian, a quantity that involves only  $\mathbf{D}w$  and not  $w$  itself. The scheme presented here was used successfully in [39, 11] to study systematically the parameterization of the turbulent enhancement of the flame speed for a variety of small scale flows. The numerical data were used to identify two distinct scalings regimes, similar to those observed in experiments with real flames. The transition between the two regimes was shown to depend essentially on a non-dimensional "flame residence time" that relates an intrinsic flame response time to a time scale related to the flame passage-time through a periodic cell; this

qualitative analysis inspired by the numerical data was explained theoretically via a formal asymptotic analysis.

Ultimately, one objective is to use the asymptotic speed enhancement as a basis for a subgrid-scale model in large eddy simulations of turbulent flames, where the effect of the unresolved turbulent flow scales must be accounted for as a modelled enhanced burning speed. The feasibility of such strategy is demonstrated in [40] for an idealized case : the scheme introduced in this paper is used to generate a complete database or "flamelet library" which can then be used repeatedly as an input to a level-set formulation for the flame front at large scales. Results of such computation are shown in [40] to be in excellent agreement with detailed direct simulation predictions for the wrinkled flames, with the large eddy simulations requiring only a small fraction of the computational cost of the detailed simulations.

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# Chapitre 4

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## DYNAMIQUE DU FRONT EN DEUX DIMENSIONS

### 4.1. INTRODUCTION

Dans ce chapitre, on applique la méthode numérique développée au chapitre 3 au cas d'une flamme soumise à un écoulement périodique en deux dimensions. La dynamique du front est décrite de façon qualitative par des séquences d'instantanés de la flamme. Les illustrations représentent les résultats obtenus à l'aide de la théorie de l'homogénéisation de Majda et Souganidis [46] (voir le chapitre 1) où le schéma numérique qui préserve le gradient présenté au chapitre 3 est utilisé pour résoudre le problème cellulaire.

Dans le régime d'application de la théorie, le front d'une flamme prémélangée sous le régime des flammelettes consiste en une interface infiniment mince séparant les gaz brûlés des gaz non brûlés qui avance en direction du mélange frais. Dans des conditions laminaires, la vitesse de propagation (la vitesse de combustion) est déterminée par la nature de la réaction chimique et est connue sous le nom de vitesse de combustion laminaire, mais en présence d'un écoulement turbulent (écoulement non constant qui varie sur plusieurs échelles), le front de la flamme est plissé, ce qui se traduit par une augmentation de la vitesse de combustion. Intuitivement, cette augmentation de vitesse de combustion est due au fait qu'une flamme plissée présente une surface de zone de réaction plus grande que celle d'une flamme lisse. L'augmentation de vitesse de combustion due à un écoulement donné

est d'autant plus importante que les plissements du front de la flamme causés par cet écoulement sont importants.

Dans le chapitre 2, nous avons décrit la paramétrisation systématique de l'augmentation de la vitesse de combustion en fonction des temps caractéristiques de la flamme pour le cas d'un cisaillement qui dépend du temps. Dans ce chapitre, nous considérons le cas d'une flamme soumise à un écoulement bi-dimensionnel de type Childress-Soward (une combinaison de cisaillements et de tourbillons). En s'inspirant des résultats du chapitre 2, nous présentons ici une analyse qualitative des résultats afin de comprendre le phénomène de plissement du front dans un cadre plus général et tentons de donner une réponse aux questions suivantes :

1. Comment le front de la flamme se plisse t-il ?
2. À quels endroits ?
3. Quel type d'écoulement favorisent les plissements ?
4. Est ce que les plissements sont toujours proportionnels à l'intensité de la turbulence ?
5. Est-ce que l'alignement de la flamme par rapport à l'écoulement est important ?

## 4.2. PARAMÈTRES ÉTUDIÉS

On considère une flamme initialement plane soumise à un écoulement turbulent bi-dimensionnel. Pour simplifier on suppose que l'écoulement moyen est nul. Le champ de vitesse choisi ainsi que l'orientation du front moyen sont décrits ci-dessous.

### a) Le champ de vitesse : écoulement de Childress-Soward

Les écoulements de Childress-Soward sont décrits par la famille de fonctions de courant

$$f_{\delta}(x, y) = \lambda C[\sin(2\pi x) \sin(2\pi y) + \delta \cos(2\pi x) \cos(2\pi y)] \quad (4.2.1)$$

où  $\delta$  est un paramètre qui varie dans l'intervalle  $[0, 1]$  et  $C$  est une constante qui dépend de  $\delta$  fixée telle que la norme max du champ de vitesse

$$\mathbf{v}(x, y) = (-\partial_y f_\delta(x, y), \partial_x f_\delta(x, y)) \quad (4.2.2)$$

soit égale à  $\lambda$ .  $\lambda$  est un paramètre positif qui mesure l'intensité de "la turbulence". Dans la suite on jouera sur les deux paramètres  $\lambda$  et  $\delta$  qui caractérisent l'écoulement et son intensité. Lorsque  $\delta$  varie dans l'intervalle  $[0, 1]$  on obtient des champs de vitesse de différentes natures, susceptibles d'avoir des impacts totalement différents sur la flamme. Une simple reproduction des lignes de courant, dans la figure 4.1, nous permet de voir que quand  $\delta = 1$  l'écoulement généré est un cisaillement incliné à  $45^\circ$  par rapport à l'axe des  $x$ . Quand  $\delta = 0$  nous avons un écoulement cellulaire constitué par un réseau de tourbillons. Les valeurs intermédiaires  $0 < \delta < 1$  correspondent à des écoulements hybrides cisaillement-tourbillons. Dans ce dernier cas, les tourbillons ont la forme d'une ellipse et sont séparés par des canaux (qui sont la trace des lignes de cisaillement) où le fluide passe très vite tandis que des poches de fluide sont "piégées" dans les tourbillons. Quand  $\delta$  est proche de 1, les canaux s'élargissent et tendent vers des lignes droites tandis que les tourbillons s'allongent et s'amincissent et tendent à disparaître. Quand  $\delta$  s'approche de zéro les canaux deviennent étroits et se referment éventuellement sur les tourbillons qui deviennent de plus en plus circulaires.

### **b) L'orientation du front moyen**

On considère une flamme initialement plane qui fait un angle  $\theta$  avec l'axe des abscisses tel que la normale dirigée vers le mélange frais est donnée par (voir la figure 4.2)

$$\mathbf{n} = (\cos \theta, \sin \theta).$$

Étant donné que le champ de vitesse moyen est nul, le front moyen (qui se propage avec la vitesse de combustion turbulente moyenne) est toujours parallèle à ce front initial. Dans la suite on joue sur le paramètre  $\theta$  pour changer l'orientation



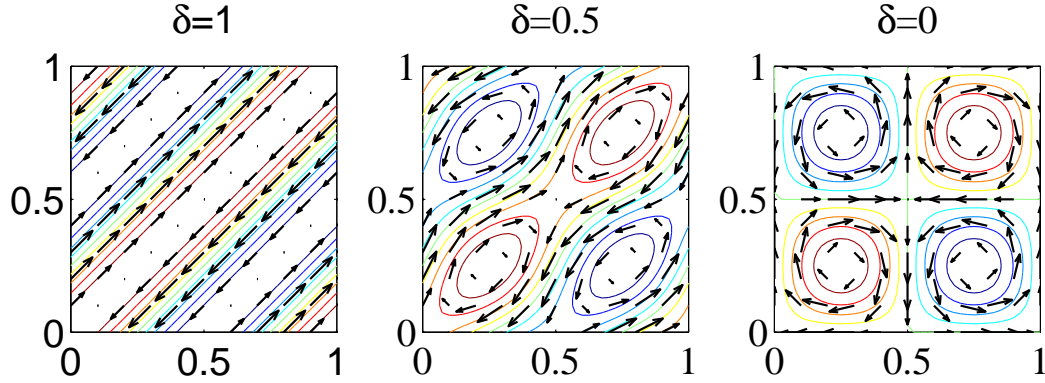


FIG. 4.1. Écoulement de Childress-Soward.

$\delta = 1$  est un cisaillement tourné à 45 degrés,  $\delta = 0.5$  c'est un écoulement hybride cisaillement-tourbillons et  $\delta = 0$  forme une collection de tourbillon.

du front moyen. La réponse du front à l'écoulement aux petites échelles dépend fortement de cette inclinaison, par exemple, dans le cas d'un cisaillement pur, l'effet maximal est observé si la normale au front et le cisaillement ont la même direction tandis que si la normale au front est perpendiculaire au cisaillement, celui-ci n'a absolument aucun effet sur le front.

### 4.3. LE FRONT INSTANTANÉ

Soit  $w$  la fonction propre solution du problème cellulaire,

$$-|\mathbf{D}w + \mathbf{p}|^2 + \mathbf{v} \cdot (\mathbf{D}w + \mathbf{p}) = -H(\mathbf{p}), \quad (4.3.1)$$

$$\mathbf{p} = r_0(\cos \theta, \sin \theta)$$

avec  $\theta$  l'angle que fait la normale à la flamme initiale (plane) avec l'axe des abscisses,  $r_0$  est un nombre réel positif qui intervient dans la minimisation, voir ci-dessous. Les fronts instantanés de la flamme sont donnés par les lignes de niveau de la fonction

$$\bar{Z}(x, y, t) = r_0 x \cos \theta + r_0 y \sin \theta + w(x, y). \quad (4.3.2)$$

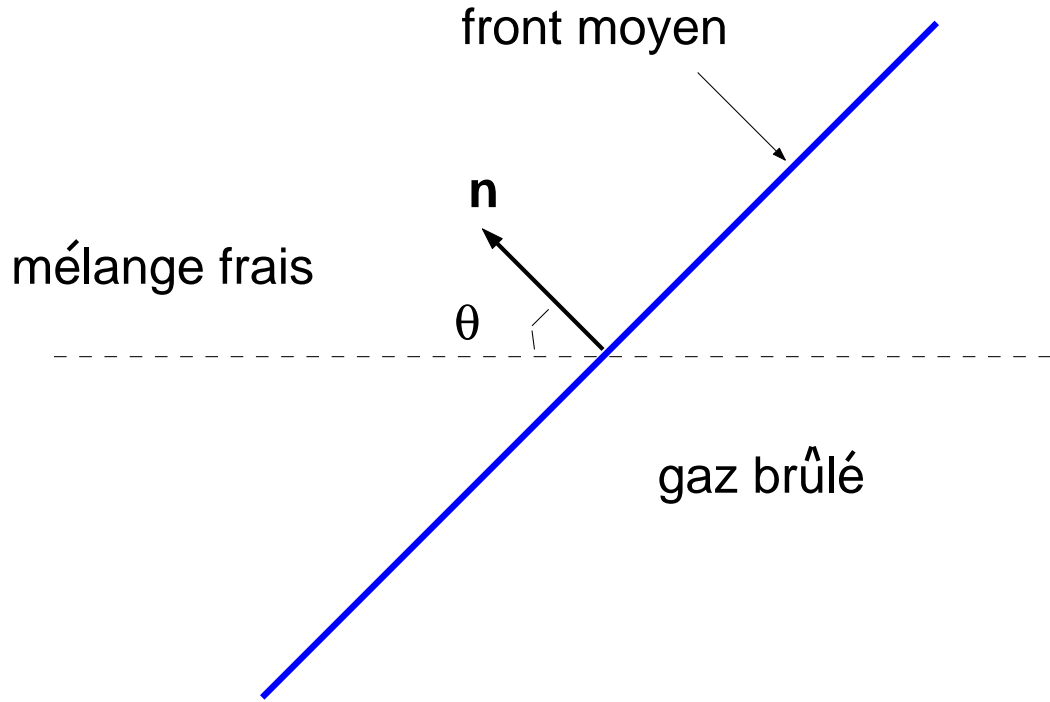


FIG. 4.2. Orientation du front moyen.

Cette conception du front instantané peut paraître un peu hasardeuse car  $w$  est en fait la solution du problème cellulaire qui est “un problème dual pour le problème homogénéisé” [46] dont la signification physique n’a pas été clarifiée par la théorie. Après l’homogénéisation, seul le front de la flamme aux grandes échelles est défini par la solution de l’inéquation variationnelle. Or, on sait, d’après la même théorie, que lorsque le champ de vitesse à grande échelle est constant, le front moyen obéit au principe d’Huygens donc il est et restera tout le temps une ligne droite, parallèle au front initial, qui se déplace avec la vitesse de combustion,

$$F = \min_{r>0} \frac{H(r(\cos \theta, \sin \theta)) - f'(0)}{r} = \frac{H(r_0(\cos \theta, \sin \theta)) - f'(0)}{r_0}. \quad (4.3.3)$$

En posant

$$\tilde{Z}(x, y, t) = Ft + x \cos \theta + y \sin \theta + \frac{1}{r_0} w(x, y). \quad (4.3.4)$$

Il est clair que quand  $w = 0$  les lignes de niveaux de  $\tilde{Z}$  sont des droites parallèles donnant le front aux grandes échelles à chaque instant  $t$ . Ainsi la quantité  $w(x, y)/r_0$  est vue comme une perturbation du front moyen.

En remplaçant dans le problème cellulaire (4.3.1), on obtient l'équation suivante pour  $\tilde{Z}$

$$(r_0\tilde{Z})_t - |\mathbf{D}(r_0\tilde{Z})|^2 + \mathbf{v} \cdot \mathbf{D}(\tilde{Z}) - f'(0) = 0. \quad (4.3.5)$$

Dans la zone de préchauffage où  $T$  est proche de zéro, on a

$$f'(0) \approx -\frac{f(T)}{T} \quad (4.3.6)$$

car le terme de réaction,  $f$ , est de type KPP (voir le chapitre 1). On peut "inverser" la procédure de l'homogénéisation :

1. en rajoutant à droite de l'équation (4.3.5) un petit terme de viscosité  $\epsilon\Delta Z^\epsilon$ ,
2. en remplaçant  $r_0\tilde{Z}$  par  $Z^\epsilon$
3. en utilisant (4.3.6) (en supposant qu'on est dans la zone de préchauffage et que  $0 < \epsilon \ll 1$ ).

On obtient

$$Z_t^\epsilon - \epsilon\Delta Z^\epsilon - |\mathbf{D}Z^\epsilon|^2 + \mathbf{v}(x, y) \cdot \mathbf{D}Z^\epsilon + f(T)/T = 0, \quad (4.3.7)$$

i.e, on obtient l'équation de départ de la théorie rigoureuse [46] (voir le chapitre 1) avec  $\epsilon^\alpha = 1$  (car, ici, notre échelle de longueur est la période de l'écoulement aux petites échelles qui est fixé à un). Le front de la flamme à grande échelle est défini dans la théorie asymptotique par la frontière  $\partial\{Z < 0\}$ . Donc, pour  $\epsilon \ll 1$ ,  $\partial\{Z^\epsilon < 0\}$  serait le résultat de la perturbation du front asymptotique par l'effet des petites échelles, i.e, le front plissé. Ce dernier coïncide avec le niveau zéro de  $\tilde{Z}$ . Comme (4.3.5) est invariante par l'ajout d'une constante à  $\tilde{Z}$ , chacun des niveaux de la solution  $\tilde{Z}(x, y, t)$  pour  $t$  fixe (en particulier  $t = 0$ , i.e.,  $\bar{Z}$ ) définit une forme possible pour le front instantané. D'une façon équivalente, en faisant varier  $t$  de  $-\infty$  à  $+\infty$  et en définissant le front de la flamme comme étant le

niveau zéro de  $\tilde{Z}$  à chaque instant, comme la dérivée  $\tilde{Z}_t$  est une constante, ce niveau zéro (le front de la flamme) passera par chacun des niveaux de  $\bar{Z}(x, y)$  défini en (4.3.2).

Vu la nature périodique (dans l'espace) de la fonction  $w$ , lors de sa propagation, le front de la flamme aussi adopte une dynamique périodique dans le temps. Ainsi dans les figures ci-après, nous illustrons à l'aide d'images instantanées la dynamique du front durant une seule période de temps (réduite par la suite à une demi-période à cause de l'anti-symétrie des écoulements de Childress-Soward) sur deux périodes de l'espace (pour mieux illustrer).

#### 4.4. CAS TESTS ET ILLUSTRATIONS

Étant donné que le cas d'un écoulement unidimensionnel qui caractérise un cisaillement a été étudié au chapitre 2, nous n'allons pas considérer ici le cas  $\delta = 1$  qui peut se ramener à un écoulement unidimensionnel par une simple rotation de  $45^\circ$ . Nous allons nous limiter aux deux valeurs  $\delta = 0$  et  $\delta = 1/2$ . Le cas  $\delta = 0$  où on a seulement des tourbillons présente un nouveau type d'écoulement dont la topologie est complètement différente de celle du cisaillement vu au chapitre 2 tandis que le cas  $\delta = 1/2$  constitue un pont qui nous permettra de passer du cas simple du cisaillement à celui des tourbillons. Un autre paramètre important à faire varier, avec l'intensité de la turbulence  $\lambda$ , bien sûr, est l'angle  $\theta$  de la normale au front initial par rapport à l'axe des  $x$ .

Nous savons (voir le chapitre 2) que dans le cas d'un simple cisaillement, l'augmentation de vitesse atteint sa valeur théorique maximale si la flamme est initialement perpendiculaire aux lignes du cisaillement et elle est nulle si le front est initialement parallèle au cisaillement.

Pour ces raisons, nous commençons par le cas  $\delta = 1/2$  où la composante du cisaillement dans l'écoulement de Childress-Soward est importante et nous considérons A) le cas  $\theta = \pi/4$  qui correspond à une flamme perpendiculaire au cisaillement, B) le cas  $\theta = -\pi/4$  où la flamme est parallèle au cisaillement et C) le

cas  $\theta = 0$  qui constitue un état intermédiaire entre les deux. Afin d'analyser l'effet de l'intensité de la turbulence nous considérons chacun des cas cités ci-dessus avec deux valeurs différentes de  $\lambda$ ,

- i)* une valeur plus grande que la vitesse de combustion laminaire, normalisée à  $S_L = 1$ , qui correspond à un cas de forte turbulence et
- ii)* une valeur plus petite que  $S_L$  correspondant à un cas de faible turbulence.

Nous reprenons les cas A)  $\theta = 0$  et B)  $\theta = \pi/4$  combinés avec

- i)* une faible et
- ii)* une forte turbulence

avec la valeur  $\delta = 0$  qui constitue une collection de tourbillons. On notera qu'ici le cas  $\theta = -\pi/4$  est équivalent au cas B),  $\theta = \pi/4$  par symétrie.

## I. Écoulement hybride cisaillement-tourbillons

On considère une flamme initialement plane soumise à un écoulement de type Childress-Soward avec  $\delta = 1/2$ . Rappelons que l'écoulement ainsi choisi est composé d'un cisaillement à 45 degrés combiné avec une collection de tourbillons, où le cisaillement et les tourbillons ont une contribution comparable dans la topologie de l'écoulement total, voir la figure 4.1. Nous savons d'après le chapitre 2 et ses références que dans le cas d'un simple cisaillement l'alignement de la flamme par rapport aux lignes du courant joue un rôle important en ce qui concerne la distorsion du front et par conséquent l'augmentation de la vitesse de combustion. Quand le front est perpendiculaire au cisaillement, l'augmentation de vitesse atteint sa borne supérieure théorique et quand la flamme est parallèle au cisaillement, il n'y a rien qui se passe, l'augmentation de vitesse est nulle. En partant de ces considérations, nous considérons ci-dessus les cas où l'angle que fait la normale au front avec l'axe des  $x$  est : A)  $\theta = \pi/4$  qui correspond à une flamme perpendiculaire à la composante-cisaillement de l'écoulement de Childress-Soward avec, B)  $\theta = -\pi/4$  qui est un cas où la flamme est parallèle à ce cisaillement ainsi que le cas médian C)  $\theta = 0$ .

**A) La flamme est perpendiculaire à la composante-cisaillement :  $\theta = \pi/4$**

Rappelons que dans le cas  $\delta = 1/2$ , les lignes de cisaillement dans l'écoulement de Childress-Soward représentent des canaux ouverts où les particules du fluide peuvent circuler tandis que les tourbillons constituent des points d'arrêt où les particules sont coincées et ne font que tourner autour d'elles même. Dans les figures 4.3 et 4.4 on représente les fronts instantanés associés pour deux différentes valeurs de  $\lambda$ . La flamme qui est initialement perpendiculaire aux canaux s'engage vers l'avant aux endroits où le flot se dirige de son côté et est retenue vers l'arrière là où le flot est opposé. Ainsi la flamme qui se retrouve tirée d'un côté et de l'autre, se déforme. Dans le tour de force qui oppose la flamme qui avance vers le mélange frais et le courant qui essaye de l'entraîner d'un côté vers l'arrière et de l'autre côté vers l'avant, le front de la flamme se plisse et forme une pointe vers l'arrière tout comme dans le cas d'un simple cisaillement vu au chapitre 2. Toutefois, la forme des plissements, tout comme leurs longueurs respectives, dépend fortement de l'intensité de la turbulence  $\lambda$ .

*i) Faible turbulence :  $\lambda = 0.8$*

Sur la figure 4.3, on illustre la dynamique du front d'une telle flamme avec  $\lambda = 0.8$ . On voit que dans le cas de faible intensité de turbulence, la flamme ne semble pas être affectée par la présence des tourbillons. Elle présente une topologie semblable à celle d'une flamme soumise à un simple cisaillement (voir le chapitre 2), excepté qu'ici la structure du front oscille à cause des jets qui ne sont pas droits mais qui zigzaguent entre les tourbillons.

*ii) Forte turbulence :  $\lambda = 6.4$*

Sur la figure 4.4, on illustre le cas de forte intensité de turbulence,  $\lambda = 6.4$ .

