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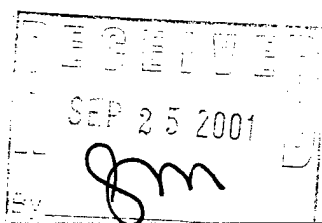
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Analytical validation of flamelet-based models
for non-premixed turbulent combustion
(Final progress report - DAAG 55-98-1-0220)
A.Bourlioux

15 September, 2001

1 Foreword

The aim of the project was to validate various implementations of the flamelet approach to turbulent combustion modeling in particular in the context of large eddy simulations of turbulent flames. A hybrid mathematical, numerical, asymptotics approach has been used by Bourlioux and her students, in collaboration with Majda, to systematically exploit Majda and co-workers theoretical results in an applied computational framework. The idealized models utilized in the project were amenable to rigorous asymptotic predictions regarding the effective behavior at large scales in terms of the flame overall burning rate. New numerical tools were designed to carry on the asymptotic procedures for relevant test-cases. A strong emphasis was placed on providing the physical intuition behind the various turbulent regimes identified by the theory. The asymptotic predictions were compared with ad-hoc modeling procedures to identify the pros and cons of those methods. Additionally, direct numerical simulations were carried on for the idealized test-cases to provide practitioner with some intuition regarding the relationship between the abstract asymptotic results and finite parameters realizations.

2 Statement of the problem studied

Flamelets are a key ingredient in the modeling of turbulent flames when the flame thickness is expected to be much smaller than all other significant length scales. Computationally, it would be very expensive to attempt to resolve that very small scale, so it is convenient to treat it as infinitely thin and account for its behavior through a laminar flamelet model. When the flame is indeed laminar, the computational application of the rigorous asymptotic concept is straightforward. However, many practical applications occur in the turbulent regime and there are important issues regarding the overall soundness and feasibility of extending laminar flamelets in that regime, as well as issues regarding the validation of such approach. The general theme of the research carried on in this project was to investigate systematically the relevance of rigorous asymptotic results regarding turbulent advection-diffusion-reaction equations for scalars to the issues relevant to people designing practical large eddy simulation codes for turbulent flames.

3 Summary of the most important results

Here is a summary of the specific scientific accomplishments:

In [1], a systematic investigation was carried on to assess the fundamental soundness of three flamelet models for a very wide range of Peclet and Damköhler numbers, including regimes which are well beyond the capacity of DNS. An important question was addressed regarding the impact of the approximation of the flamelet dissipation in finite-rate models meant to improve on the lower order equilibrium model. An explicit connection between the dissipation and the turbulent diffusion was identified that explained the surprisingly good performance of flamelet models outside their theoretical asymptotic range of validity: in regimes with relatively low Peclet (i.e. low turbulence intensity) and Damköhler (i.e. relatively thick flame) such as the ones direct numerical simulations are typically limited to, the crude models for dissipation have been reported to perform surprisingly well and this is indeed the case also for our idealized model. A straightforward explanation was provided in terms of the strong mixing at the scale of the flame thickness, consistent with the results in recent work by Majda and Souganidis. On the other hand, our idealized model allowed us to explore regimes for which DNS

are not affordable, in particular the proper highly turbulent flamelet regime to which diesel engines are expected to belong. In that regime, we show that the crude models for dissipation provide only a marginal asymptotic improvement over the low order model, mostly in the exceptional cases when the symmetry in the data leads to error cancellations in finite rate models. This result is to be contrasted with what is usually feasible with direct numerical simulations for the full set of reactive compressible Navier-Stokes equations, for which simulations are so expensive that very few test cases can be afforded with the consequence that it is impossible to extract asymptotic trends. An example of test-case is given in Figure 1.