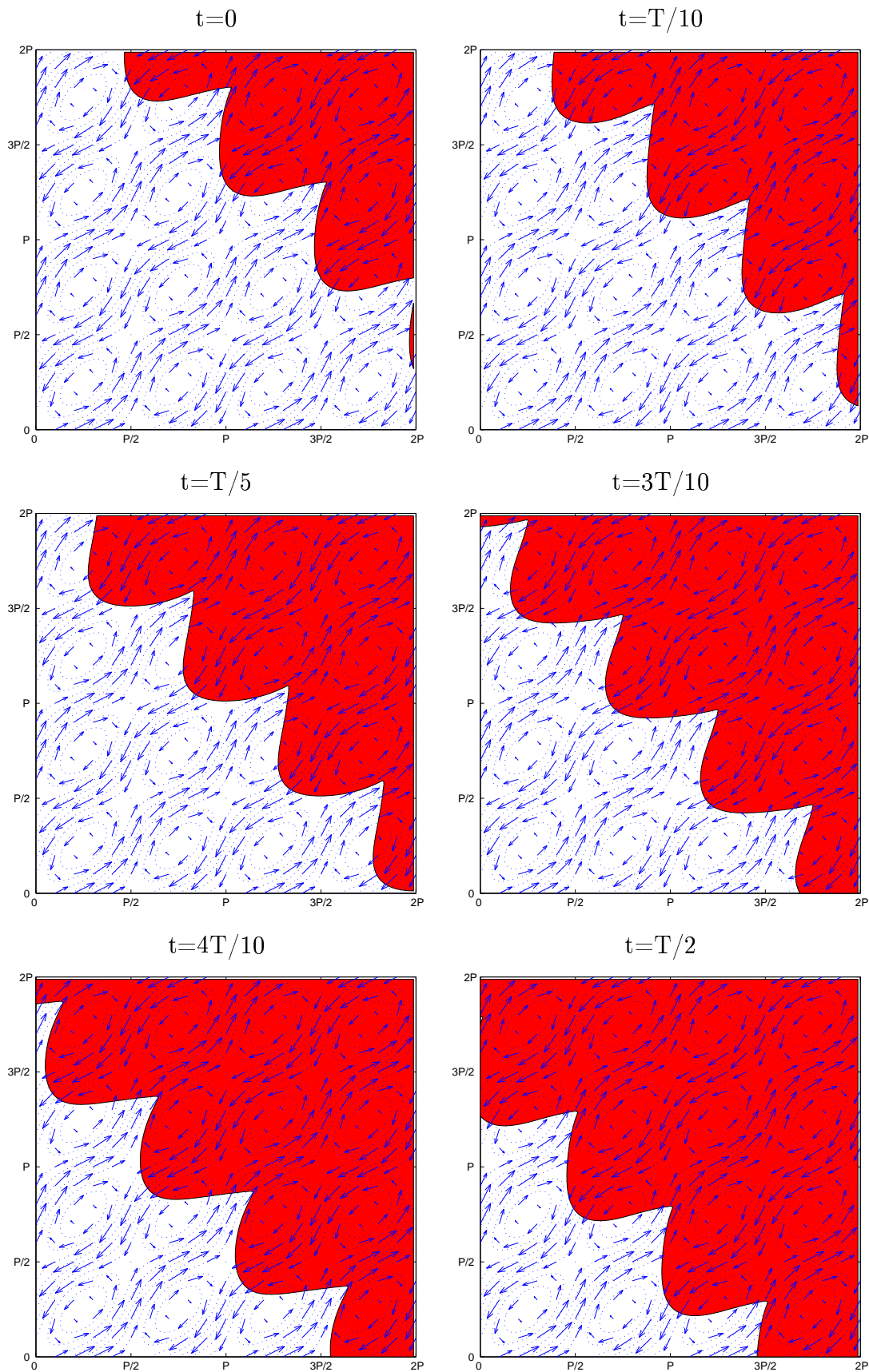


FIG. 4.3. Cas I. A) *i*):  $\delta = 1/2$ ,  $\theta = \pi/4$ ,  $\lambda = 0.8$ .

Contrairement au cas de faible turbulence, dans ce cas, on distingue clairement l'effet des tourbillons qui forcent la flamme à se replier sur elle-même pour former des poches de gaz non brûlé à l'intérieur de la zone brûlée. Dans le cas de faible turbulence *i)*, le front reste le graphe d'une fonction dans le repère défini par le front moyen (initiale, droit) donc facile à suivre lors d'une simulation, ce qui n'est pas le cas ici à cause du fait que la flamme se replie sur elle-même. On notera aussi que la longueur des plissements est beaucoup plus importante dans ce dernier cas.

**B) La flamme est parallèle à la composante-cisaillement :  $\theta = -\pi/4$**

Maintenant on change l'angle  $\theta$  à  $\theta = -\pi/4$  de telle sorte que la flamme soit grosso-modo parallèle au cisaillement et on refait l'expérience précédente.

*i) Faible turbulence :  $\lambda = 0.4$*

Sur la figure 4.5, on présente le cas d'une flamme dont la normale (moyenne) fait un angle  $-\pi/4$  avec l'axe des x pour une faible intensité de turbulence,  $\lambda = 0.4$ . Comme dans le cas  $\theta = \pi/4$ , quand la turbulence est faible les plissements de la flamme ressemblent à ceux associés à un cisaillement perpendiculaire.

*ii) Forte turbulence :  $\lambda = 6.4$*

Sur la figure 4.6, on reprend le cas précédent avec  $\lambda = 6.4$ . Ici on voit apparaître les effets des tourbillons mais l'amplitude des plissements est très petite.

**Interaction de deux cisaillements perpendiculaires**

La dynamique de la flamme dans le cas de faible intensité ressemble étrangement à son homologue de la figure 4.3 ( $\theta = \pi/4$ ,  $\lambda = 0.8$ ) malgré qu'apparemment il n'y a pas de cisaillement qui lui est perpendiculaire. Ceci n'est qu'une illusion car une simple manipulation algébrique de la fonction de courant,  $f_\delta$ , montre qu'en fait l'écoulement de Childress-Soward s'écrit comme la somme de deux



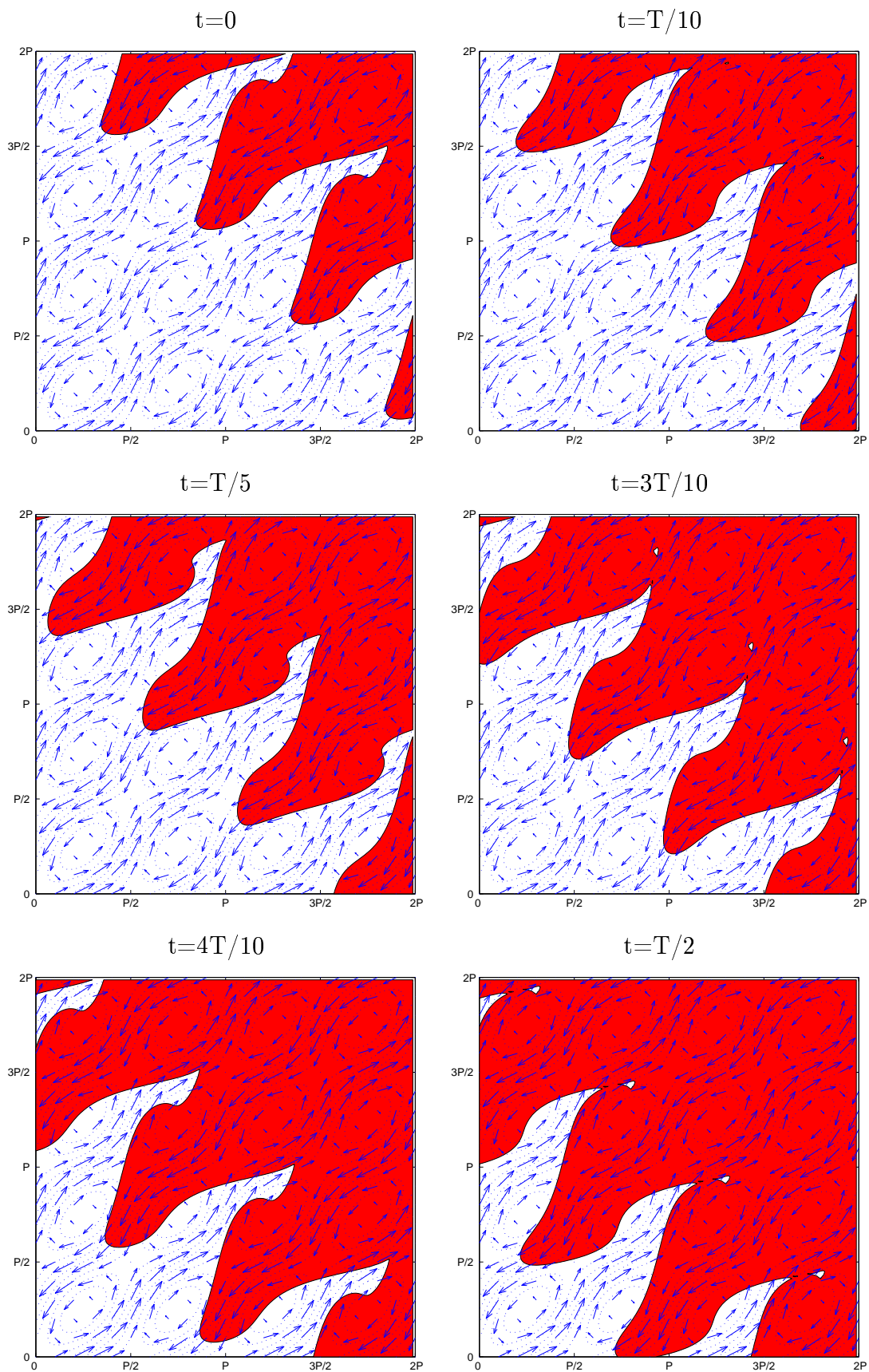


FIG. 4.4. Cas I. A) *ii*):  $\delta = 1/2$ ,  $\theta = \pi/4$ ,  $\lambda = 6.4$ .

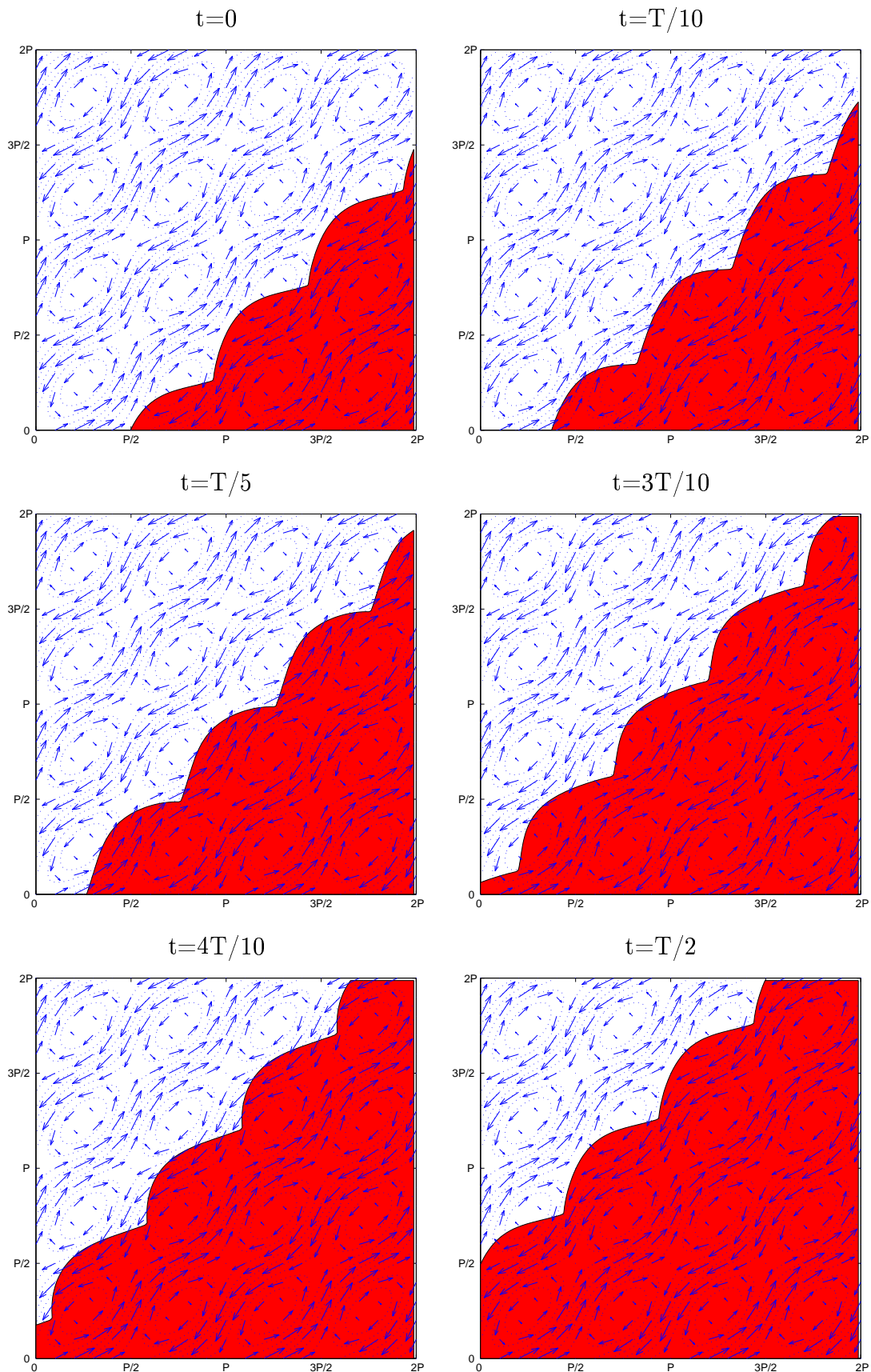


FIG. 4.5. Cas I. B) *i*) :  $\delta = 1/2$ ,  $\theta = -\pi/4$ ,  $\lambda = 0.4$ .

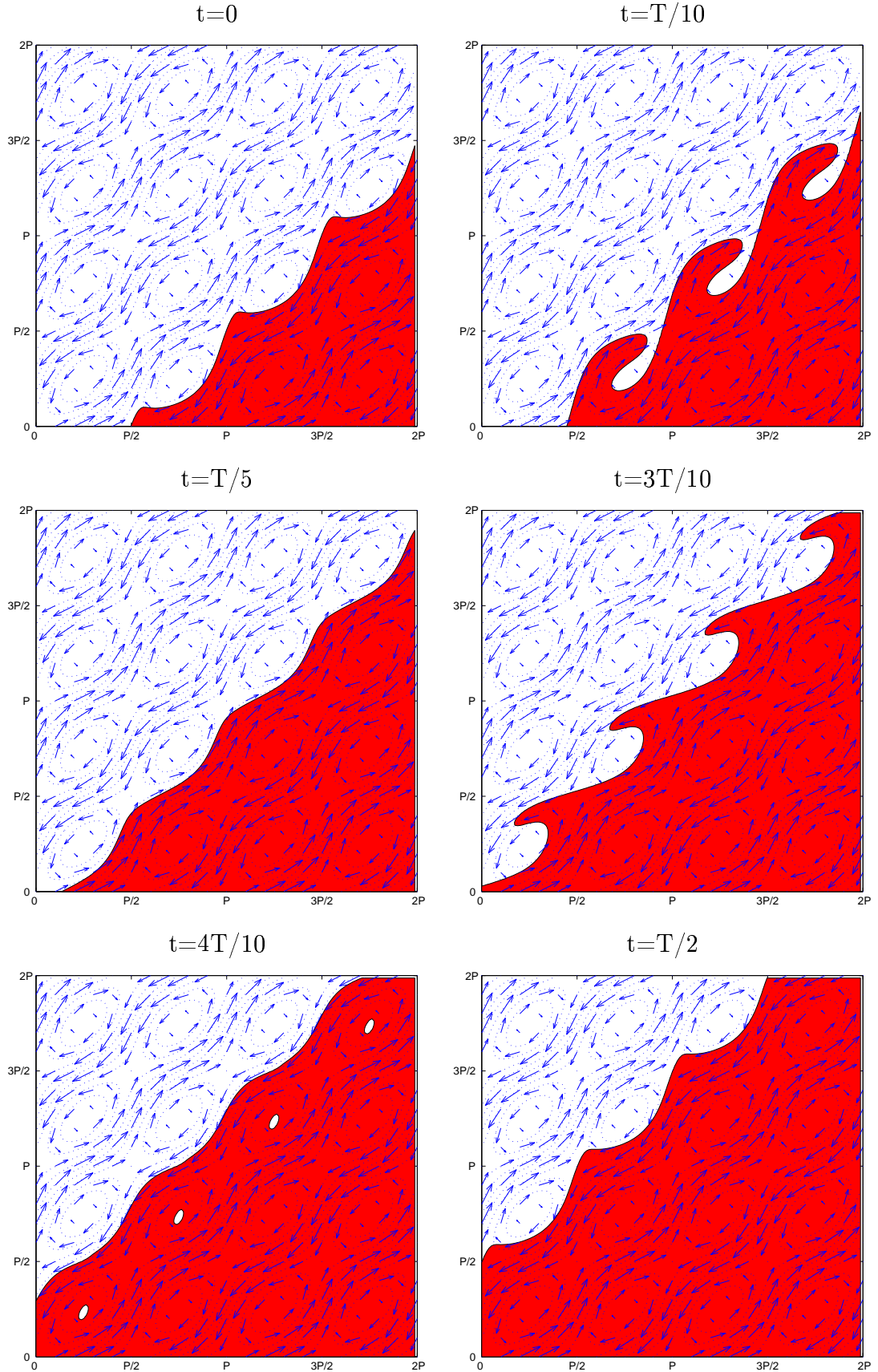


FIG. 4.6. Cas I. B) *ii*) :  $\delta = 1/2$ ,  $\theta = -\pi/4$ ,  $\lambda = 6.4$ .

cisaillements. On a

$$\sin 2\pi x \sin 2\pi y + \delta \cos 2\pi x \cos 2\pi y = \frac{1 + \delta}{2} \cos 2\pi(x - y) + \frac{\delta - 1}{2} \cos 2\pi(x + y).$$

Il est facile de voir que les fonctions  $f_1(x, y) = \cos 2\pi(x - y)$  et  $f_2(x, y) = \cos 2\pi(x + y)$  représentent deux fonctions de courant dont les lignes de niveaux sont des lignes droites parallèles aux première et deuxième bissectrices respectivement. De plus les écoulements associés sont des simples cisaillements respectivement parallèles aux deux bissectrices. Ainsi l'écoulement de Childress-Soward se décompose en deux cisaillements perpendiculaires, le premier est parallèle à la première bissectrice et le second est parallèle à la deuxième bissectrice. L'intensité du premier est amplifié par un facteur  $(1 + \delta)/2$  tandis que celle du second est amortie par un facteur  $(1 - \delta)/2$ . Quand la normale de la flamme moyenne fait un angle  $\theta = \pi/4$  (cas précédent) avec l'axe des x, la flamme se retrouve donc perpendiculaire au cisaillement de plus forte intensité, le front se déforme selon ce cisaillement et ensuite l'autre cisaillement intervient, avec une plus faible intensité, pour seulement la faire osciller suivant la direction perpendiculaire dans le cas de faible turbulence ( $\lambda = 0.8$ ) mais il parvient à la faire déformer quand  $\lambda = 6.4$ .

Tandis que dans le cas présent ( $\theta = -\pi/4$ ) la flamme est perpendiculaire au cisaillement de plus faible intensité donc c'est celui là qui la déforme en premier. Ensuite quand le front se présente face au cisaillement de plus forte intensité ce dernier intervient pour modifier les plissements. Quand l'intensité de turbulence est faible, voir la figure 4.5 ( $\lambda = 0.4$ ), le cisaillement parallèle à la flamme ne la fait qu'osciller tandis que dans le cas de forte turbulence, en bas de la figure ( $\lambda = 6.4$ ), la flamme est repliée sur elle-même par l'action du cisaillement de plus forte intensité. Notez que dans le cas  $\theta = -\pi/4$ ,

1. le cisaillement qui se trouve parallèle à la flamme agit sur l'avant de la flamme en l'entraînant à l'intérieur des canaux qui sont perpendiculaires à la normale de la flamme moyenne ce qui l'empêche ainsi d'avancer plus

vite dans la direction normale au front moyen, contrairement au cas précédent, où la formation de poches se fait vers l'arrière. Ici, les jets associées avec le cisaillement parallèle à la deuxième bissectrice sont fermés par le cisaillement transversal qui a une plus forte intensité.

2. Contrairement au cas  $\theta = \pi/4$ , on voit sur la figure 4.6 que la flamme n'est pas beaucoup plus plissée dans le cas de forte turbulence qu'elle est dans le cas de faible turbulence, donc on y gagne pas beaucoup en matière d'augmentation de vitesse de combustion lorsque on augmente l'intensité de turbulence. Voir la sous-section 4.5 pour plus de discussion.

**C) La flamme est à 45 degrés par rapport à la composante-cisaillement :**  
 $\theta = 0$

*i) Faible turbulence :  $\lambda = 0.5$*

Sur la figure 4.5, on présente le cas d'une flamme dont la normale (moyenne) fait un angle  $\theta = 0$  avec l'axe des x pour une faible intensité de turbulence,  $\lambda = 0.5$ . Comme dans le cas  $\theta = \pi/4$ , quand la turbulence est faible les plissements de la flamme ressemblent à ceux associés à un cisaillement perpendiculaire.

*ii) Forte turbulence :  $\lambda = 4$ .*

Sur la figure 4.6, on reprend le cas précédent avec  $\lambda = 4$ . Ici on voit apparaître les effets des tourbillons mais l'amplitude des plissements est très petite. Avec  $\theta = 0$ , l'alignement initial de la flamme ne favorise pas nécessairement l'un ou l'autre des deux cisaillements perpendiculaires qui composent l'écoulement de Childress-Soward (mis en évidence ci-dessus). Ainsi on voit sur la figure 4.7 que dans le cas de faible turbulence (en haut de la figure) la flamme ne sent pas la présence des tourbillons (ou d'une façon équivalente le cisaillement à -45 degrés) elle est

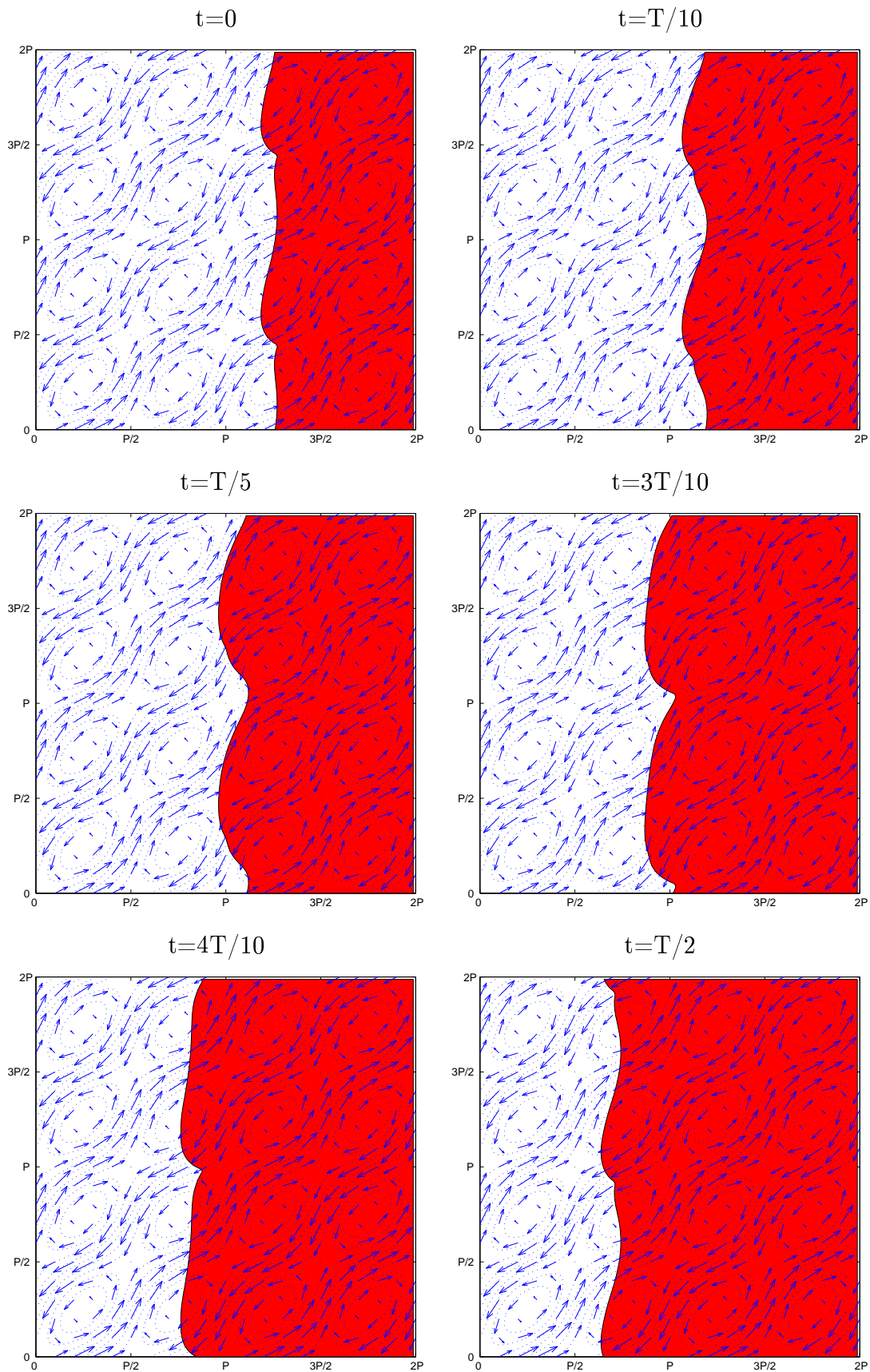


FIG. 4.7. Cas I. C) *i*) :  $\delta = 1/2$ ,  $\theta = 0$ ,  $\lambda = 0.5$ .

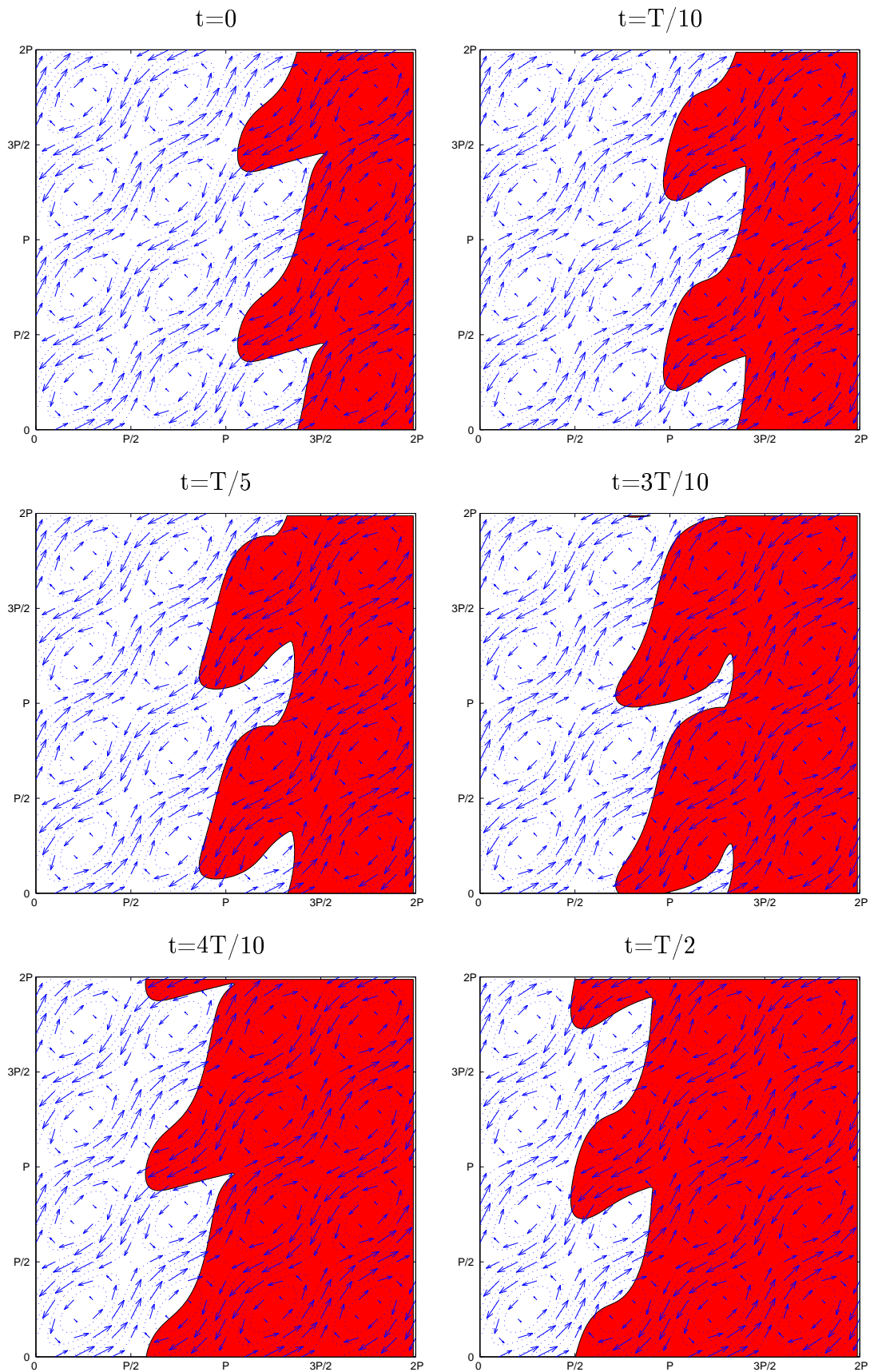


FIG. 4.8. Cas I. C) *ii*):  $\delta = 1/2$ ,  $\theta = 0$ ,  $\lambda = 4$ .



seulement légèrement déformé par le cisaillement à 45 degrés. Mais dans le cas de forte turbulence, la figure 4.8, la flamme est très plissée et est entraînée par les canaux d'écoulement associés au cisaillement de plus forte intensité (à 45 degrés) tandis que les tourbillons l'affectent légèrement vers l'arrière. Ainsi ce cas est très semblable au premier ( $\theta = \pi/4$ ) dans la mesure où c'est l'effet du cisaillement à 45 degrés qui domine.

## II. Écoulement cellulaire : tourbillons

On considère une flamme initialement plane soumise à un écoulement de type Childress-Soward avec  $\delta = 0$ . Dans ce cas les deux cisaillements qui composent l'écoulement de Childress-Soward, voir ci-dessus, sont d'intensités égales donc les angles  $\theta = \pi/4$  et  $\theta = -\pi/4$  représentent le même cas, de plus les lignes de cisaillement associées se sont mutuellement fermées donc on s'attend à ce que la distorsion du front soit faible et qu'il n'y ait pas beaucoup d'augmentation de vitesse quel que soit l'angle du front. On considère ici les angles A)  $\theta = 0$  et B)  $\theta = \pi/4$ .

### A) La flamme est parallèle aux axes : $\theta = 0$

#### *i) Faible turbulence : $\lambda = 0.8$*

Sur la figure 4.9, on illustre la dynamique du front d'une flamme initialement parallèle à l'axe vertical avec une faible turbulence.

#### *ii) Forte turbulence : $\lambda = 6.0$*

Le cas de forte turbulence est repris dans la figure 4.9 avec  $\lambda = 6.0$ .



Lorsque  $\lambda = 0.8$  (turbulence faible), la flamme est légèrement plissée et il est difficile de dire avec quelle partie de l'écoulement ce plissement est réellement associé. Par contre quand  $\lambda = 6$  (forte turbulence), on voit clairement l'effet des tourbillons. Un plissement de la flamme entraînée dans les canaux d'écoulement vers l'avant à un certain moment est vite déviée vers l'arrière par l'effet du tourbillon repliant ainsi la flamme sur elle-même ce qui provoque la formation de poches.

**B) La flamme est perpendiculaire à la première bissectrice :  $\theta = \pi/4$**

Dans le cas où la flamme est parallèle à la première bissectrice, un des deux cisaillements formant l'écoulement de Childress-Soward se trouve plus favorisé que l'autre.

*i) Faible turbulence :  $\lambda = 0.1$*

Sur la figure 4.11, on illustre la dynamique du front d'une telle flamme avec une faible turbulence ( $\lambda = 0.1$ ).

*ii) Forte turbulence :  $\lambda = 6.4$*

Le cas de forte turbulence est représenté dans la figure 4.12 en fixant  $\lambda = 6.4$ .

Dans le cas de faible turbulence la flamme ne voit que le cisaillement qui lui est perpendiculaire tandis que quand  $\lambda = 6.4$  la flamme est interceptée par le cisaillement transversal et l'effet des tourbillons la fait replier sur elle-même et encore une fois on voit apparaître des poches de gaz non brûlé vers l'arrière.

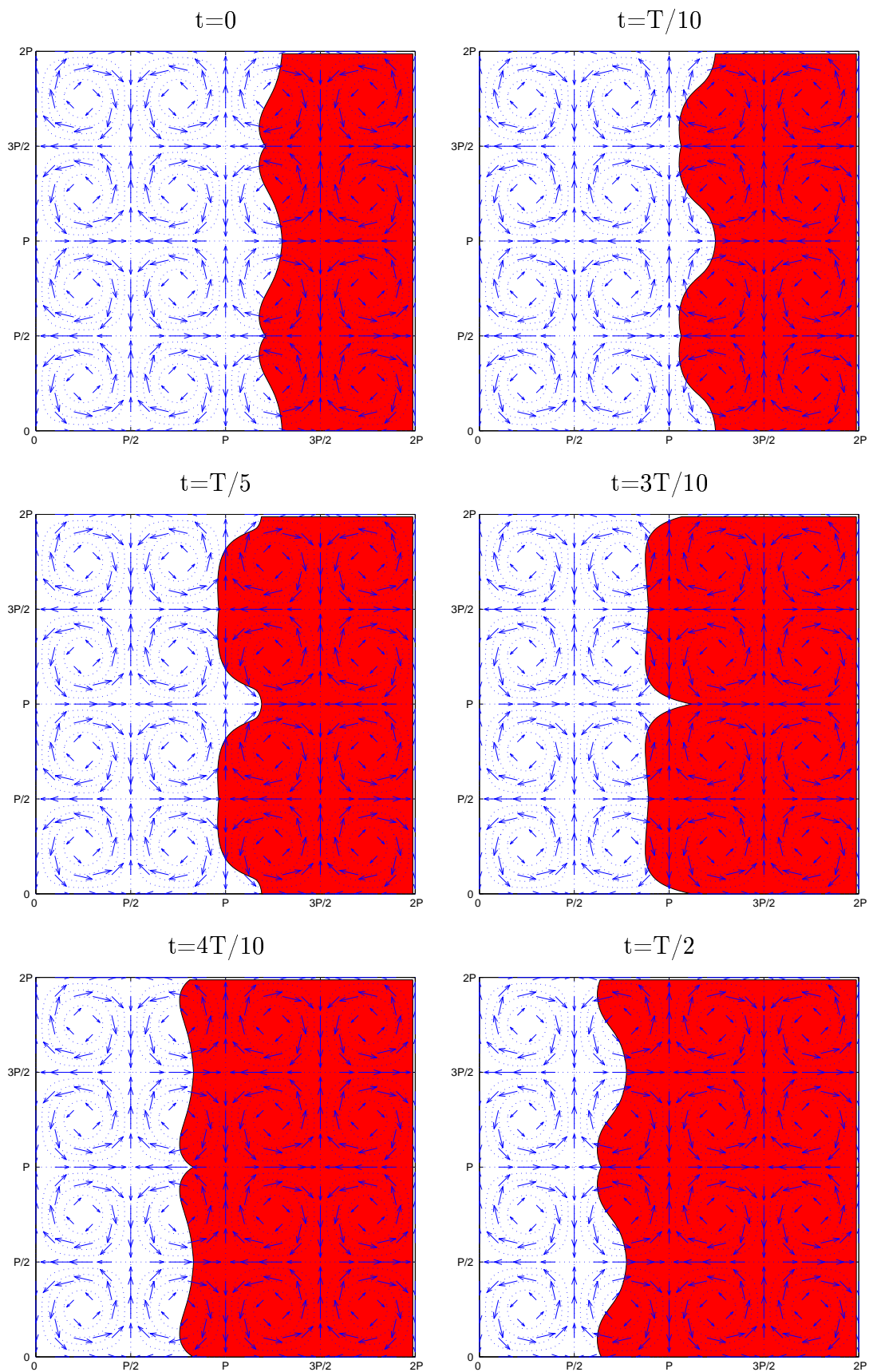


FIG. 4.9. Cas II. A)  $i$ ) :  $\delta = 0$ ,  $\theta = 0$ ,  $\lambda = 0.8$ .

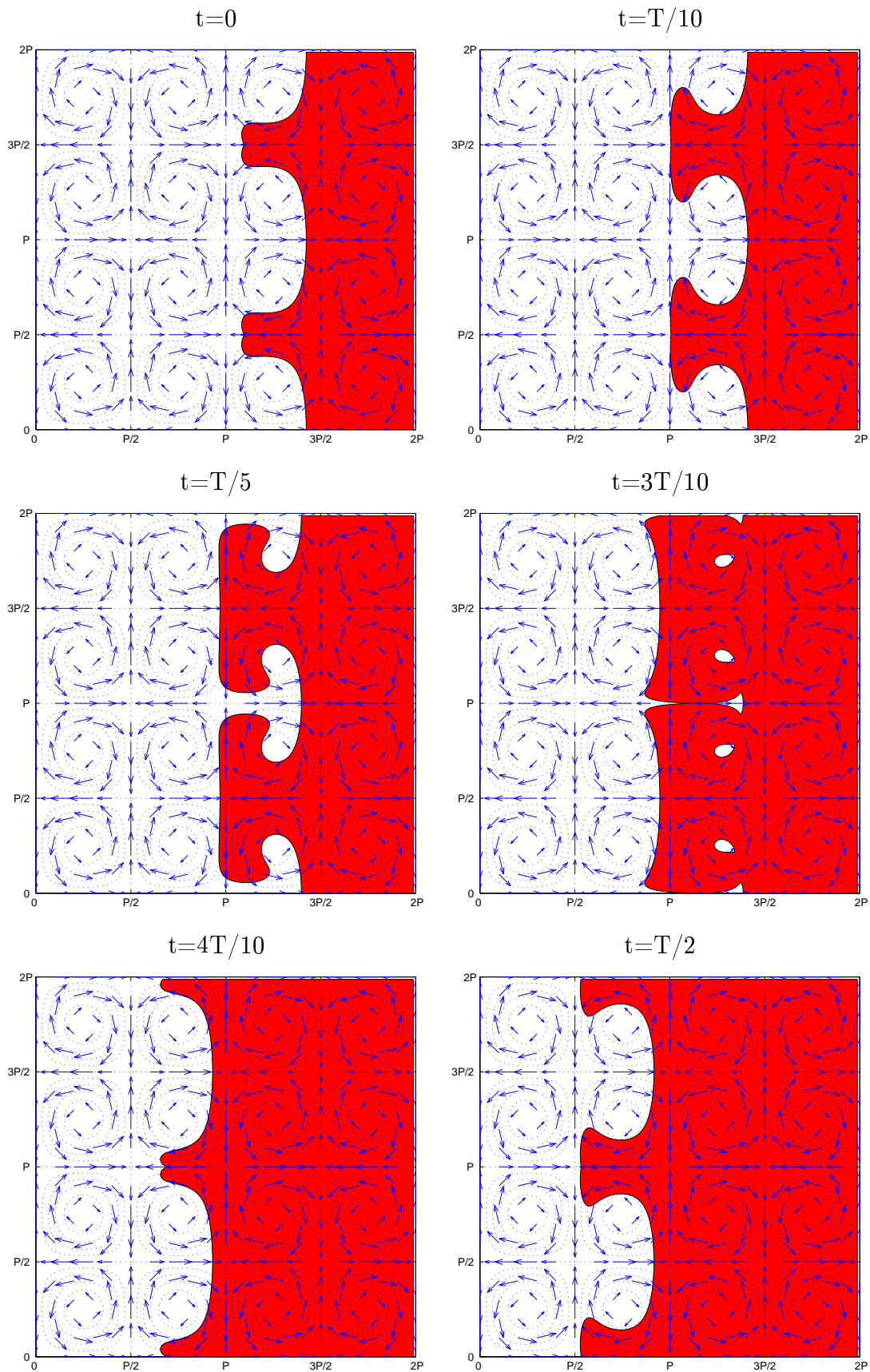


FIG. 4.10. Cas II. A) *ii*) :  $\delta = 0$ ,  $\theta = 0$ ,  $\lambda = 6.0$ .

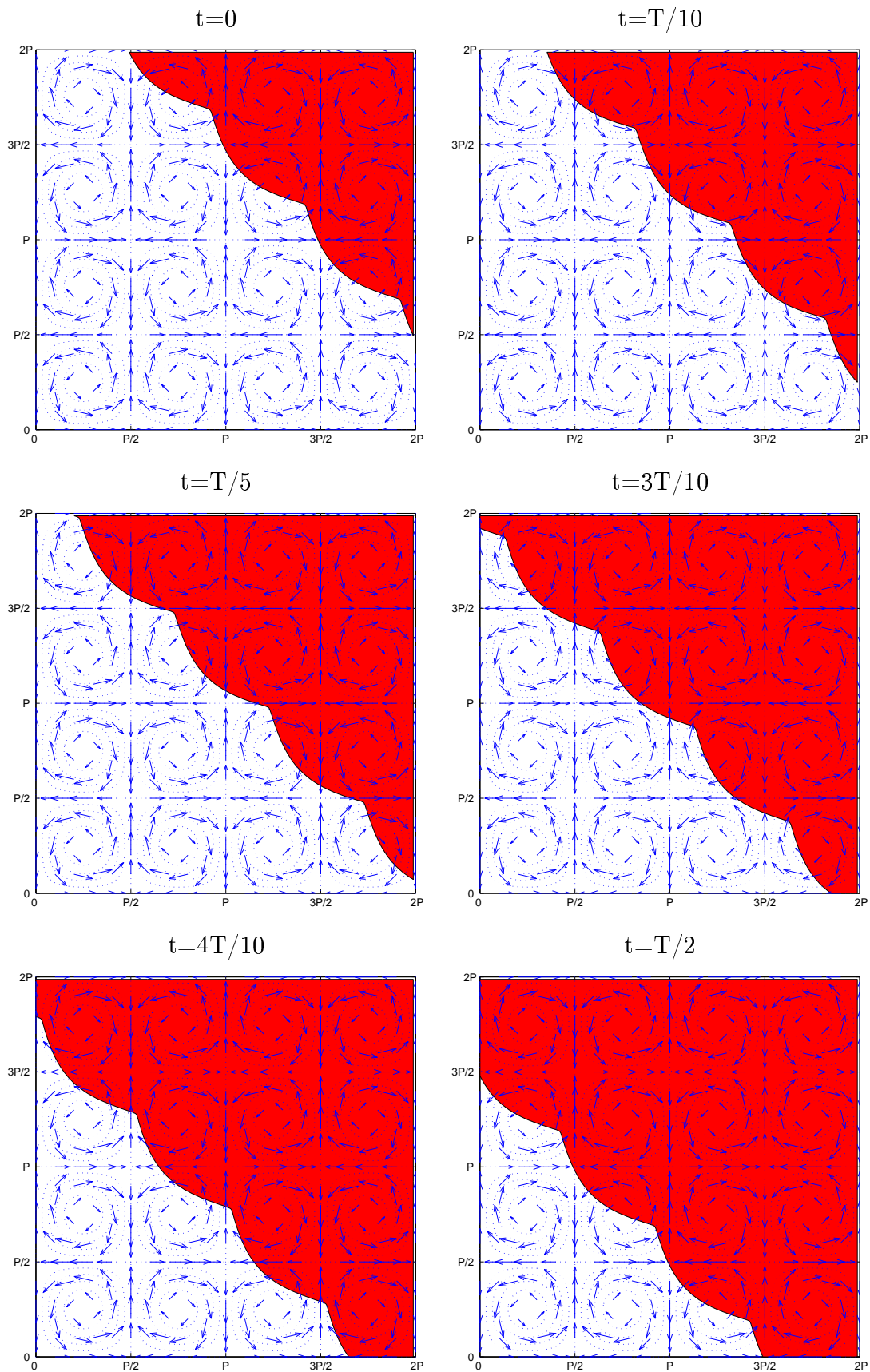


FIG. 4.11. Cas II. B) *i*) :  $\delta = 0$ ,  $\theta = \pi/4$ ,  $\lambda = 0.1$ .

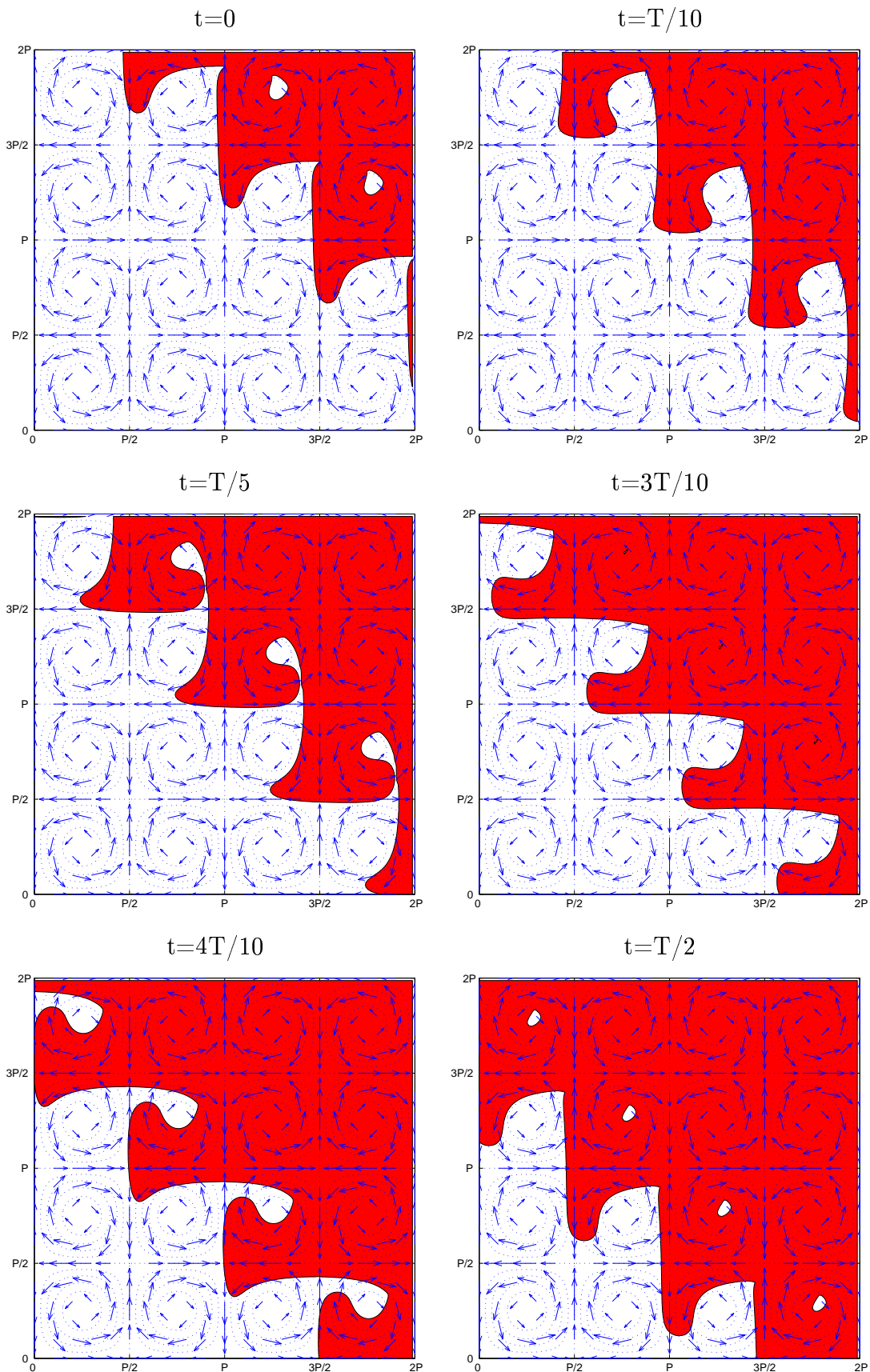


FIG. 4.12. Cas II. B) *ii*):  $\delta = 0$ ,  $\theta = \pi/4$ ,  $\lambda = 6.4$ .