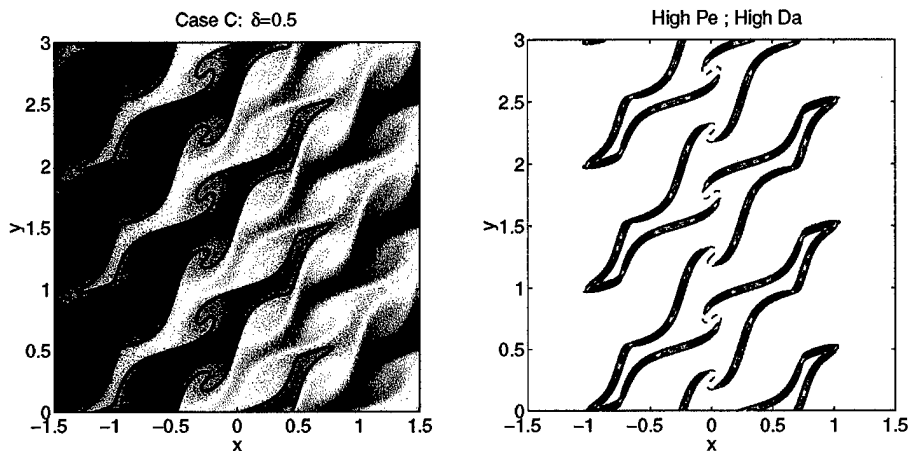


Figure 1: On the left: passive scalar; on the right, reaction rate (see [1])

In [2], the performance of a dynamic subgrid model for the turbulent burning speed of a flame was investigated for a series of idealized test cases where the flame front is wrinkled by a multiple-scale shear flow. The main result is the identification of a break-down of the self-similarity assumption at the core of the dynamic model which corresponds to a scaling transition for the flame speed. An improved model is proposed to explicitly account for this transition which improves significantly the performance of the dynamic model for some regimes.

In [3], a more systematic investigation of the scaling transition is performed. A combination of asymptotic analysis and high resolution numerical

simulations is used to provide for a definite explanation of the *bending* of the turbulent flame speed for the idealized problem. The result is interpreted in a general framework as a manifestation of the competition between the turbulent time scale of the deforming flow and the intrinsic response time of the flame. The results for the idealized model agree qualitatively with experimental observations so that one might hope that the new results might provide a new perspective on turbulent speed bending and Gibson scale cut-off for practical flames. Both issues are very important when formulating subgrid models for the large eddy simulations of turbulent flames. Figure 2 illustrates the bending between the two burning regimes.

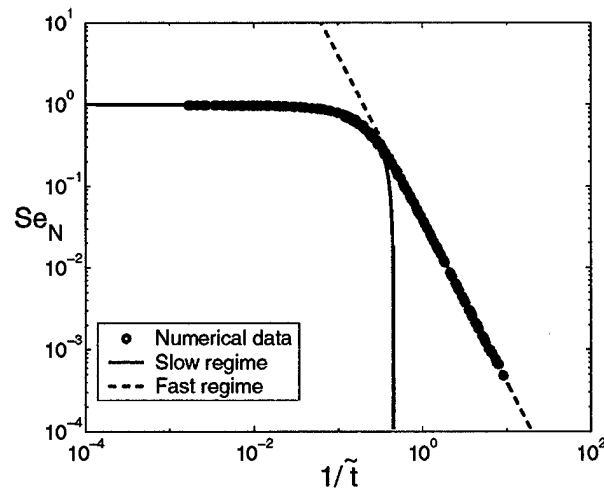


Figure 2: Fast and slow regimes for enhanced burning rate of a flame advected by a time-modulated shear (see [3])

In [4], in order to provide a bridge between important theoretical results by Majda and Souganidis (1994), a robust numerical method was designed by Bourlioux and her student Khouider so that the impact of the theory could be explored for more complex small scale flows (previously applied only to small scale shears as in [2], [3]). The computational problem to be solved is that of computing the effective Hamiltonian, as the eigenvalue of a nonlinear Hamilton-Jacobi partial differential equations. The novel method is based on the computation of the eigenfunction gradient.

In [6] (also, in a more detailed article to be submitted to JCP by Bourlioux and Khouider), this numerical tool is used to generate a subgrid library that is used as the key ingredient for the large eddy simulations of premixed flames with outstanding agreement with reference DNS results for highly distorted flames. Direct numerical simulations were carried on to show the asymptotic convergence of the thin wrinkled flame to the predicted asymptotic front. One important result is that, for KPP flames, the convergence path shows that the asymptotic front actually represents the cold-side envelop of the wrinkled front with finite thickness. This result settles an issue debated in the past by researchers dealing with large databases of resolved flames: how to interpret direct simulation results for resolved flames in terms of an unresolved flame fronts. Figure 3 shows the excellent convergence of direct numerical simulations to the predicted asymptotic front.