#### 4.5. EFFETS SUR L'AUGMENTATION DE VITESSE

Comme il a été mentionné plusieurs fois dans cette thèse, on sait que les plissements du front de la flamme par la turbulence en combustion prémélangée se traduisent par l'augmentation de la vitesse de combustion. Cette augmentation de vitesse est en partie due au fait qu'une flamme plissée présente une zone de réaction plus importante que celle d'une flamme lisse. Par ce principe, on déduit que plus les plissements de la flamme sont importants plus l'augmentation de la vitesse de combustion est grande. Ceci est confirmé dans le tableau 4.1, où on rapporte la valeur de l'augmentation de vitesse de combustion pour chacun des cas illustrés ci-dessus.

Au vu des illustrations, du tableau 4.1 et des résultats du chapitre 2, en plus du fait que l'action principale de la turbulence en combustion prémélangée est le plissement de la flamme et que ces plissements se traduisent par une augmentation de la vitesse de combustion, les points suivants sont retenus, pour le cas d'une réaction chimique de type KPP.

##### 1. Relation entre l'augmentation de la vitesse de combustion et les plissements

La théorie rigoureuse met en garde contre l'utilisation quantitative d'arguments géométriques pour prédire l'augmentation de vitesse de combustion en fonction des plissements du front. Néanmoins, une interprétation qualitative est utile et en voici un résumé.

L'augmentation de la vitesse de combustion est une fonction croissante des plissements du front de la flamme. L'expression de l'augmentation de la vitesse de combustion peut donc se faire si on trouve une mesure adéquate pour les plissements du front ainsi qu'une fonction qui relie cette mesure à l'augmentation de vitesse. En effet dans la théorie de l'homogénéisation de Majda-Souganidis, la vitesse de combustion est définie à travers le problème de minimisation en fonction de la valeur propre,  $H$ , dans (4.3.1).

Cette valeur propre est une fonction linéaire de la moyenne quadratique  $\langle |\mathbf{D}w|^2 \rangle$  de  $\mathbf{D}w$  (voir les chapitres 1 ou 3), avec  $w$  la fonction propre de (4.3.1). En partant du fait que les contours de  $w$  décrivent les formes possibles du front de la flamme, la quantité  $\langle |\mathbf{D}w|^2 \rangle$  sert donc à communiquer l'importance des plissements du front. Notez que pour une flamme plane on a  $\mathbf{D}w \equiv 0$  et ceci traduit automatiquement une augmentation de vitesse nulle, d'après l'expression du hamiltonien  $H$  en fonction de  $\mathbf{D}w$ .

**2. L'augmentation de vitesse ne dépend pas seulement de l'intensité de turbulence à travers le simple paramètre  $\lambda$ , mais aussi de plusieurs autres paramètres**

Bien que théoriquement l'augmentation de la vitesse de combustion soit une fonction non négative de l'intensité de la turbulence, cette fonction n'obéit pas à une loi de puissance universelle évidente. Nos calculs ont révélé qu'en plus de l'intensité de turbulence qui évidemment marque le premier point du fait qu'à une intensité de turbulence zéro est associés zéro augmentation de vitesse de combustion, plusieurs autres paramètres qui définissent le type d'écoulement ainsi que l'alignement de la flamme par rapport au lignes de courants, interviennent dans cette loi de puissance. Typiquement nous avons d'une part les cisaillements qui donnent une augmentation de vitesse maximale lorsqu'ils sont perpendiculaires à la flamme moyenne et une augmentation zéro quand ils sont parallèles à la flamme moyenne et d'autre part nous avons les tourbillons qui sont responsables du repliement de la flamme sur elle-même et de la formation des poches qui n'ont pas beaucoup d'effets positifs sur l'augmentation de la vitesse. Ainsi donc la vitesse de combustion est loin d'être une fonction très simple (linéaire) du seul paramètre  $\lambda$ .

On sait que dans le cas d'un cisaillement stationnaire [24], par exemple, l'augmentation de la vitesse de combustion est une fonction linéairement croissante de l'intensité de la turbulence pour les grandes intensités mais

cette pente diminue pour les faibles valeurs. Ce comportement est connu en combustion et est appelé *l'effet de flexion* (en anglais; *bending effect*) [3, 5, 22, 23]. Dans [3], il a été suggéré que cette diminution du taux d'accroissement est associée à la formation de poches par les tourbillons, tandis que dans [23] ce phénomène est associé à la variation du temps de corrélation de l'écoulement en fonction de l'intensité de turbulence. Cette dernière idée est confirmée dans le chapitre 2 pour le cas d'un cisaillement qui dépend du temps, où ce temps de corrélation dicte le temps de résidence de la flamme qui avec le temps de plissement contrôlent la transition entre deux régimes lent et rapide (voir ci-dessous). Or, on sait (voir le chapitre 2) que la présence d'un écoulement transversal sert à diminuer ce temps de résidence, comme il est aussi affecté par l'angle que fait la flamme avec le cisaillement. Étant donné la complexité des écoulements turbulents dans la réalité, le pourquoi de ce phénomène est resté longtemps sans réponse. Dans le chapitre 2, nous apportons les explications relatives au cas d'un cisaillement unidimensionnel qui peuvent être utilisées pour comprendre ce phénomène dans un cadre plus général. Dans la suite, on se réfère aux résultats du chapitre 2 pour classifier les cas considérés ici avec l'écoulement plus complexe de Childress-Soward.

### 3. Régime lent et régime rapide

Dans le chapitre 2, la vitesse de combustion est fonction d'un nombre sans dimension donné par le rapport de deux temps caractéristiques : (1) le temps de résidence de la flamme donné par le temps caractéristique du champ de vitesse et (2) le temps de plissement de la flamme qui est le temps relatif que met une flamme plane pour se plisser par un cisaillement stationnaire qui lui est perpendiculaire. Ce temps de plissement est inversement proportionnel à la racine carrée de l'intensité du cisaillement. Une loi de puissance pour la vitesse de combustion en fonction de ce nombre a



été établie pour le cas d'un simple cisaillement qui est périodique dans le temps, donc un temps caractéristique bien connu.

Le résultat du chapitre 2 se résume comme suit. Quand le temps de résidence de la flamme est plus grand que le temps de plissement, la flamme est suffisamment exposée dans le temps à l'effet de cisaillement (il reste plissé pendant longtemps), on enregistre alors une augmentation de vitesse de combustion importante. Dans ce cas, l'augmentation de vitesse est une fonction linéaire de l'intensité de turbulence,  $\lambda$ , plus une petite correction. Par contre, lorsque le temps de résidence est plus petit que le temps de plissement, la flamme ne subit pas l'effet du cisaillement pendant assez de temps, elle n'est donc que très peu plissée. Ceci se traduit par une augmentation de vitesse très faible. C'est une fonction quadratique du rapport entre le temps de résidence et le temps de plissement. Le premier cas est nommé un régime lent et le second un régime rapide. Dans le cas lent la flamme est suffisamment exposée au cisaillement, donc suffisamment plissée pour engendrer une grande augmentation de vitesse, tandis que dans le cas rapide elle passe très vite et ne subit que peu l'effet du cisaillement. Dans la suite, nous examinons cas par cas les exemples ci-dessus pour voir quels sont les cas qui correspondent à des cas lents et quels sont ceux qui correspondent à des cas rapides. À l'occasion, nous allons aussi essayer de justifier la topologie des plissements observés.

- Le cas I. A) correspond à des cas lents car la flamme moyenne est (toujours) perpendiculaire à la composante-cisaillement de plus forte intensité qui la stabilise en l'entraînant à travers les canaux. Ainsi, le temps de résidence de la flamme est infini ; il est plus grand que le temps de plissement qui est toujours fini.
- Les deux cas I. B) (figures 4.5 et 4.6) sont des cas rapides. La flamme est parallèle au cisaillement de plus forte intensité qui la fait osciller, d'une façon permanente et violente, il ne la "laisse" pas se faire plisser par le

cisaillement qui lui est perpendiculaire. Ainsi le temps de résidence de la flamme par rapport à ce dernier cisaillement est petit devant le temps nécessaire pour son plissement.

- Les cas I. C) (figures. 4.7 et 4.8) sont aussi des cas rapides. Les plissements causés par le cisaillement à 45 degrés sont vite rattrapés par la région brûlée à cause de la flamme moyenne qui passe dessus les canaux de l'écoulement à mesure qu'elle avance. D'où un temps de résidence petit.
- En II. (figures 4.9, 4.10, 4.11 et 4.12) l'écoulement de Childress-Soward ne contient que des tourbillons. Donc, indépendamment de l'angle  $\theta$  et de l'intensité de la turbulence  $\lambda$ , on ne peut engendrer que des cas rapides dans ce cas-ci car les déformations (plissements) du front causées à l'approche d'un tourbillon suivent les lignes de courant vers l'arrière et sont vite rattrapées par la flamme moyenne. Donc même si la flamme se plisse par un tourbillon, les plissements ne durent pas longtemps.

#### 4.6. CONCLUSION

D'après les illustrations ci-dessus on conclut ce qui suit.

1. Le front de la flamme se plisse essentiellement grâce à l'effet de l'étirement causé par les cisaillements qui lui sont perpendiculaires. Quand aux cisaillements parallèles, leur effet combiné avec celui des cisaillement perpendiculaires tend plutôt à replier la flamme sur elle-même et à former des poches, comme c'est typiquement le cas avec les tourbillons, qui se décomposent, du moins localement, en cisaillements parallèles et perpendiculaires à la fois.
2. Le front de la flamme se plisse donc aux endroits où les cisaillements perpendiculaires au front changent de signes, car c'est là que la flamme est tirée de part et d'autre vers l'arrière et vers l'avant.
3. L'importance des plissements du front dépend essentiellement de l'importance des cisaillements qui lui sont perpendiculaires.

4. Il est clair d'après 1 2 et 3 que l'alignement de la flamme par rapport à l'écoulement joue un très grand rôle dans la manière dont la flamme se plisse.

De plus, on voit dans le tableau 4.1, que seulement dans les deux cas en I. A) (correspondants aux figures 4.3 et 4.4), qui sont des cas lents, qu'on enregistre une augmentation importante de la vitesse de combustion, relativement à sa borne théorique maximale donnée par la valeur de l'intensité de turbulence  $\lambda$  :  $F_e \approx 0.75$  pour  $\lambda = 0.8$  et  $F_e \approx 6$  pour  $\lambda = 6.4$ . Le rapport  $F_e/\lambda$  est proche 1. Dans tous les autres cas, classés comme des cas rapides, l'augmentation de vitesse est petite par rapport à  $\lambda$ , dans certains cas (notamment les cas I.B) :  $\theta = -\pi/4$ ,  $\delta = 1/2$  et II.B) :  $\theta = \pi/4$ ,  $\delta = 0$ ) le rapport  $F_e/\lambda$  décroît avec  $\lambda$ , ce qui confirme le fait que dans ces cas  $F_e$  n'est plus une fonction linéaire de  $\lambda$ , du moins il ne le reste pas pour longtemps quand  $\lambda$  croît. Ou bien on est tous le temps dans le régime rapide ou bien on passe d'un régime moins rapide, intermédiaire entre lent et rapide, à un régime rapide.

C'est souvent de cette façon que le phénomène de flexion est observé dans les expériences de laboratoire et dans les simulations numériques : quand l'intensité de turbulence augmente le taux d'accroissement de l'augmentation de vitesse par rapport à la turbulence diminue [1, 3, 5, 23]. Une question ouverte en combustion est d'expliquer pourquoi ce phénomène apparaît de cette façon précise dans les applications et non le contraire comme dans le cas d'un cisaillement synthétique étudié au chapitre 2 où souvent les grandes intensités de turbulence sont liées à des cas lents et les petites à des cas rapides. Ci-dessous, on essaie de s'approcher de la réponse à cette question dans le cadre des écoulements synthétiques 2d étudiés ici. On est conscient du fait que c'est une question extrêmement complexe et que les cas réalistes peuvent se comporter distinctement, néanmoins, on espère apporter un certain stimulant à l'intuition.

Supposons que l'écoulement turbulent se décompose (uniformément, 'turbulence isotrope') en deux composantes-cisaillements, de telle sorte qu'une composante soit perpendiculaire à la flamme et l'autre parallèle à la flamme : les deux

cisaillement sont supposés avoir une intensité comparable ; voir le cas  $\delta = 0$  dans l'écoulement de Childress-Soward, type d'écoulement considéré dans [3]. Ce sont les cisaillements perpendiculaires à la flamme principalement qui favorisent des plissements susceptibles d'engendrer une augmentation de la vitesse de combustion ; les cisaillements transversaux quand à eux ne font que replier la flamme sur elle-même ; cet effet combiné avec la propagation propre à la combustion réduit l'amplitude des plissements causés éventuellement par les cisaillements perpendiculaires. Quand l'intensité de la turbulence,  $\lambda$ , est faible, la composante qui forme un cisaillement parallèle à la flamme est aussi faible comparativement à la vitesse de propagation du front qui est supérieure ou égale à la vitesse de combustion laminaire,  $S_L$  ( $\lambda \ll S_L$ ), fixée à  $S_L = 1$ . Donc l'échelle temporelle de cet écoulement parallèle (de l'ordre  $1/(\lambda + S_L) \approx 1/S_L$ ) est plus petite que le temps de plissement de la flamme (qui est de l'ordre  $1/\sqrt{\lambda}$ ), donc la flamme ne voit pratiquement pas cette composante transversale pendant qu'elle se laisse plisser par la composante qui va dans sa direction de propagation à moins que l'écoulement dans cette direction change de signe avec une très grande fréquence (comme dans le cas du cisaillement qui dépend du temps avec  $\omega \gg 1$  vu au chapitre 2), ainsi donc on est dans le régime lent où l'augmentation de vitesse serait linéaire par rapport à  $\lambda$ . Par contre quand l'intensité de turbulence est grande ( $\lambda \gg S_L$ ), la composante transversale est aussi grande et son échelle temporelle ( $1/(\lambda + S_L) \approx 1/\lambda$ ) est donc comparable au temps de plissement de la flamme. Par conséquent la flamme subit l'effet de l'écoulement transversal qui l'empêche de se laisser plisser par le cisaillement perpendiculaire. Ainsi, l'augmentation de vitesse est amortie par l'effet de l'écoulement transversal et on se retrouve subitement dans un régime rapide où l'augmentation de vitesse serait non-linéaire. Noter que les cas I. B) et II. B) sur le tableau 4.1 traduisent bien ce phénomène (le rapport  $F_e/\lambda$  diminue avec  $\lambda$ ), bien qu'une extension à une base de données exhaustive est souhaitable. Ainsi, la partition uniforme de l'écoulement dans les deux directions (parallèle et perpendiculaire à la flamme) fait en sorte que quand

l'intensité de la turbulence augmente on observe le phénomène de flexion, i.e., le passage d'un régime lent (linéaire ou proche de linéaire) au régime rapide (avec un taux d'accroissement plus faible), comme il a été constaté dans les expériences en laboratoire et dans les simulations numériques [1, 3, 5, 23]. Dans une tentative d'expliquer le phénomène de ralentissement de l'augmentation de vitesse, par le cisaillement transversal, en terme géométrique, sur la figure 4.13 on fait la caricature d'une flamme, a) initialement plane, soumise à un double cisaillement, un perpendiculaire et un autre parallèle à la flamme moyenne. En premier lieu, b) la flamme subit un étirement par l'action du cisaillement perpendiculaire, ensuite, c) la flamme s'ajuste grâce au fait qu'elle avance normalement à elle-même vers le mélange frais par l'effet de la vitesse de combustion, ce qui fait apparaître une pointe vers l'arrière du front. Finalement, en d) on montre l'action du cisaillement initialement parallèle qui se trouve maintenant localement perpendiculaire en certains endroits avec la flamme et la fait plier sur elle-même pour former des poches qui vont brûler rapidement, ne laissant qu'un front pratiquement lisse (en pointillés). (On notera qu'en réalité les actions b), c) et d) ont eu lieu en même temps et non étape par étape comme sur le dessin.)

TAB. 4.1. Augmentation de vitesse de combustion,  $F_e$ , en fonction des paramètres  $\theta$ ,  $\lambda$  et  $\delta$ .

	$\delta$	$\theta$	$\lambda$	$F_e$	$F_e/\lambda$	Régime
I. A) <i>i</i> )	1/2	$\pi/4$	0.8	0.7425720951	0.9282	Lent
I. A) <i>ii</i> )	1/2	$\pi/4$	6.4	5.7600722148	0.9000	Lent
I. B) <i>i</i> )	1/2	$-\pi/4$	0.4	0.1189545302	0.2974	Rapide
I. B) <i>ii</i> )	1/2	$-\pi/4$	6.4	0.6711900239	0.1049	Rapide
I. C) <i>i</i> )	1/2	0	0.5	0.0991778336	0.1984	Rapide
I. C) <i>ii</i> )	1/2	0	4	2.3060618324	0.5765	Rapide
II. A) <i>i</i> )	0	0	0.8	0.2686988266	0.3359	Rapide
II. A) <i>ii</i> )	0	0	6	2.4217256857	0.4036	Rapide
II. B) <i>i</i> )	0	$\pi/4$	0.1	0.0676491585	0.6765	Rapide
II. B) <i>ii</i> )	0	$\pi/4$	6.4	3.6391790968	0.5686	Rapide

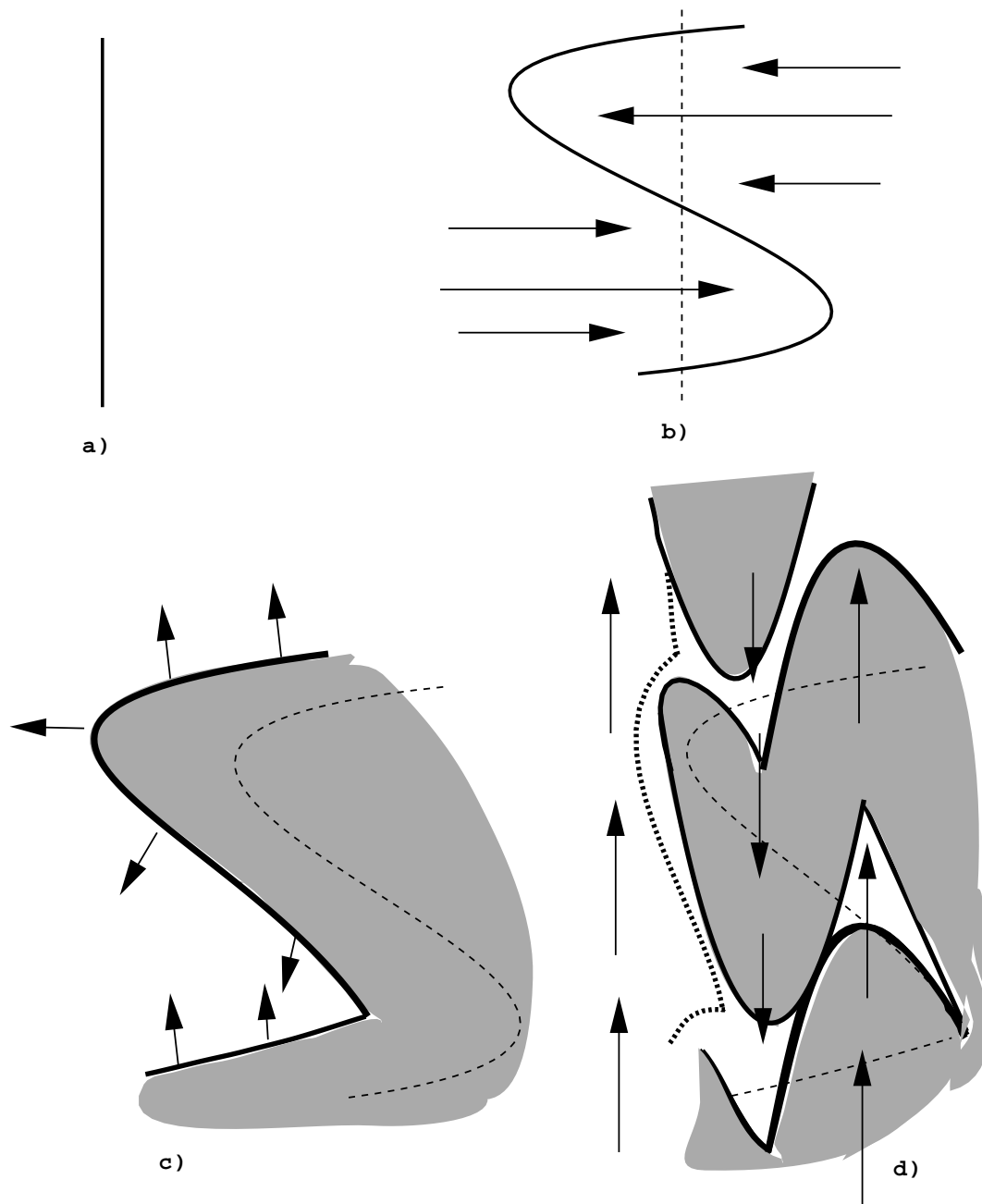


FIG. 4.13. Dessin d'une flamme initialement plane soumise à deux cisaillements perpendiculaires.

## Chapitre 5

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# MODÈLE ASYMPTOTIQUE RIGoureux POUR LA SIMULATION AUX GRANDES ÉCHELLES

Ce chapitre est constitué de l'article “ A rigorous asymptotic perspective on on the large scale simulations of turbulent premixed flame fronts” par Boualem Khouider et Anne Bourlioux qui sera soumis à *SIAM Journal on Applied Mathematics*.

Voici la liste des contributions principales de B.K. à cet article :

- choisir le cas test ;
- générer la base de données des flammelettes en utilisant la méthode numérique introduite dans le chapitre 3 ;
- mise en œuvre numérique de la stratégie LES en utilisant la base de données et le schéma ENO d'ordre supérieure pour les équations de Hamilton-Jacobi d'Osher et Shu pour résoudre l'équation G ;
- comparer les résultats DNS avec les résultats LES.



# A rigorous asymptotic perspective on the large scale simulations of turbulent premixed flame fronts

Boualem Khouider & Anne Bourlioux

*To be submitted to SIAM Journal on Applied Mathematics*

## ABSTRACT

*An idealized model for turbulent premixed flames is introduced. It consists of a scalar advection-reaction-diffusion equation that describes the interaction of a thin flame with a turbulent-like flow field acting on two separate scales. Rigorous asymptotic results as well as affordable and reliable direct numerical simulations are available to describe the effective large scale behavior of the idealized front. A strategy is proposed to use this framework as an modeling approach to the large scale simulations of turbulent fronts. That such a rigorous asymptotic approach for an idealized problem is actually relevant to practical computations is illustrated by applying it to address three unresolved issues related to practical closure models for more realistic turbulent flames : regimes in the parameterization of the flame speed; relationship between the front at large scales and the resolved reaction zone in a direct simulation; accuracy and efficiency of the large scale flamelet approach.*

## 5.1. INTRODUCTION

Turbulent premixed flames play an important role in applications such as spark ignition engines and power plants [54, 31]. Most of those applications are actually expected to take place in the so-called flamelet regime, characterized by the fact that the flame thickness is very small compared to any other relevant length scales in the problem, in particular smaller than the smallest active turbulent length scale. In a practical computation of an engine for example, it is clear that one cannot afford to resolve explicitly the entire turbulent spectrum because this would require an excessively fine mesh resolution; resolving the very thin flame

would only worsen the resolution requirements. Instead, recent research efforts have focussed on designing effective and reliable large eddy simulation (LES) methods for turbulent premixed flames, where only large scales are resolved while subgrid scales are modeled - for premixed flames, subgrid scales involve both the unresolved turbulent length scales and the reaction zone thickness. The fact that the flame front is so thin can actually become an asset in designing such a strategy by relying on the *laminar flamelet approach*: the key assumption is that the front is so thin that it can be viewed as a sharp interface separating fresh and burnt gas. Microscopically, with the flame thickness smaller than the smallest turbulent eddies, its fine scale transverse structure is undisturbed compared to the laminar case; an ad-hoc view of the macroscopic behavior of the front can then be formulated by simply viewing it as a wrinkled front moving normal to itself with the local laminar burning speed. There are various ways of accounting for the wrinkling of the front by the turbulent eddies and also various numerical strategies to represent numerically such a front and coupling it to the rest of the flows. Examples can be found in refs. [14], [15], [56], [55], [41], [60]. A systematic validation of such approaches remains a major challenge. One approach is to compare with experiments, but the large eddy simulation of turbulent flames is still at a fairly early stage of development so that most likely, one will attempt to validate the results by comparing with direct numerical simulations (DNS), where all the scales are resolved so that no model is needed [56, etc]. Direct numerical simulation is a very valuable tool to explore the dynamics of a turbulent flame but it has also limitations due to the cost of such computation. What is discussed in this paper is a complementary approach where one transposes the laminar flamelet strategy as a subgrid model to a simpler, idealized test-case. It is accessible to theoretical analysis and to comparatively cheap computations so that systematic validation is much more tractable, with the potential that the key results could be transposed back to the original problem. How to design such an idealized test-case is described next.

## 5.2. OVERALL STRATEGY

The topic of numerical turbulent combustion is very challenging if one views it as simulating turbulent flows with the additional difficulty of accounting for the interaction of turbulence with combustion. A lot of progress has been made regarding the design of large eddy simulation strategies for nonreactive turbulent flows, but it is still an active area for research. With the additional complexity of combustion in a turbulent flame simulation, it is very hard, when evaluating the performance of a model, to sort out the effects of the turbulence model itself and those of the model for the interaction combustion-turbulence. The strategy to be described next is designed so that all the modeling and computing efforts are focussed on the later point, excluding all the classical nonreactive turbulent issues. We first describe it in very general terms, applicable to all types of flames in the flamelet regime. The model consists of a single equation as introduced in [46] that describes the evolution of the reactive scalar  $T$ , where  $T$  can be viewed as either the temperature field or a reactant mass fraction. The scalar is assumed to obey an advection-diffusion-reaction equation of the form :

$$\frac{\partial T}{\partial t} + (\bar{\mathbf{v}}(\mathbf{x}, t) + \mathbf{v}(\mathbf{x}/\epsilon^\alpha, t/\epsilon^\alpha)) \cdot \nabla T = \epsilon \Delta T + \frac{1}{\epsilon} f(T) \quad (5.2.1)$$

with  $\epsilon > 0$  and  $0 < \alpha < 1$  given. The nonlinear reaction rate function  $f(T)$  must also be given ; an example of reaction rate corresponding to a nonpremixed flame can be found in [12] while an example for a premixed flame is given in the next section. The scaling in the equation is such that, in the absence of turbulent advection, the combination of slow diffusion (order  $\epsilon$ , with  $\epsilon$  small) and fast reaction (reaction rate  $f(T)/\epsilon$ ) leads to a very thin flame whose width scales like  $\epsilon$ .

The synthetic velocity field on the left hand side is also specified a priori. The velocity field has two components, both assumed to be incompressible : a large scale flow  $\bar{\mathbf{v}}$  and a perturbation  $\mathbf{v}$  that acts at the scale  $\epsilon^\alpha$  intermediate between

the flame thickness  $\epsilon$  and the large scale (normalized here to be of order 1). An example of such flow is given in the next section.

One central issue in turbulent combustion is to account properly for the turbulent mixing by the intermediate scale velocity as it always leads to an enhancement of the large-scale effective burning rate. There are two related point-of-views as far as characterizing that enhancement, and more generally describing the solution for  $T$  at large scales :

1. **mathematical statement of the problem** : what is the solution for  $T$  in the limit of  $\epsilon, \epsilon^\alpha \rightarrow 0$ , i.e. what is the effective behavior of the thin flame front at large scales, taking into account the effects of its distortion at the intermediate scale by the velocity perturbation  $\mathbf{v}$ ?
2. **practical statement of the problem** : what is an efficient procedure to compute numerically the solution for  $T$  at large scales when both the very small flame thickness  $\epsilon$  and the intermediate scale  $\epsilon^\alpha$  associated with the turbulent flow  $\mathbf{v}$  are smaller than the discretization grid size?

The practical formulation of the problem in 2 is the classical closure problem that one must tackle in large eddy simulations : the challenge is to account properly for the subgrid effects that contribute to the solution at large scales. There are two such effects - the first one is advection, which corresponds to the classical non-reactive turbulence closure problem, in the non-reactive case it is dealt with by specifying an enhanced diffusivity. The second one is specific to reactive turbulence and is associated with the nonlinear reaction rate function  $f(T)$ . There have been many propositions for ad-hoc closure in the reactive cases that capitalize on the fact that, at least in the flamelet regime, the reaction zone is very thin compared to all turbulent length scales. The strategy proposed here is to exploit the rigorous results from the mathematical approach as stated in 1 to offer a fresh perspective on the practical closure issue as stated in 2.

This asymptotic approach to closure validation proposed here has two key advantages, both direct consequences of the relative simplicity of Eq.5.2.1 compared with the full reactive Navier-Stokes equations :

- Rigorous asymptotic results are available to provide useful information regarding the effective behavior at large scales, for example : scaling of subgrid models, upper bounds on effective transport coefficients, etc. ;
- Eq.5.2.1 is orders of magnitude easier to solve numerically than the full reactive Navier-Stokes equations so that cheap, extensive, reliable numerical databases can be generated.

The approach has of course intrinsic limitations. Eq.5.2.1 could be derived from the full reactive Navier-Stokes equations under a number of assumptions, most importantly : zero heat release, equal diffusivity for temperature and chemical species (i.e. Lewis number unity), simple one-step irreversible chemistry, prescribed two separated velocity scales. It is therefore obvious that the idealized model will not be appropriate to validate any modeling issue related to any of those topics. Nevertheless, it has been used very successfully in the past in the case of passive scalar turbulent advection - see [45] for a self-contained introduction to that topic, with results that are directly relevant to the validation of flamelet models for large eddy simulations of nonpremixed flames [12]. Below, the strategy is applied to an idealized turbulent premixed flame. The detailed set-up for that application is described in Section 5.3. The asymptotic perspective on the problem is explained in detail in Section 5.4, including a summary of the relevant homogenization results, their practical implementation, and a numerical validation of the asymptotic predictions. Section 5.5 describes the results obtained when applying the strategy to three practical premixed flame LES questions.

### 5.3. SPECIFIC SET-UP

### 5.3.1. Idealized test-case

The type of flame described by Equation 5.2.1 depends on the specific choice for the reaction rate  $f(T)$ . In the rest of this paper, we assume a KPP type reaction rate:  $f(T) = KT(1-T)$  with  $K > 0$ . This choice corresponds to a premixed flame, where the temperature has been normalized so that the unburnt gas temperature corresponds to  $T = 0$  and the burnt temperature to  $T = 1$ . Notice that  $T = 1$  is a stable equilibrium point of the ODE  $T_t = KT(1 - T)$ ,  $0 \leq T \leq 1$  ( $K > 0$ ) while  $T = 0$  is an unstable equilibrium point; the irreversible conversion from fresh gas (unstable  $T = 0$ ) to burnt gas (stable  $T = 1$ ) corresponds to the propagation of the flame front towards the fresh gas ([12, 48]).

We solve Equation 5.2.1 for  $T(x, y)$  in a rectangular domain. The initial condition is such that  $T$  is independent on  $y$  so that initially, the computational domain is divided in two parts with unburnt gas on the left side and burnt gas on the right side as shown on Fig. 5.1. Periodic conditions in  $y$  are assumed throughout the simulation, with the mean flame moving from right to left.

The large scale velocity field is a simple horizontal shear,

$$\bar{\mathbf{v}}(x, y) = \bar{\lambda}(\sin(2\pi y), 0) \quad (5.3.1)$$

with  $\bar{\lambda} > 0$  the constant intensity of the large scale shear. The intermediate scale flow field is obtained, on the bi-periodic box of length  $\epsilon^\alpha$ , from the Childress-Soward stream function

$$\psi(\xi, \eta) = \sin(2\pi\xi) \sin(2\pi\eta) + \delta \cos(2\pi\xi) \cos(2\pi\eta)$$

with  $(\xi, \eta) = (\frac{x}{\epsilon^\alpha}, \frac{y}{\epsilon^\alpha})$ ,  $0 \leq \delta \leq 1$ . i.e,

$$\mathbf{v}(\xi, \eta) = \lambda \left( -\frac{\partial\psi(\xi, \eta)}{\partial\eta}, \frac{\partial\psi(\xi, \eta)}{\partial\xi} \right) \quad (5.3.2)$$

with  $\lambda$  the intensity of the small scale turbulence. This intermediate scale box is used to tile the large scale rectangular domain as illustrated in Fig. 5.1. The streamlines of the Childress-Soward flow in each box are represented in Fig. 5.2

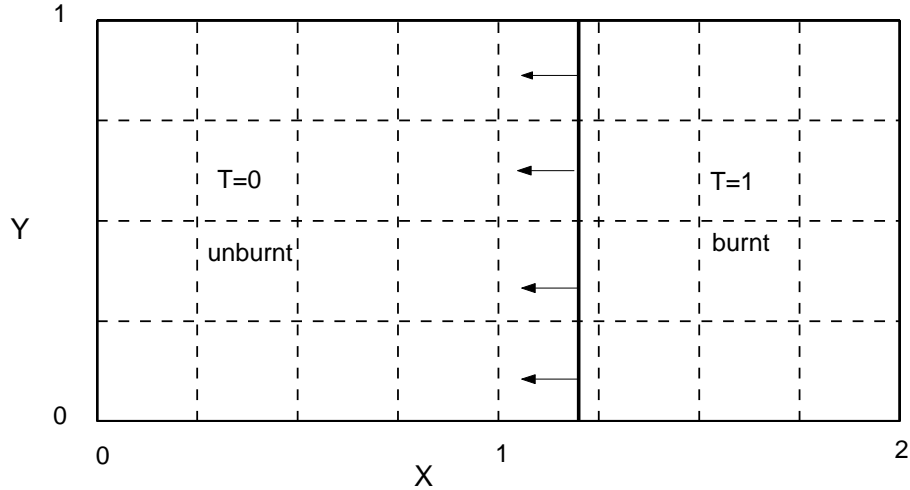


FIG. 5.1. Geometric set-up for test case and initial data.

for the values  $\delta = 0$ ,  $\delta = 0.5$  and  $\delta = 1$ . The value of  $\delta = 1$  corresponds to a pure shear tilted at 45 degrees and the value of  $\delta = 0$  corresponds to an array of eddies. An intermediate value  $0 < \delta < 1$  corresponds to a combination of shears and eddies; this is the value selected for the computations in this paper.

The choice of an horizontal shear for the large scale flow is motivated by the following arguments. It is a computationally convenient choice as, in the limit of an infinitely thin reaction zone, the large scale flame front emanating from the initial conditions above will be independent of  $x$  so that the large eddy simulation will be reduced to a one-dimensional computation. Despite its simplicity, this large scale flow leads to the typical "tulip-shape" flame front observed for instance in practical flame configurations due to the shear in a channel or at the outlet of a pipe. The choice for the intermediate flow consisting of shears and eddies is a reasonable choice to generate a non trivial (even though synthetic) flow somewhat representative of what can be expected at small turbulent scales.

### 5.3.2. Numerical method for resolved reference computations

The numerical algorithm used for the direct resolution of (5.2.1) is as follow. Given a time step  $\Delta t$ , we rely on the Strang splitting finite difference method to

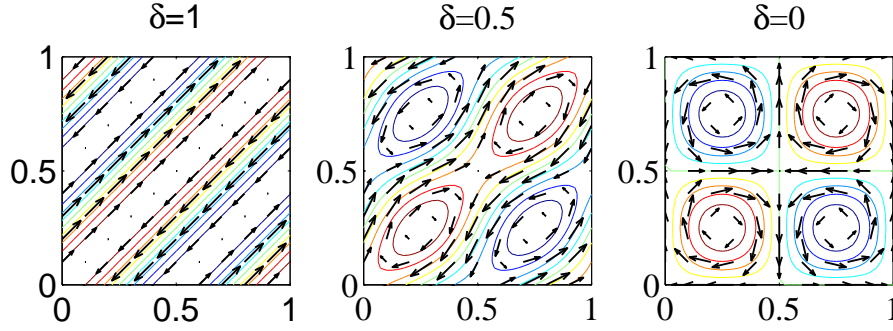


FIG. 5.2. Streamlines for the Childress-Soward flow (intermediate scale flow).

integrate from time  $t$  to  $t + \Delta t$ .

$$T(., t + \Delta t) \approx \mathcal{A}(\Delta t/2)\mathcal{R}(\Delta t/2)\mathcal{D}(\Delta t)\mathcal{R}(\Delta t/2)\mathcal{A}(\Delta t/2)T(., t)$$

where  $\mathcal{A}(\Delta t/2)$  is the numerical advection operator used to integrate the advection term  $(\bar{\mathbf{v}}(x, y) + \mathbf{v}(x/\epsilon^\alpha, y/\epsilon^\alpha)) \cdot \nabla T$  from a given time  $t$  to  $t + \Delta t/2$ ,  $\mathcal{D}(\Delta t)$  is the numerical approximation for the diffusion operator corresponding to the term  $\epsilon(T_{xx} + T_{yy})$  and  $\mathcal{R}(\Delta t/2)$  is the discretized reaction operator corresponding to the reaction term.

The advection term is approximated by a fourth order essentially non-oscillatory upwind scheme [43, 53] and the diffusion term uses a combination of the spectral (in the  $y$  direction) and the Crank-Nicholson methods [see the appendix at the end of this paper for the details] whereas the reaction term is integrated exactly,

$$T_t = \frac{K}{\epsilon}T(1 - T) \implies T(t + \Delta t) = \frac{T(t)}{T(t) + (1 - T(t)) \exp(-\frac{K}{\epsilon}\Delta t)}$$

Notice this later formula remains robust even in the stiff limit when  $\epsilon$  becomes small.

### 5.3.3. DNS results and large scale effects of small scales

In Fig. 5.3 we report a snapshot of a DNS result for the temperature field,  $T$ , in (5.2.1) with the velocity field given by (5.3.1) and (5.3.2) for the typical set of parameters  $\epsilon = 1/16$ ,  $\epsilon^\alpha = 1/4$ ,  $\bar{\lambda} = \lambda = 2$ . Yet, the picture shows a thin flame



front separating the burnt ( $T = 1$ ) and unburnt ( $T = 0$ ) regions wrinkled at both the large and intermediate scales corresponding to the two scales of the velocity field. The same simulation is run again, this time with  $\lambda = 0$ , i.e., without the intermediate scale flow. The results from both simulations are compared in Figs. 5.4 and 5.5 where, respectively, the two flame speeds and the shapes of the corresponding fronts are displayed (see Section 5.4.3 for a description on how the flame speeds are computed). Clearly, from Fig. 5.4, we see the speed up of the flame due to the intermediate scale flow and Fig. 5.5 shows how small scale turbulence can deform the shape of the flame front at large scale : actually, the large scale front that would correspond to the fully wrinkled flame is different from the front associated with the large scale flow alone.

This comparison of results with and without the intermediate scale flow shows the importance of the small scale effects on the large scale features of a premixed flame so that one cannot solve for the large scale front without modeling those effects.

## 5.4. THE RIGOROUS ASYMPTOTIC VIEW

### 5.4.1. Theoretical predictions

A mathematical theory predicting the asymptotic behavior of Equation 5.2.1 has been introduced in [46] by Majda and Souganidis. This theory relies on the viscosity solutions and homogenization theory of Hamilton-Jacobi equations to demonstrate that Equation 5.2.1 converges to a certain limit model when  $\epsilon$  becomes small. This new model generalizes the flamelet concept known in the laminar case to turbulent flows for the case of KPP type reaction rates : in the asymptotic limit, the flame front consists in an infinitely thin interface separating the burnt and unburnt sides and moving towards the unburnt gas with an overall “turbulent” combustion speed,  $S_T$ , completely determined by what is going on in the pre-heat zone, near  $T = 0$ , hence, generalizing the laminar flamelet regime

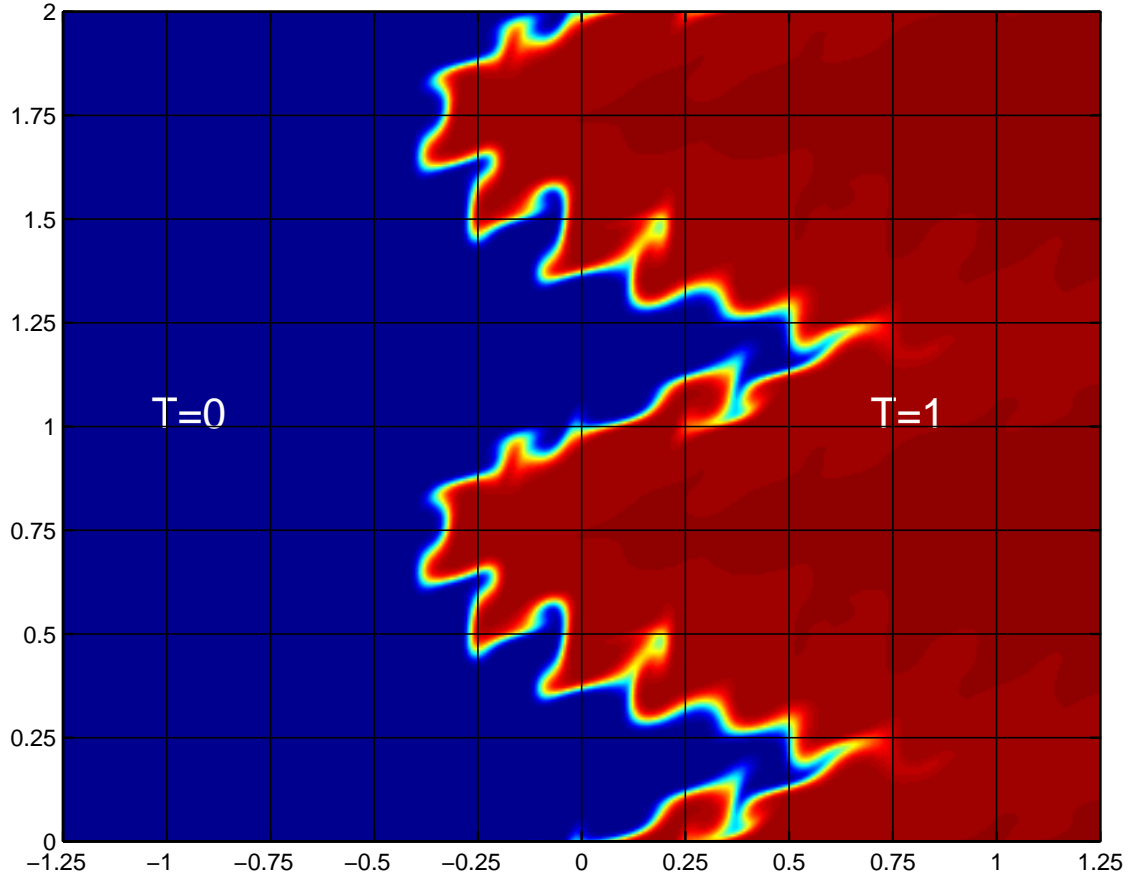


FIG. 5.3. Snapshot of DNS result for the temperature field.

where it is well known that the laminar combustion speed,  $S_L$ , is given by (set  $\bar{\mathbf{v}}(x, y) + \mathbf{v}(x/\epsilon^\alpha, y/\epsilon^\alpha) \equiv 0$  in (5.2.1))

$$S_L = 2\sqrt{f'(0)}. \quad (5.4.1)$$

Next is a qualitative discussion of the rigorous theory in [46] to provide some intuition on how this theory describes the mechanism by which turbulence leads to an enhancement of the propagation speed of the flame  $S_e = S_T - S_L$  as a result of the mixing taking place near the cold side boundary.

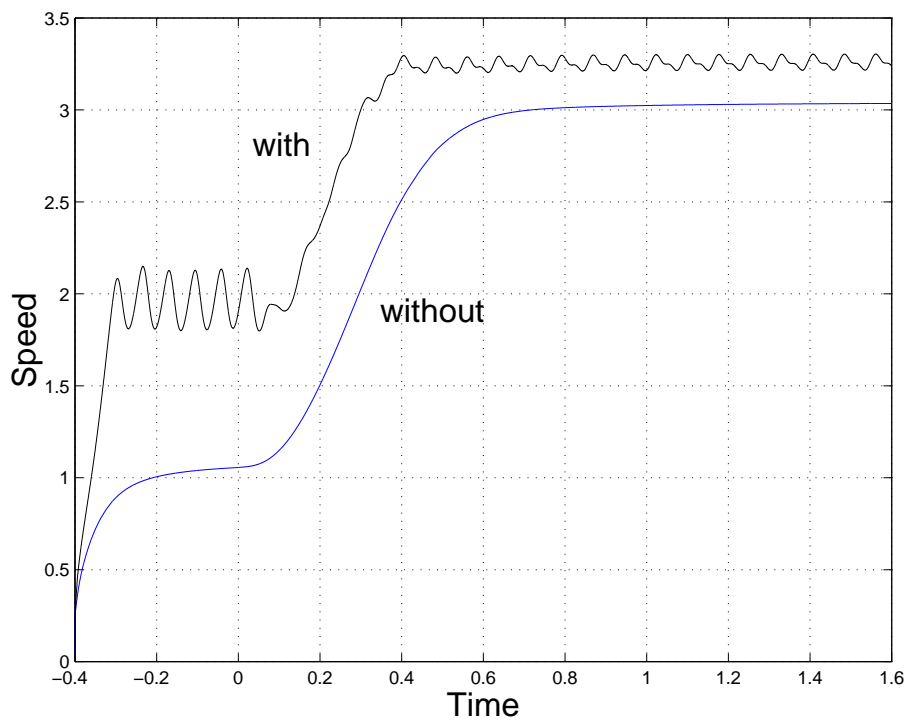


FIG. 5.4. Flame speed with and without the intermediate scale flow.