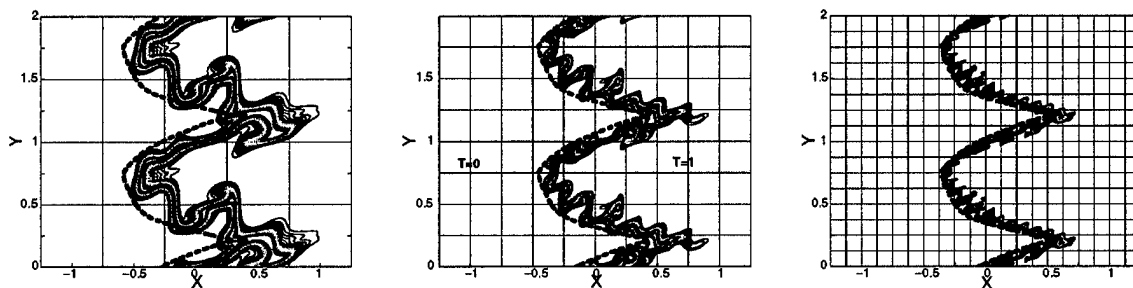


Figure 3: Direct numerical simulations to verify asymptotic convergence to the predicted front (see [6])

In [5], simple models were set-up with idealized mechanisms to generate intermittency that affects the passive scalar PDF. Since a good knowledge of the scalar PDF is at the heart of nonpremixed flamelet models, the ability to examine the response to intermittent behavior is a key topic for the combustion application. This work was carried on while A.Bourlioux was on sabbatical at Courant. The key results is the identification of an extremely simple mechanism to generate much wider than Gaussian PDF in a tracer; this is in direct contrast with the complex conditions that were previously thought to be needed for such a behavior. This is extremely interesting as far as analyzing unsteady flamelet models. Indeed, even though the work

has so far focussed exclusively on the behavior of the passive scalar under intermittent conditions - work is planned for the near future to pursue the intermittency study this time for the reactive scalar and to catalog the impact on the laminar flamelet model.

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Peer-reviewed conference proceedings

- [6] A.Bourlioux, B.Khouider, A.J.Majda, A mathematical prototype for the validation of large eddy simulations strategies for turbulent flames, selected for publication in the Proceedings of the 2001 IUTAM symposium on Turbulent mixing and combustion, Queens University.

Papers presented at meetings and seminars

- [7] Eight Siam International Conference on Numerical Combustion, March 2000, Amelia Island, Florida. *An idealized test-case for the validation of nonpremixed turbulent flamelet models.*
- [8] Eight Siam International Conference on Numerical Combustion, March 2000, Amelia Island, Florida. *Large eddy simulations of premixed flames with a rigorous asymptotic subgrid model.*
- [9] University of British Columbia, Mechanical engineering department seminar, 2000. *The mathematics of turbulent diffusion applied to burning issues in nonpremixed combustion.*
- [10] Georges Washington University, Mechanical engineering department seminar, 2000. *Large eddy simulations of turbulent flames with asymptotic subgrid flamelets .*
- [11] First Siam Computational Science and Engineering Conference, Washington DC, 2000. *Large eddy simulations of turbulent flames with asymptotic subgrid flamelets.*
- [12] Seminar at the Center of Environmental and Applied Fluid Mechanics, Johns Hopkins University, 2000. *The mathematics behind the computation of turbulent flames.*
- [13] Computations in Science Seminar, University of Chicago. *Asymptotic flamelets and large scale simulations of turbulent flames.*

4 Scientific personnel

1. B.Khouider, Ph.D. Université de Montréal expected summer 2001, now research associate at Courant under A.J.Majda's supervision. - partial support. Awarded a student travel fellowship to SIAM Numerical Combustion Conference, Amelia Island, March 2000.
2. O. Volkov, Ph.D. candidate, Université de Montréal January 2000-now, full support. Collaboration with L.Greengard to implement state-of-the-art multipole algorithm for adaptive turbulent flame solvers with application to unsteady flamelets.

3. Noah Cantin, research assistant, June-August 1999; received his Masters in Physics from Université de Montréal, 1999.
4. Xu Dong Zhang, research professional, partially supported by grant, 98-99.