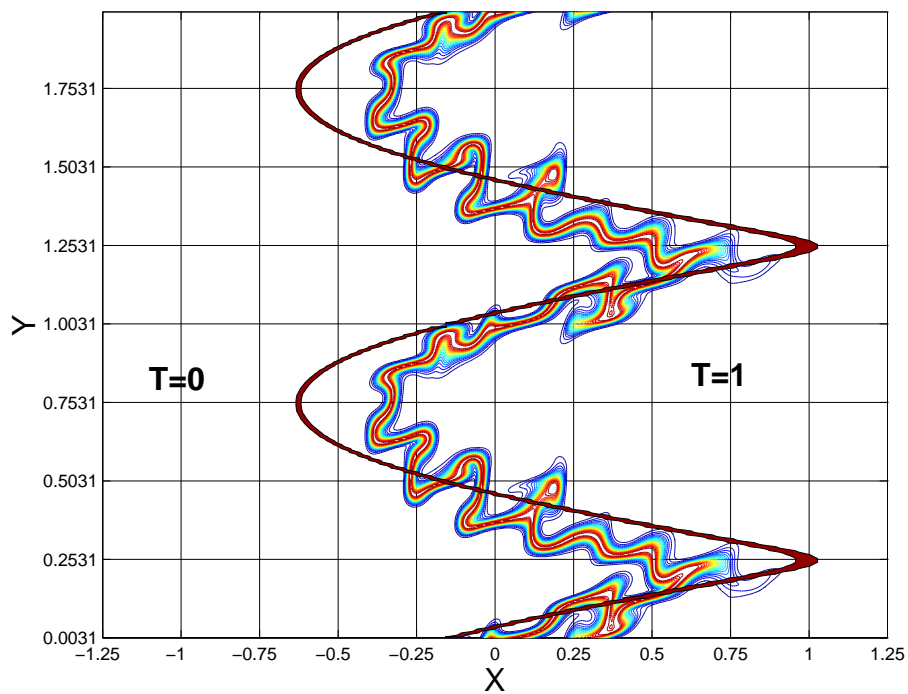


FIG. 5.5. Front shape with and without the intermediate scale flow.

The first step is to change variable in order to focus on the pre-heat zone near  $T = 0$  :

$$Z^\epsilon = \epsilon^{-1} \log T$$

This clearly emphasizes the exponential decay of  $T$  near zero. The equation for the new variable is such that the diffusion operator splits into two terms, a small (order  $\epsilon$ ) diffusion term for  $Z^\epsilon$  which is negligible in the limit of  $\epsilon \rightarrow 0$  and a new highly nonlinear term (order 1) which has the same order of magnitude as the advection term : it is this nonlinear term that, combined with the non-trivial advection term, describes the turbulent mixing mechanism in the pre-heat zone.

$$\frac{\partial Z^\epsilon}{\partial t} - |\nabla Z^\epsilon|^2 + (\bar{\mathbf{v}}(x, y) + \mathbf{v}(x/\epsilon^\alpha, y/\epsilon^\alpha)) \cdot \nabla Z^\epsilon = \frac{f(T)}{T} + \Delta Z^\epsilon.$$

When  $\epsilon$  goes to zero the solution  $Z^\epsilon$  converges uniformly on compact subsets to the viscosity solution of the variational inequality of Hamilton-Jacobi type [46],

$$\max(Z_t + H(\nabla Z, x, y), Z) = 0 \quad (5.4.2)$$

with

$$\begin{cases} Z = 0 & \text{when } T = 1 \text{ (burnt side)} \\ Z = -\infty & \text{when } T = 0 \text{ (unburnt side)} \end{cases}$$

and  $H$  is the eigenvalue of the so-called cell-problem

$$-|\mathbf{p} + \mathbf{D}w(\xi, \eta)|^2 + (\bar{\mathbf{v}}(x, y) + \mathbf{v}(\xi, \eta)) \cdot (\mathbf{p} + \mathbf{D}w(\xi, \eta)) = -H(\mathbf{p}, x, y) \quad (5.4.3)$$

here  $\mathbf{D}$  represents the gradient with respect to the variables  $(\xi, \eta)$ ,  $H$  is the eigenvalue and  $w$  is the associated eigenfunction which is assumed to be a bi-periodic solution in the viscosity sense with zero mean on one period box.

Furthermore, the theory of Majda-Souganidis states that if in addition the large scale velocity field,  $\bar{\mathbf{v}}$ , is constant, then the asymptotic flame is a pure

traveling wave obeying to the Huygens principle and evolving according to the *geometric equation*

$$G_t = F(\nabla G) \quad (5.4.4)$$

where the zero-level set  $\{G(x, t) = 0\}$  represents the flame interface and  $\nabla G$  is proportional to its unit normal,  $\mathbf{n} = (\cos \theta, \sin \theta)$ , pointing to the unburnt side with  $\theta$  being the angle between this normal and the  $x$ -axis. The function  $F$  defines for this particular case the overall turbulent combustion speed which is given by the minimization problem

$$S_T(\mathbf{n}) + \bar{\mathbf{v}} \cdot \mathbf{n} = F(\mathbf{n}) = \min_{r>0} \frac{H(r\mathbf{n}) + f'(0)}{r} \quad (5.4.5)$$

here  $H$  is the eigenvalue in (5.4.3) when  $\mathbf{p} = -r\mathbf{n}$ . Although, the gradient of  $Z$ ,  $\nabla Z$ , in (5.4.2) is actually directed to the hot region, it is more convenient to define here the burning speed with respect to the normal directed to the unburnt side. This is the reason why we have the minus sign in the last equality.

Notice that because the functional  $F$  verifies

$$F(\mu\mathbf{p}) = \mu F(\mathbf{p}), \quad \mu > 0,$$

(5.4.4) is called a geometric equation. Although, the theory [46] states that this geometric equation is only valid for the cases with constant large scale velocities,  $\bar{\mathbf{v}}$ , we still use this equation here for tracking the large scale flame interface in order to avoid the (numerical) complexity of (5.4.2). Nevertheless, it has been rigorously demonstrated in [46] that the geometric front, that is the front which is predicted by (5.4.4) for a non trivial  $\bar{\mathbf{v}}$ , is an optimal lower bound for the asymptotic front given by (5.4.2) and examples with non-constant  $\bar{\mathbf{v}}$ 's where the two fronts (the asymptotic front and its geometric lower bound) coincides are known [26].

### 5.4.2. Practical implementation

When the size of the small box,  $\epsilon^\alpha$ , is small compared to the scale of the mean flow,  $\bar{\mathbf{v}}(x, y)$ , hence to the grid size in a large eddy simulation set-up, the formula in (5.4.5) can be used to define the local turbulent combustion speed of the asymptotic flame interface at any time,  $t$ , during the simulation by setting

$$S_T(x, y, t) = \min_{r>0} \frac{H(r\mathbf{n}(x, y, t), x, y) + f'(0)}{r} - \bar{\mathbf{v}}(x, y) \cdot \mathbf{n}(x, y, t)$$

Now, it is straightforward to go through this procedure and compute the turbulent combustion speed at each position  $(x, y)$  on the flame interface given at time  $t$ , provided one has the adequate tools for solving the minimization problem in (5.4.5) and the nonlinear eigenvalue problem in (5.4.3) (see below).

The burning speed,  $S_T$ , depends only on the geometry and position of the front : this is completely specified knowing the local unit normal to the large scale front,  $\mathbf{n}(x, y) = (\cos\theta(x, y), \sin\theta(x, y))$  and the local intensity of the large scale flow,  $\bar{\mathbf{v}}$ . Hence an efficient strategy to avoid repetitive calculations is to compute and store in a database the solution  $S_T = S_T(\theta_I, \bar{\mathbf{v}}_J)$  over the expected range of values for  $\theta_I, I = 1, \dots, L$  and  $\bar{\mathbf{v}}_J, J = 1, \dots, M$ . The evaluation of  $S_T$  for any combination of values of  $\theta$  and  $\bar{\mathbf{v}}$  is obtained by simple interpolation in the database. Later on, we refer to this database as an “asymptotic flamelet library” or more simply “flamelet library”.

By symmetry arguments, it is clear that

$$S_T(\theta + \pi, \bar{\mathbf{v}}) = S_T(\theta, -\bar{\mathbf{v}});$$

in fact, this can easily be checked by using (5.4.3) and (5.4.5). Hence, when generating the flamelet library on the given mesh points  $(\theta_I, \bar{\mathbf{v}}_J)$  one can reduce by half the numerical cost by limiting the calculations to  $0 \leq \theta_I \leq \pi$  (or equivalently to  $\bar{\mathbf{v}}_J \geq 0$ ) and use the above formula to recover the values of  $S_T$  at the missing mesh points.

5.4.2.1. *Preliminary step : generating the asymptotic flamelet library*

The preliminary step of generating the flamelet library is a computationally intensive step as one needs to solve the coupled problem (5.4.3)-(5.4.5) repeatedly over the expected range of values for the parameters. The minimization in (5.4.5) is easily carried out with a standard numerical routine [13] downloaded from the web whereas the cell problem in (5.4.3) is far less standard. Except for one dimensional flows (simple shear layers) and a particular family of rotating flows [25, 46], analytical solutions for (5.4.3) are unknown and as a nonlinear eigenvalue problem its numerical resolution is a challenge. In [38], a new numerical scheme was introduced and validated specifically to solve this problem in an efficient and robust fashion. The method consists in differentiating Equation 5.4.3 with respect to the small scale variables  $(\xi, \eta)$  in order to get a system of conservation laws for the eigenfunction gradient components  $\mathbf{D}w$  :

$$\mathbf{D} \left\{ -|\mathbf{p} + \mathbf{D}w(\xi, \eta)|^2 + (\bar{\mathbf{v}}(x, y) + \mathbf{v}(\xi, \eta)) \cdot (\mathbf{p} + \mathbf{D}w(\xi, \eta)) \right\} = 0 \quad (5.4.6)$$

Differentiation has effectively removed the eigenvalue problem, which can be recovered a posteriori by using the following formula, directly derived from the cell-problem :

$$H(\mathbf{p}, x, y) = \langle |\mathbf{D}w|^2 \rangle + |\mathbf{p}|^2 - \bar{\mathbf{v}}(x, y) \cdot \mathbf{p}$$

where  $\langle |\mathbf{D}w|^2 \rangle = \int \int_{[0,1]^2} |\mathbf{D}w(\xi, \eta)|^2 d\xi d\eta$  denotes the mean of  $|\mathbf{D}w|^2$  over one period length box.

The system of equations in (5.4.6) is still a complex nonlinear system of equations ; its solution for  $\mathbf{D}w$  is obtained as the steady state solution of the following system of nonlinear conservation laws :

$$\begin{aligned} \frac{\partial u_1}{\partial s} + \frac{\partial}{\partial \xi} \left\{ -|\mathbf{p} + \mathbf{u}(\xi, \eta)|^2 + (\bar{\mathbf{v}}(x, y) + \mathbf{v}(\xi, \eta)) \cdot (\mathbf{p} + \mathbf{u}(\xi, \eta)) \right\} &= 0 \\ \frac{\partial u_2}{\partial s} + \frac{\partial}{\partial \eta} \left\{ -|\mathbf{p} + \mathbf{u}(\xi, \eta)|^2 + (\bar{\mathbf{v}}(x, y) + \mathbf{v}(\xi, \eta)) \cdot (\mathbf{p} + \mathbf{u}(\xi, \eta)) \right\} &= 0 \end{aligned} \quad (5.4.7)$$

with  $\mathbf{u} = (u_1, u_2)$  the new unknown representing  $\mathbf{D}w$  and with  $s$  the pseudo-time marching variable (not to be confused with the physical time  $t$  in (5.2.1)).

Because the system in (5.4.7) is not hyperbolic, solving it with classical methods failed [38] to lead to a converged steady state. To recover the convergence, one must take into account the essential information that the steady state vector solution we aim to reach is the gradient of a periodic function. This is a trivial requirement in one space dimension, but in two or more dimensions, it is not automatically satisfied. One way to take this constraint into account is described in [38] : there, one compensates for the lack of hyperbolicity by relying on a staggered grid to build up a “gradient preserving scheme”. The idea of essentially non-oscillatory interpolation [43] is used to achieve second order spatial accuracy whereas linear stability arguments for frozen stencils are used to construct a two-step first order method in time that converges efficiently to the steady state ; the interested reader is referred to that paper for more details and validation.

#### 5.4.2.2. *The flamelet library*

The strategy just described is used to solve (5.4.3)-(5.4.5), for each set of parameters  $(\theta_I, \bar{v}_J), I = 1, \dots, L, J = 1, \dots, M$ , leading to  $S_T = S_T(\theta_I, \bar{v}_J)$ . In Fig. 5.6, we plot the contours of the speed enhancement  $S_e(\theta, \bar{v}) = S_T(\theta, \bar{v}) - S_L$  when  $L = 41$  and  $M = 21$  for a large scale flow extended to  $\bar{\lambda} = 4$ . Increments for the large scale flow intensity are picked accordingly :  $\Delta\theta = \pi/20$  and  $\Delta\bar{v} = 0.2$ . Notice that the calculations are limited to  $\bar{v} > 0$  since the remaining values can be obtained by symmetry as noted before. The small scale flow,  $\mathbf{v}$ , is derived from the Childress-Soward stream-function where  $\delta$  is fixed to  $\delta = 0.5$  and which is renormalized such that the intensity,  $\lambda$ , of  $\mathbf{v}$  is fixed to

$$\lambda = \max_{[0,1] \times [0,1]} \mathbf{v}(\xi, \eta) = 2$$

From Fig. 5.6 we see that the speed enhancement  $S_e$  due the small scale flow  $\mathbf{v}$  attains its maximal value  $S_{e,\max} \approx 1.8$  near the points  $(-3\pi/4, 0)$  and  $(\pi/4, 0)$



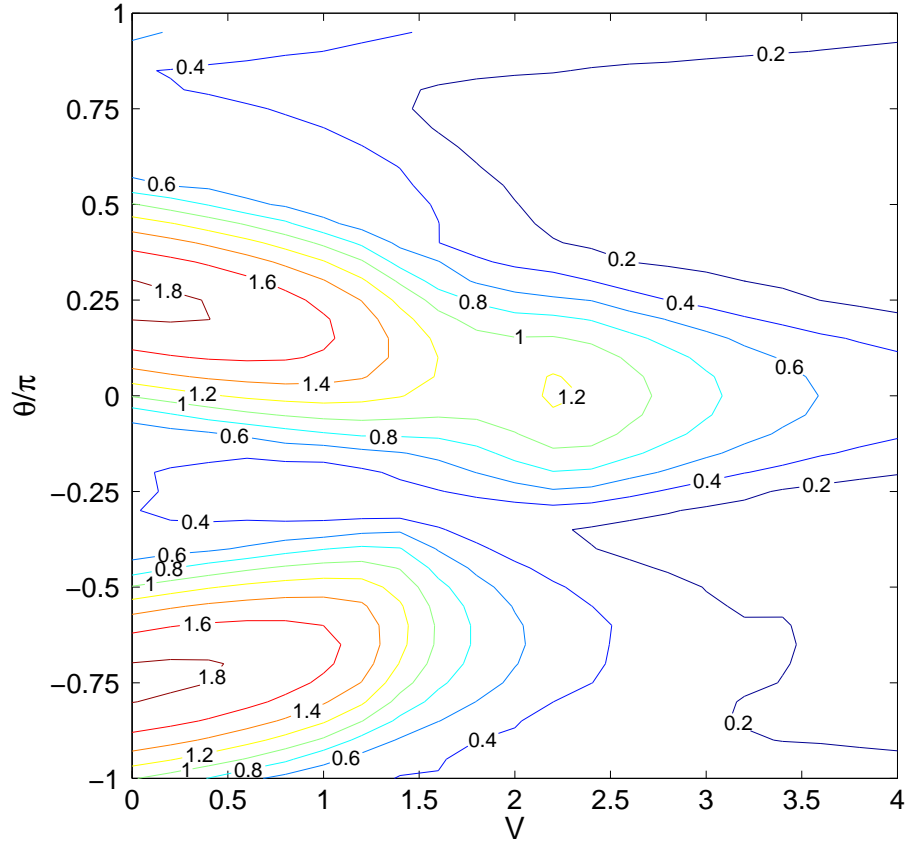


FIG. 5.6. Flamelet library : contours of  $S_e = S_T(\theta, \bar{v}) - S_L$  for a fixed intermediate scale flow of Childress-Soward with  $\delta = 0.5$  and  $\lambda = 2$ .

and  $S_e$  decreases when  $\bar{v}$  increases or  $\theta$  approaches the values  $3\pi/4$  and  $-\pi/4$ . A qualitative, intuitive explanation for this behavior is the following.

- When the intensity  $\bar{v}$  of the flow advecting the flame across the small box is large, the flame is swept so quickly that it has no time to see the small scale flow.
- The results in Fig. 5.6 confirm the fact that shear flows that are aligned with the normal  $\mathbf{n}$  of the mean front are likely the flows for which the largest enhancement speeds are achieved. The small scale flow considered here has an important component which is a shear layer tilted at 45 degrees, see Fig. 5.2. When  $\theta = -3\pi/4$  or  $\theta = \pi/4$  we are in the situation where the

shear component is aligned with  $\mathbf{n}$  so that maximum effect of that shear is felt by the flame, hence a maximum speed enhancement is achieved. When  $\theta = 3\pi/4$  or  $\theta = -\pi/4$  the mean flame itself is aligned with that shear, it sees only the eddies, hence the speed enhancement is weak.

#### 5.4.2.3. *Front evolution*

A computationally efficient strategy to implement the theoretical predictions is presented next based on the level-set formulation. Consider any level-set function,  $G$ , for which the level zero  $\{G = 0\}$  coincides with the asymptotic flame front,  $G$  is positive on the burnt side and negative on the unburnt side at some time  $t = t_0$  as shown on Fig. 5.7. By generalizing the equation in (5.4.4) for non constant  $\bar{\mathbf{v}}$  and using the equation in (5.4.5) with the fact that the unit normal to the front directed to unburnt side is given by

$$\mathbf{n} = -\frac{\nabla G}{|\nabla G|},$$

we have

$$G_t = F(\nabla G) = |\nabla G|F(\mathbf{n}) = S_T|\nabla G| + |\nabla G|\bar{\mathbf{v}} \cdot \mathbf{n}$$

and we get

$$G_t(x, y, t) + \bar{\mathbf{v}}(x, y, t) \cdot \nabla G(x, y, t) = S_T(x, y, t)|\nabla G| \quad (5.4.8)$$

which is the so popular G equation [3, 4, 5, 64, etc], where the laminar combustion speed is replaced here by the turbulent speed

$$S_T(x, y, t) = S_T(\nabla G(x, y, t), \bar{\mathbf{v}}(x, y)) = S_T(\theta(x, y, t), \bar{\mathbf{v}}(x, y)).$$

Because, the large scale velocity field is imposed to be a shear flow that depends only on  $y$ , the level-set function can be chosen such that  $\nabla G$  depend only on  $y$  by setting

$$G(x, y, t) = x + g(y, t)$$

and the equation (5.4.8) becomes

$$g_t + \bar{\lambda} \sin(2\pi y) = S_T(\theta(y, t), t) \sqrt{1 + g_y^2} \quad (5.4.9)$$

with  $\theta(y, t)$  being the angle shown in Fig. 5.7.

The numerical resolution of (5.4.9) is carried out by using the high order (two to four) essentially non oscillatory scheme for Hamilton-Jacobi equations of Osher and Shu [53]. This numerical method is based on an upwind finite difference discretization so that the numerical solution converges to the right limit solution in the viscosity sense. The method is quite efficient at capturing the cusps developed by the flame front ; these cusps correspond to singularities in the first order derivative of  $g$  that are typical for the viscosity solutions of Hamilton-Jacobi equations. Strictly speaking, because the large scale flow  $\bar{v}(y)$  here is not constant, one can only demonstrate theoretically that the front computed using the strategy described in this section is a lower bound for the actual flame. There are for instance examples where the flame does not obey a geometric propagation law as assumed here ([26, 46]). The numerical experiments to be described next confirm however that for the present case, the front asymptotically coincides with the geometric front predicted following the strategy above.

### 5.4.3. Validation

Here, we validate the asymptotic large eddy simulation discussed in details above by using results from the direct numerical simulation presented in Section 5.3.2. Precisely, we compare the flame predicted by the geometric equation in (5.4.9) supplemented by the flamelet library from Section 5.4.2.2 with the flame obtained by Equation 5.2.1 for sufficiently small  $\epsilon$ . This requires

1. computing and comparing the effective speeds at which each one of the flames is moving ;
2. comparing the detailed shapes of the the fronts at the large scales (resolved even in the LES).

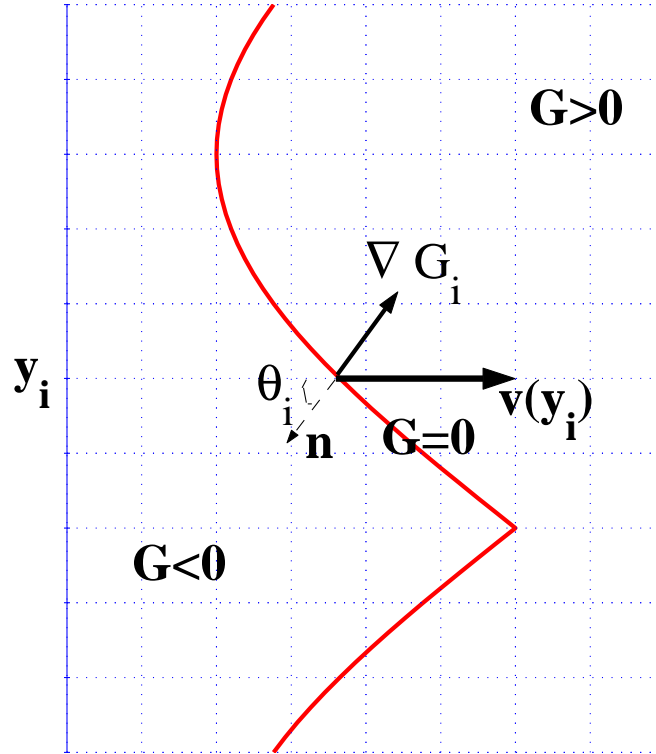


FIG. 5.7. Illustration for the level-set tracking procedure for the asymptotic front. The zero-level curve,  $G = 0$ , indicates the location of the front.

The speed of propagation of the asymptotic front is always trivial to compute as it is directly related to the time derivative of the average  $x$ -position of the front. The speed of propagation for the finite thickness reaction zone can be obtained indirectly via a conservation principle, whereas the change in mean temperature in the domain must result from flame propagation through burning.

In Fig. 5.8 we plot the reaction rate contours,  $f(T) = c$ ,  $c = .01, .02, \dots, .1$ , given by the direct numerical simulation of Equation 5.2.1 along with the LES front (dashed line) predicted by the geometric equation in (5.4.9) and using the flamelet library from Section 5.4.2.2, for the values  $\epsilon = 1/8$  (top),  $\epsilon = 1/16$  (middle) and  $\epsilon = 1/32$  (bottom) with the number of small boxes being fixed to  $N_p = 1/\epsilon^\alpha = 2, 4$  and  $8$  respectively. In Fig. 5.9, we compare the speed computed in each one of these three cases,  $(\epsilon = 1/8, N_p = 2)$ ,  $(\epsilon = 1/16, N_p = 4)$ ,  $(\epsilon =$

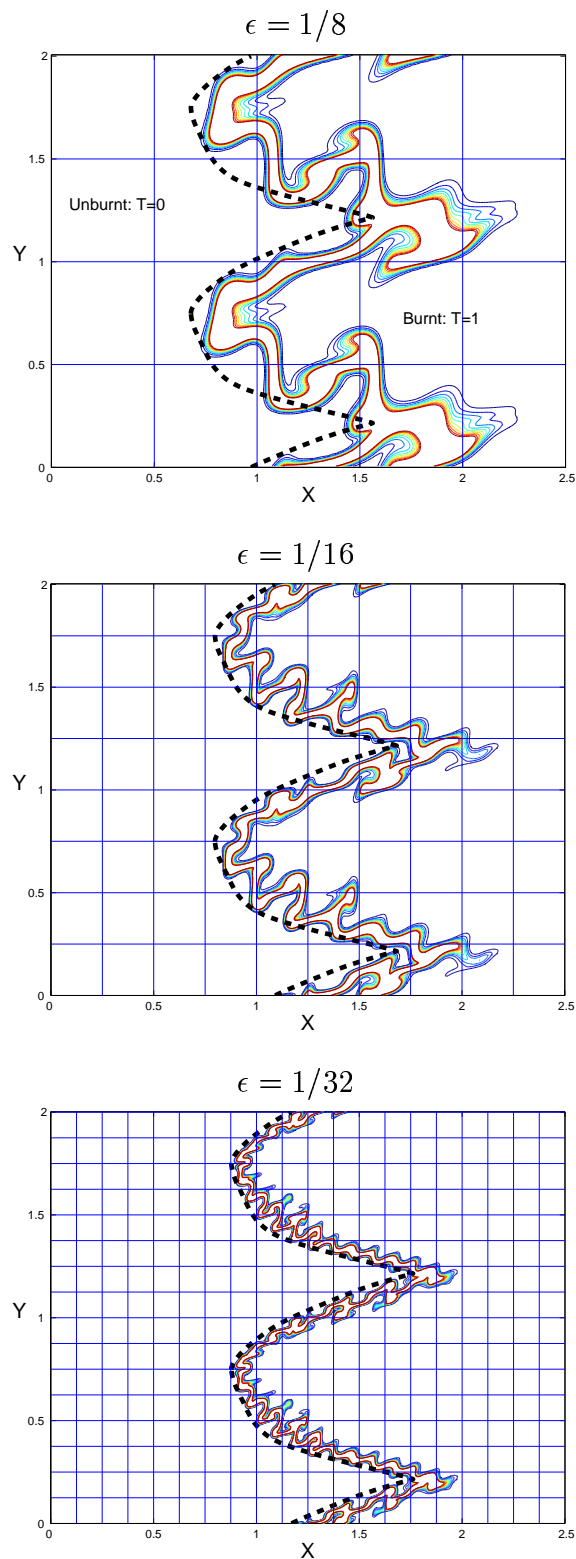


FIG. 5.8. Validation 1). Contours of the reaction rate,  $f(T) = c$ ,  $c = .01 : .01 : .1$ , for decreasing values of  $\epsilon$  and  $\epsilon^\alpha$  showing the asymptotic convergence to a limit which is in agreement with the LES front (dashed line). The small squares within each chart indicate the small period boxes of size  $\epsilon^\alpha$ .

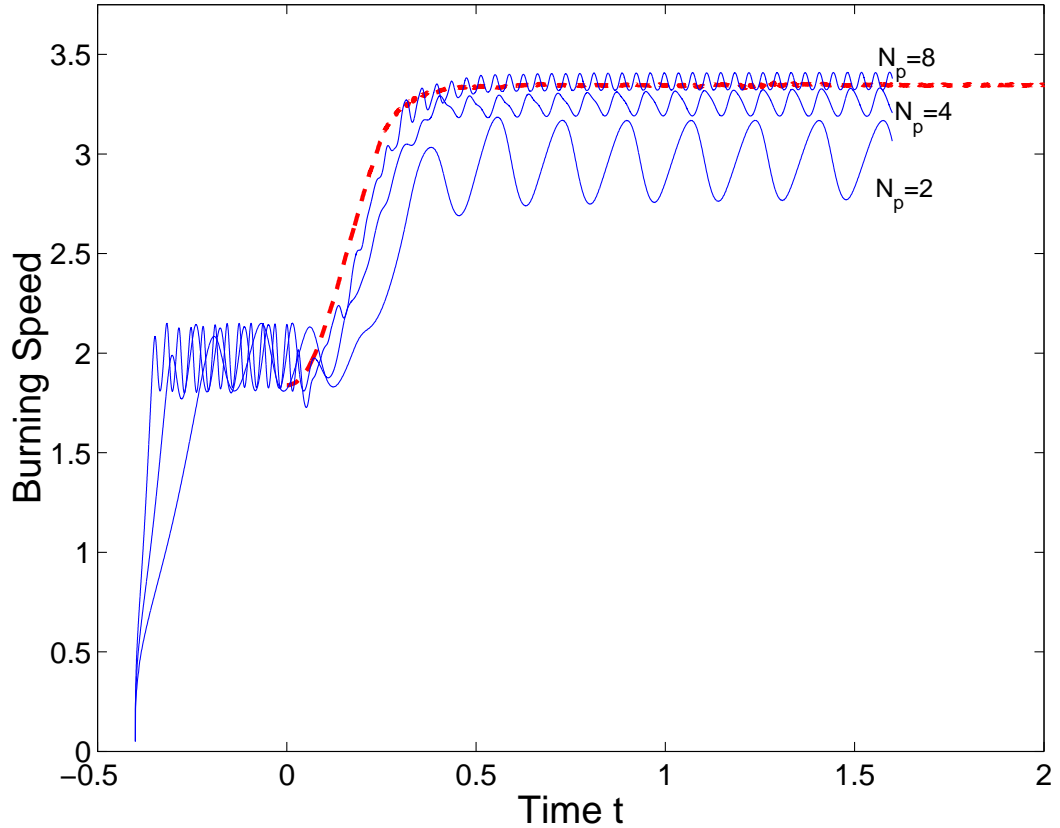


FIG. 5.9. Validation 2). History of the effective burning speed. For  $\epsilon = 1/8$ ,  $\epsilon = 1/16$ ,  $\epsilon = 1/32$  corresponding to the number of small boxes  $N_p = 2, 4$  and  $8$  respectively, and LES front (dashed line). From  $t = -0.5$  to  $t = 0$  only the intermediate scale velocity,  $\mathbf{v}$ , is active.

$1/32, N_p = 8$ ) with the speed of the LES front (dashed line). There are two phases in the computations : from  $t = -0.5$  to  $t = 0$ , only the intermediate scale velocity,  $\mathbf{v}$  is activated, the large scale flow  $\bar{\mathbf{v}}$  is turned on at time  $t = 0$  and the computations are carried out until the flame speed converges to a steady mean. (In this sequence,  $\alpha$  is not fixed, this would have required  $\epsilon = 1/64$  in the last set of simulation, which would have been too costly for direct simulation. This does not affect the convergence, which basically depends only on the facts that  $\epsilon < \epsilon^\alpha < 1$ ,  $\epsilon \rightarrow 0$  and  $\epsilon^\alpha \rightarrow 0$ ).

Fig. 5.8 and Fig. 5.9 demonstrate that as  $\epsilon \rightarrow 0$  and  $\epsilon^\alpha \rightarrow 0$ , both the effective speed of the flame and its shape converge to the asymptotic limit predicted by the geometric equation in (5.4.9) using the flamelet library from Section 5.4.2.2 - the agreement is quite remarkable. This indicates unambiguously that this particular problem set-up is a case where the front is actually described by the theoretical lower bound even though the large scale speed is not constant. In 5.8, the large scale front was systematically positioned to correspond with the cold side of the flame, a choice validated by the fact that the wrinkled front with decreasing wrinkle length scale appears to effectively collapse from the right onto the asymptotic large scale front. This particular point will be discussed further in Section 5.5 (Issue II) below.

## 5.5. REVISITING PRACTICAL LES ISSUES

The results from the previous section validate unambiguously the asymptotic theory in the limit of  $\epsilon$  going to zero as well as its practical implementation via a flamelet library : the agreement between the asymptotic large scale front and the direct simulations is quite spectacular by the standards of LES validation. However, in a practical case, the flame thickness as well as the characteristic length scale(s) of the subgrid turbulent flow are small but finite and the relevance of the asymptotic theory is not straightforward. The purpose of this section is to illustrate the type of information that can be obtained from the idealized test-case with direct relevance to the practical cases.

### **Issue I : parameterizing the turbulent burning speed**

The LES results in Section 5.4 required the generation of an extensive database for the subgrid enhancement. For more realistic cases, this would be too costly. Instead, one might want to use an inexpensive subgrid model of the type :  $S_T = S_L + K\lambda^\beta$ , with  $\lambda$  the subgrid turbulence (units of velocity) while the pre-constant  $K$  and the exponent  $\beta$  are parameters to be adjusted statically or

dynamically (see for instance [8, 9, 15] regarding the feasibility of adjusting  $\beta$  dynamically rather than specifying it a priori). Experimental results indicate that typically  $S_T$  will be linear in the turbulence intensity for “large” intensities (i.e.  $\beta = 1$  at large intensities) but that  $\beta > 1$  at small intensities; the transition between the two regimes is known as the bending effect. A better understanding of the possible regimes for  $S_T(\lambda)$  would be very helpful in designing an efficient subgrid parameterization. A step in that direction is achieved with unambiguous results obtained for the model problem using a combination of careful numerical simulations and asymptotics (see [11] for details). The results can be stated for fairly general velocity fields of the type used with the model, but for simplicity, we will restrict the presentation here only to the case when the perturbation velocity field  $\mathbf{v}$  is a time modulated shear normal to the front :  $\mathbf{v} = (v, 0)$  with  $v(y, t) = \lambda \sin(2\pi y) \cos(\omega t)$ . The results are as follows :

- in the limit  $\omega \rightarrow 0$ , the burning speed enhancement corresponds exactly to  $S_{E,0} = 2\lambda/\pi$  so that in that case, the scaling exponent is  $\beta = 1$ .
- when  $\omega > 0$ , the normalized speed enhancement  $S_{E,N} = S_e/S_{e,0}$  is a function only of the nondimensional number  $\tilde{t} \sim \sqrt{\lambda}/\omega$ . This nondimensional number is the ratio of the modulation period  $T \sim 1/\omega$  to the flame deformation time  $t_{ref} \sim 1/\sqrt{\lambda}$  defined as the time it takes a steady shear to deform to steady state an initially planar flame.
- when  $\tilde{t}$  is large (hence the flow frequency is very slow, so that the steady solution is a good approximation),  $S_{e,N} = 1 - C/\tilde{t}$  so that, to leading order,  $S_e$  is proportional to  $\lambda$  and  $\beta = 1$ .
- when  $\tilde{t}$  is small (hence the shear oscillates very fast, so that the flame has no time to respond and the enhancement is very small),  $S_{E,N} = \tilde{t}^2/4$  so that  $S_e$  is to leading order proportional to  $\lambda^2$  and  $\beta = 2$



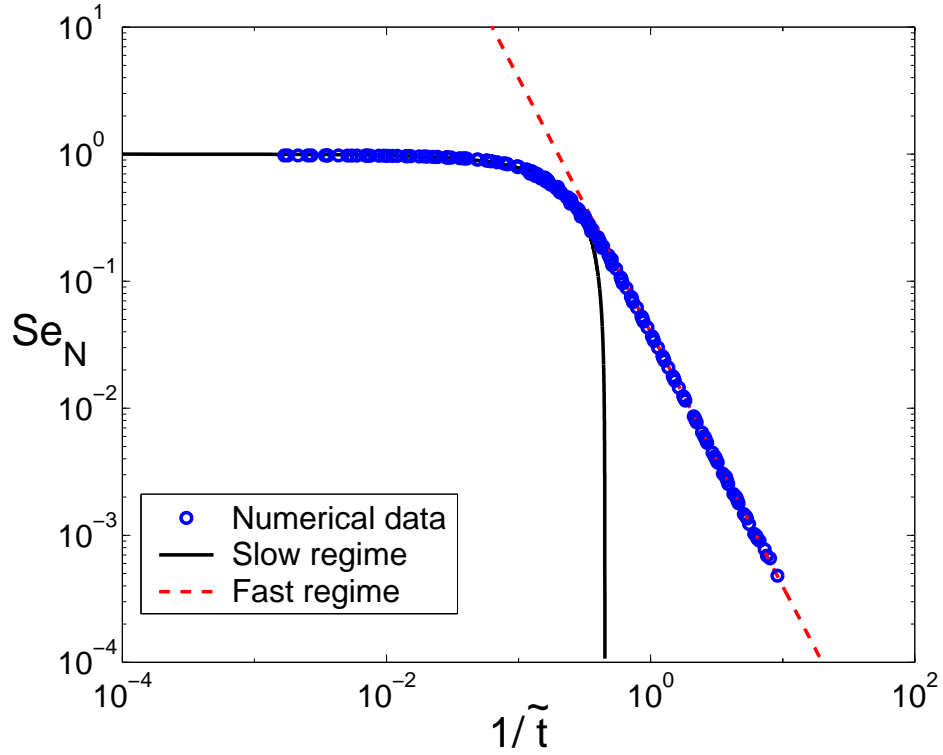


FIG. 5.10. Normalized burning speed enhancement  $S_{e,N} = S_e/\tilde{t}$  as a function of the non-dimensional flame residence time  $\tilde{t}$  for the case of a time-modulated horizontal shear  $v(y) = \lambda \sin(2\pi y) \cos(\omega t)$ .

Those predictions of two distinct regimes for  $S_{E,N}(\tilde{t})$  are verified in Fig. 5.10 where the flame propagation speed has been processed from numerical simulations with a wide range of values of  $\omega$  and  $\lambda$ .

For instance, the analysis of the flamelet library from Section 5.4.2.2 can be reformulated in terms of the non-dimensional flame residence time.

- The condition  $t_w < t_r$  corresponds to the slow regime where the flame has all the time to wrinkle to its maximum distortion, hence, considerable amount of speed enhancement can be achieved : the neighborhoods of  $(-3\pi/4, 0)$  and  $(\pi/4, 0)$  in Fig. 5.8 correspond to parameter values that give rise to a slow regime,

- The condition  $t_w > t_r$  corresponds to the fast regime where the flame has not sufficient residence time in order to achieve a lot of wrinkling, so that the speed enhancements encountered in this regime are very weak : in Fig. 5.6, we have a fast regime at large values of  $\bar{v}$  and close to  $\theta = \pi/4$  and  $\theta = -\pi/4$

### **Issue II : identifying the LES front - the asymptotic view and the averaging view**

Direct numerical simulations are one of the preferred strategy to validate large eddy simulations. In a direct numerical simulation of a premixed flame, all the scales, down to the very small reaction zone thickness, are explicitly resolved. An open question is the following : how should one use the DNS data a priori to predict the shape of a LES flame front, i.e. how do you extrapolate the resolved results to a zero-thickness front? For instance, if one were to identify the infinitely thin front with a specific value of the reaction progress variable  $c$  ( $c = 1$  representing the reaction being complete and  $c = 0$  the reaction not yet started), which contour of  $0 \leq c \leq 1$  should be identified with the large scale front? In practical databases, different contours can have very different geometric behavior [56, etc]; this ambiguity complicates attempts at devising ad-hoc subgrid models for the front speed because such models account explicitly for the geometry of the front contour, for example to propose a model for the subgrid "wrinkling" or to quantify curvature effects to control the smoothness of the front.

Theoretically, it is well known that, in the laminar case, the burning speed of KPP flames is governed by the behavior of the reaction rate on the cold side (near  $T = 0$ ). The rigorous asymptotic theory of Majda and Souganidis generalizes this argument : the cell-problem that leads to the prediction of the turbulent burning speed describes the interaction of mixing, diffusion, and reaction near the cold side of the flame [46, 11].

As mentioned in Section 5.4.3, the sequence of pictures in Fig. 5.9 confirms the theoretical considerations as it appears that the reaction contour snapshots converge to the asymptotic front prediction from the right : at small but finite size wrinkles and reaction zone thickness, the asymptotic front was shown to coincide with the cold side envelop of the wrinkled flame front.

The asymptotic view is a very rigorous strategy to extract the large scale behavior as the fluctuations shrink as  $\epsilon \rightarrow 0$ . This abstract strategy is however very remote from the practical view so an alternate approach to extracting the large scale behavior is discussed here. A series of numerical experiments were carried where Eq. 5.2.1 is solved with the velocity field in (5.3.1) and (5.3.2) except that the small scale flow alignment with respect to the large scale flow and the initial data has been shifted randomly :

$$\mathbf{V} = \bar{\mathbf{v}}(x, y) + \mathbf{v}((x + x_i)/\epsilon^\alpha, (y + y_i)/\epsilon^\alpha)$$

with  $x_i, y_i$  independent and uniformly distributed in  $[0, 1]$ . This random phase shift is illustrated in Fig. 5.11. Fig. 5.12 shows the flame speed history for 20 realizations of that phase shift for  $\epsilon = 1/16$  and  $\epsilon^\alpha = 1/4$ . In the limit of  $\epsilon \rightarrow 0$ , the phase shift has no influence on the results but it definitely influences the finite  $\epsilon$  realizations. Also shown is the average over all those realizations : this illustrates that the phase averaging is an effective procedure to remove the fluctuations observed in the realizations ensemble as well as the unsteadiness of each realization (only a fraction of the time modulation is still observed in the average curve). Fig. 5.13 compares this flame speed phase average with the asymptotic speed prediction : agreement is remarkable, indicating that, in a statistical sense, the asymptotic theory is an excellent predictor for the finite  $\epsilon$  behavior for values of  $\epsilon, \epsilon^\alpha$  as large as  $1/16$  and  $1/4$  respectively ! The agreement is even more remarkable by considering the geometry of the front as indicated by the reaction rate contours averaged over all 20 realizations. The contours are shown in Fig. 5.14, where the agreement between the asymptotic large scale front and the cold side contour for

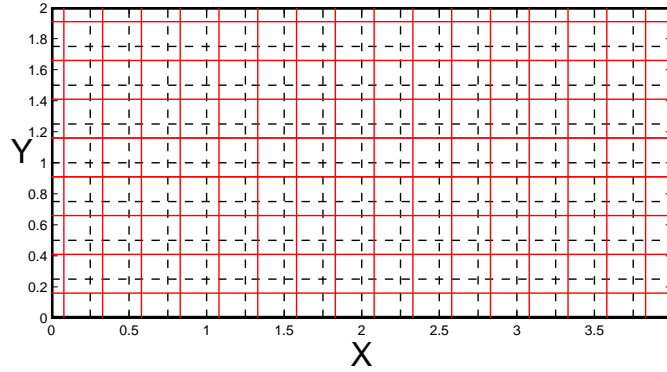


FIG. 5.11. Set-up for phase-averaging.

the reaction rate is demonstrated unambiguously, confirming the intuition from the theoretical predictions and from the numerical asymptotic convergence study. Here are some practical remarks to conclude the discussion regarding this topic :

- If one is considering DNS data, the large scale front cannot be identified with any specific contour of the temperature or reaction rate ; rather, at least for a KPP type chemistry, it will more likely coincide with the cold-side envelop of the resolved reaction zone.
- If the large scale front is an envelop, it might not be smooth but display cusps as it is the case for the example considered here. One direct consequence of this observation is that the popular *filtering* strategy might not be appropriate as it smoothes out any singularity such as cusps.
- The phase averaged front is not infinitely thin, instead its width in the example considered here is on the order of the volume over which the phase shift occurred. In a practical computation, this width would nevertheless still appear as a sub-scale effect, so that the front would appear as a sudden jump in the data, which requires the use of the appropriate numerical methodology for capturing or tracking fronts ([33],[41],[60]).

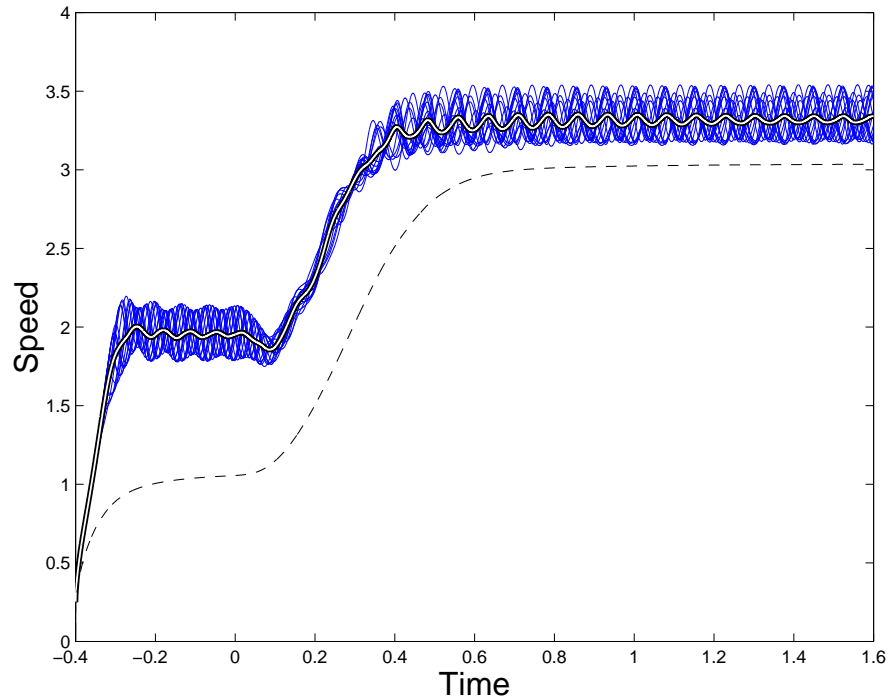


FIG. 5.12. Flame speed for many phase realizations along with their average and the laminar speed.

### **Issue III : reducing effectively the requirement for numerical grid refinement**

The purpose of a large eddy simulation strategy is to be able to represent accurately the large scale behavior without resolving the fine scale details. Here we verify the feasibility of effectively reducing the grid refinement by relying on the subgrid modeling strategy. So far, the large scale behavior (for instance the front shape and the front speed) has been predicted using a resolution of 80 points per vertical period. Transposed to a practical computation, this resolution would be quite excessive. Fig. 5.15 and Fig. 5.16 illustrate that it is indeed not needed. As little as 5 points per period are sufficient to capture the large scale flame front (see Fig. 5.15) but seem insufficient to fall into the convergence range for the flame speed (see Fig. 5.16); however, 10 points per period are already adequate

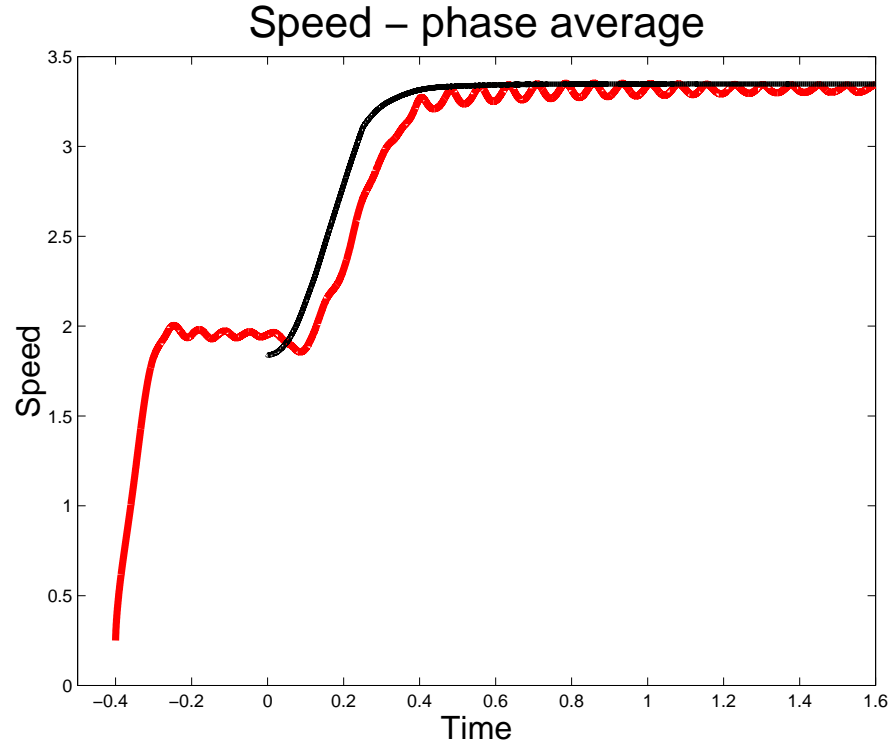


FIG. 5.13. Flame speed averaged over many phase realizations along with LES speed.

on both accounts. This confirms convincingly the potential of the subgrid flamelet strategy for the large eddy simulations of premixed flames with very reduced resolution.

## 5.6. CONCLUSION

New, unambiguous answers to a number of important practical issues regarding the large scale simulations of turbulent premixed flames have been obtained using a hybrid asymptotic-numerical approach applied to an idealized test-case. Implementing the rather abstract mathematical theory required the design of specialized numerical tools, in particular to build an *asymptotic flamelet library*. The excellent results achieved for a practical case somewhat outside the strict conditions of applicability of the theory demonstrate its robustness and relevance.

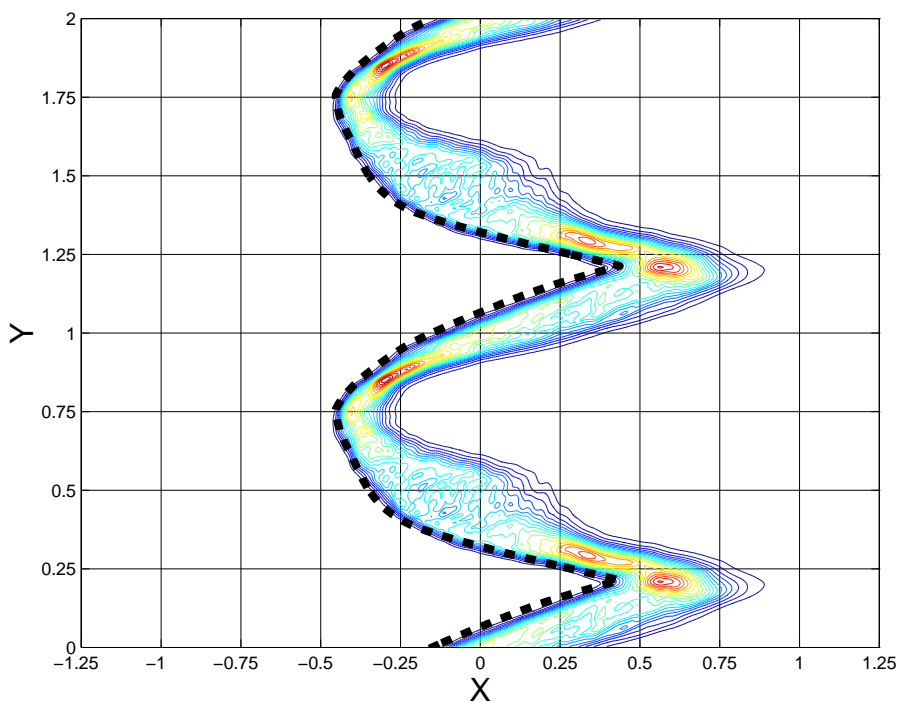


FIG. 5.14. Reaction rate from phase-averaged temperature along with LES front.

Furthermore, the asymptotic predictions are shown to be very valuable in the more practical sense of phase-averaged predictions suggesting for instance new perspectives to re-examine direct numerical simulation databases. Further work will extend the results presented here to more complex small scale flows (multiple-scale rather than two-scale, stochastic etc.) and reaction rate.

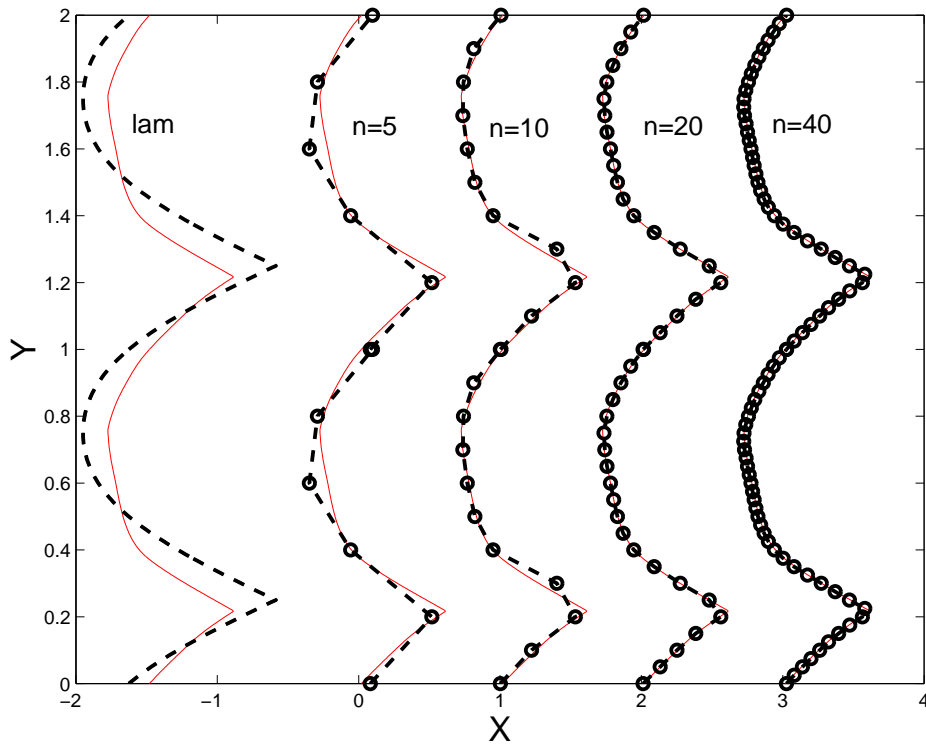


FIG. 5.15. LES front shape with reduced resolution ( $n$  = number of points per vertical period, two periods are shown).



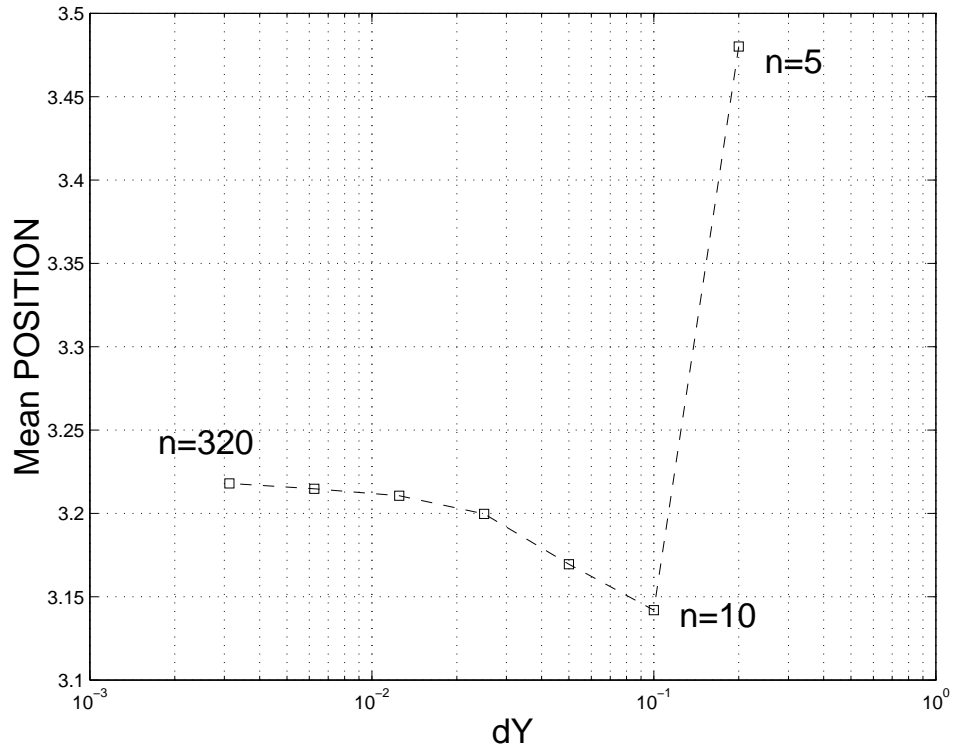


FIG. 5.16. LES flame speed with reduced resolution - same as Fig. 5.15.

## APPENDIX : NUMERICAL ALGORITHM FOR THE DIFFUSION OPERATOR IN 2D

Her we give the numerical algorithm used in this work to solve diffusion part of the reaction-diffusion-advection equation in (1). Consider the diffusion equation

$$T_t = D(T_{xx} + T_{yy}) \quad T(x, y, 0) = T_0(x, y)$$

where  $T_0$  is periodic in  $y$ .  $D$  replaces the term  $\epsilon\kappa$ . We exploit the semi-periodicity and use the spectral method to reduce the derivative in  $y$  then the Crank-Nicholson scheme for  $(x, t)$ .

- the spectral method in the direction  $y$  is based on the Fast-Fourier-Transform (FFT) algorithm from [61] where the forward Fourier transform, `dfft`, and backward Fourier transform, `dftb`, are defined as follow. Given the vector  $r(1 : N)$  say representing the values of a real periodic function  $r$  on the grid  $y_j, j = 1, \dots, N$ , we represent by  $R(1 : N)$  the Fourier-Transform of  $r(1 : N)$ . Suppose that  $N$  is even, we have

$$r(1 : N) \begin{array}{c} \xrightarrow{\text{dfft}} \\ \xleftarrow{\text{dftb}} \end{array} R(1 : N)$$

with

$$r_j = R_1 + (-1)^{j-1} R_N + \sum_{k=2}^{N/2} 2R_{2k-2} \cos[(k-1)(j-1)2\pi/N] - 2R_{2k-1} \sin[(k-1)(j-1)2\pi/N]. \quad (5.6.1)$$

Below we set  $\theta_j = 2(j-1)\pi/N$  for simplicity. Suppose we approximate the second derivative in  $y$  by using the second order approximation

$$\left. \frac{\partial^2 r}{\partial y^2} \right|_{y=y_j} \approx \frac{r_{j+1} - 2r_j + r_{j-1}}{\Delta y^2}$$

then, by replacing  $r_{j-1}, r_j, r_{j+1}$  by their Fourier series as in (5.6.1) and using some trivial trigonometric identities, we obtain the following expansion for the second derivative of  $r$

$$\frac{\partial^2 r}{\partial y^2} \Big|_{y=y_j} \approx \sum_{k=2}^{N/2} \frac{1}{\Delta y^2} \left( 2(\cos(2(k-1)\pi/N) - 1) R_{2k-2} \cos[(k-1)\theta_j] - 2(\cos(2(k-1)\pi/N) - 1) R_{2k-1} \sin[(k-1)\theta_j] \right)$$

- the equation  $T_t = D(T_{xx} + T_{yy})$  (here  $D = \epsilon\kappa$ ) resumes to  $N$  1D-diffusion equations with sources terms

$$\partial_t \hat{T}(K) = D \partial_{xx} \hat{T}(K) + C(K) D \hat{T}$$

where  $C(K) = 2(\cos(K\pi/N) - 1)/\Delta y^2$  if  $K = 2, 4, \dots, N-2$ ,  $C(K) = (\cos((K-1)\pi/N) - 1)/\Delta y^2$  if  $K = 3, 5, \dots, N-1$  and  $C(K) = 0$  if  $K = 1, N$ .

- the equation  $\partial_t \hat{T}(K) = D \partial_{xx} \hat{T}(K) + C(K) D \hat{T}$  is integrated by using the Crank-Nicholson method

$$\frac{\hat{T}_i^{n+1} - \hat{T}_i^n}{\Delta t} = \frac{D}{2} \left[ \frac{\hat{T}_{i+1}^{n+1} - 2\hat{T}_i^{n+1} + \hat{T}_{i-1}^{n+1}}{\Delta x^2} + C(K) \hat{T}_i^{n+1} + \frac{\hat{T}_{i+1}^n - 2\hat{T}_i^n + \hat{T}_{i-1}^n}{\Delta x^2} + C(K) \hat{T}_i^n \right]$$

where the variable  $K$  is dropped for simplicity,

- hence, the diffusion term reduces to  $N$  tridiagonal  $N \times N$ -linear systems.

# CONCLUSION

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L'étude menée dans cette thèse porte sur trois volets principaux : 1) la paramétrisation systématique de l'augmentation de la vitesse de combustion d'une flamme prémélangée due à la turbulence pour le cas d'un cisaillement instationnaire ainsi que son extension, du moins qualitative, à des écoulements bidimensionnels de type Childress-Soward, 2) l'élaboration d'une méthode numérique pour résoudre le hamiltonien effectif de la théorie de Majda-Souganidis [46] et, finalement, 3) la mise en œuvre numérique d'une stratégie LES pour un cas test utilisant le modèle asymptotique de M-S pour modéliser l'effet des petites échelles afin de démontrer l'utilité du modèle asymptotique dans un cadre global.

## PARAMÉTRISATION DE LA VITESSE DE COMBUSTION

Dans cette étude, nous avons montré que l'augmentation de la vitesse de combustion d'une flamme prémélangée idéalisée soumise à un cisaillement périodique aux petites échelles dépendant du temps subit une transition contrôlée par un temps de résidence non-dimensionnel de la flamme. Quand le temps de résidence est grand (ce qui a tendance à être le cas quand l'intensité de turbulence est grande), l'augmentation de la vitesse de combustion est linéaire par rapport à l'intensité de turbulence tandis que, quand le temps de résidence est petit (ceci est typiquement le cas quand l'intensité de turbulence est petite ou aux très petites échelles temporelles), l'augmentation de vitesse est non-linéaire (ici quadratique) par rapport à l'intensité de turbulence. Cette transition ressemble considérablement à l'effet de flexion (*bending effect*) observé dans les expériences.

Ce travail a été effectué dans le contexte asymptotique rigoureux développé dans [46] pour des flammes de type KPP. Un modèle contemporain plus populaire

pour décrire la propagation d'un front de flamme est l'approche de l'équation G (utilisée par exemple dans [5, 22]). Alors que le modèle asymptotique de Majda Souganidis et l'équation G peuvent mener dans quelques régimes à des prédictions très différentes, ils s'accordent qualitativement dans d'autres [24]. Le travail en progrès de A. Bourlioux et R. Touma [8, 62] semble indiquer un excellent accord avec ce présent travail, en ce qui concerne la dépendance de l'augmentation de vitesse de combustion par rapport à l'intensité de turbulence. Les deux modèles affichent une transition qualitativement semblable entre un régime lent (linéaire) et rapide (non-linéaire, quadratique).

La robustesse du mécanisme de transition par rapport à la variation dans le modèle aussi bien que la similitude avec l'observation expérimentale sont des indices encourageants à ce que le résultat principal de ce travail soit pertinent pour des applications plus pratiques. Tandis que beaucoup de simplifications ont été faites pour dériver un modèle favorable à l'analyse asymptotique systématique aussi bien qu'accessible à des calculs fiables, on peut espérer que les résultats s'étendent à une classe de configurations plus réalistes.

Un des objectifs de la paramétrisation est de fournir un modèle sous grille pour les simulations aux grandes échelles de flammes turbulentes prémélangées, d'où le besoin d'étendre cette paramétrisation à des écoulements turbulents aux petites échelles plus réalistes. Une étape dans cette direction est faite dans [11] où on étudie l'augmentation de vitesse de combustion pour des écoulements idéalisés aux petites échelles avec une structure spatiale plus complexe. Déjà l'étude qualitative faite dans le chapitre 4 démontre la faisabilité d'une telle extension. Ultimement, les études comme celles présentées ici peuvent être employées comme guides pour choisir des configurations génériques appropriées pour des simulations numériques directes pour les équations de Navier-Stokes réactives avec toute la complexité de la chimie. Ceci permettrait d'aborder explicitement des questions au delà de la portée du modèle idéalisé utilisé ici—les exemples pour de telles perspectives sont les effets sur la vitesse de combustion du nombre de Lewis quand il n'est pas égal

à un, de la complexité de la chimie, de la libération de chaleur/compressibilité, de l'écoulement turbulent réaliste avec un aspect aléatoire et plusieurs échelles temporelles et spatiales, etc. Les calculs avec de tels modèles réalistes sont extrêmement coûteux—on espère que l'intuition gagnée par l'étude du présent modèle idéalisé sera utile dans ce contexte.

### SCHÉMA NUMÉRIQUE POUR LE HAMILTONIEN EFFECTIF

Une méthode numérique a été présentée pour résoudre le problème-cellulaire aux valeurs propres non linéaire surgissant dans la théorie de l'homogénéisation des fronts de flammes turbulentes prémélangées [46]. Le schéma tient compte du calcul efficace du hamiltonien effectif (c-à-d. la valeur propre) et de la fonction propre (liée aux réalisations successives du front de la flamme plissée) avec une précision de second ordre. Le problème de valeur propre est résolu en utilisant la technique du pseudo-temps marchant à l'infini pour un système de lois de conservation pour le gradient de la fonction propre. Des arguments théoriques concernant l'importance de satisfaire la contrainte que ce vecteur-solution soit effectivement le gradient d'une fonction scalaire sont présentés. En exploitant la symétrie du problème, une formulation de grilles décalées est présentée pour satisfaire automatiquement cette contrainte dans un certain sens discret approprié si les données initiales la satisfont. Des expériences numériques confirment les prévisions théoriques en démontrant que (i) la propriété de préserver le gradient (*gradient-preserving*) est nécessaire pour garantir la convergence vers l'état stationnaire—voir la figure 3.3, (ii) un schéma d'intégration dans le temps ayant de bonnes propriétés “d'amortissement” (*damping*) pour converger rapidement vers l'état stationnaire à été élaboré en se basant sur l'étude de la stabilité linéaire des stencils-gelés (*frozen-stencils*)—voir la figure 3.4, (iii) le schéma réalise exactement la précision d'ordre deux, avec un gain significatif pour les faibles résolutions comparativement au schéma du premier ordre—voir les tableaux 3.1, 3.2 et 3.3.

L'idée de convertir une équation de Hamilton-Jacobi multi-dimensionnelle en un système de lois de conservation pour le gradient de la solution  $w$  à été également employée par Jin et Xin [35]. Leur schéma impose également dans une certaine mesure la condition du gradient dans une formulation qui a beaucoup d'avantages pour des cas généraux. Le schéma présenté ici est différent à plusieurs égards : il exploite la structure spécifique du hamiltonien pour imposer la contrainte du gradient exactement, pas dans un sens de relaxation comme dans [35], néanmoins, il se généralise facilement à une large classe d'équations de Hamilton-Jacobi ; les deux composantes de la solution discrète sont représentées sur des grilles décalées, par contre dans [35] elles sont définies sur une même grille, seulement  $w$  est décalée ; le schéma présenté ici est adapté pour le calcul efficace d'une solution à l'état stationnaire pour le hamiltonien effectif, une quantité qui implique seulement  $\mathbf{D}w$  et pas  $w$  elle-même. Le schéma présenté ici est employé avec succès tout au long de cette thèse pour l'étude systématique de la paramétrisation de l'augmentation de la vitesse de flammes turbulentes pour une variété d'écoulements aux petites échelles ainsi que pour générer une base de données utilisées en guise de modèle sous-grille pour faire un calcul LES.

## SIMULATION AUX GRANDES ÉCHELLES

Une approche hybride asymptotique-numérique de simulations aux grandes échelles des flammes turbulentes prémélangées est proposée et validée pour un cas test idéalisé. La stratégie consiste à utiliser la technique des iso-surfaces pour suivre le front de la flamme à grande échelles (i.e., le front de la flamme est représenté par le niveau zéro d'une certaine fonction de niveau qu'on suit dans le temps) en se basant sur la théorie de l'homogénéisation de Majda-Souganidis afin de modéliser d'une façon rigoureuse l'effet des petites échelles.

De nouvelles réponses à un certain nombre de questions pratiques importantes, relatives aux simulations aux grandes échelles de flammes prémélangées en général, sont apportées, sans ambiguïté, pour le cas test idéalisé :

- “l’extraction” du front à grande échelle d’une flamme prémélangée à partir de données DNS, qui a toujours été une question ouverte, est clarifiée, du moins pour le cas des réactions KPP, par l’introduction de l’enveloppe du champ de température du côté froid ;
- un des avantages de la définition du front à grande échelle comme étant l’enveloppe du côté froid est que la flamme ainsi définie n’est pas lisse mais contient des points de rebroussement, tels que constaté dans les expériences, qui sont typiques aux flammes turbulentes, tandis que l’approche classique qui consiste à “filtrer” les données DNS débouche sur un “front aux grandes échelles” qui est lisse.

La résolution précise des points de rebroussements présentés par le front à grande échelle, qui sont des singularités pour le gradient de la fonction de niveaux, est rendue possible par l’utilisation des méthodes numériques adéquates (schémas ENO d’ordre supérieur). La mise en application de la théorie mathématique abstraite a exigé la conception d’outils numériques spécifiques, en particulier pour construire *la base de données asymptotique des flammelettes (flamelet asymptotic library)*. Les résultats pour un cas pratique en quelque sorte en dehors des conditions strictes de l’applicabilité de la théorie démontrent la robustesse et la pertinence de la procédure utilisée. En outre, les prédictions asymptotiques s’avèrent très fiables dans le sens plus pratique de la moyenne des phases suggérant ainsi de nouvelles perspectives pour examiner de nouveau les bases de données des simulations numériques directes. Une première extension des résultats présentés ici peut être obtenue en considérant des écoulements aux petites échelles plus complexes (multi-échelles plutôt que deux échelles, aléatoires etc...) et à d’autres types de réactions chimiques.

La fonction de courant de Childress-Soward que nous avons utilisée dans ce travail est aussi utilisée dans [49] pour le problème cellulaire dans le cas du scalaire passif. Aussi, on retrouve dans [7] une analyse quasi-stationnaire pour l’étude



asymptotique du problème cellulaire dans le cas du scalaire passif semblable à celle que nous avons utilisée au chapitre 2.

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