Numerical Simulation of Two–Dimensional Laminar Flames with Special Finite Element Method

W. Wang

Lehrstuhl für Strömungsmechanik, Institut für Thermo- und Fluiddynamik Ruhr-Universität Bochum, D-44780, Bochum, Germany Email: wang@lstm.ruhr-uni-bochum.de

Abstract

Full governing equations for two-dimensional reactive flows are discretized and solved with finite element method (FEM). In order to fully explore FEM for reactive flow problems, some new concepts are introduced. Special quadrilateral elements and their corresponding interpolation functions are created to handle the interface between different refinement levels resulting from local refinement. A new strategy for constructing adaptive criterion based on the local discontinuity is developed for adaptive finite element method (AFEM). From modeling side, reduced mechanism and detailed transport models have been implemented to simulate the chemical reaction and the transport processes, respectively. To test the effectiveness of the newly introduced methods, two-dimensional as well as one-dimensional laminar flames have been calculated and satisfactory results have been obtained, which shows that the proposed concepts have great potential in solving convection-diffusion-reaction (CDR) systems.

Introduction

Numerical simulation of two-dimensional laminar flames has not yet reached to a stage at which the full governing equations can be tackled in a realistic and effective way as for one-dimensional cases. Combustion is multi-dimensional in most engineering applications. The solutions of one-dimensional equations involve not only geometric simplifications, but also unrealistic mass, momentum and energy transports caused by the presumption that all the transports act only in a single dimension. On the other hand, less simplifications in two-dimensional simulations indicate more realistic geometry as well as more truthful models for the transport phenomena. Therefore, numerical simulations for multi-dimensional laminar flames will reveal more insight and help greatly in understanding practical combustion processes, such as turbulent combustion.

In the present paper, attention is mainly focused on the numerical simulation of two-dimensional laminar flames. Compared to one-dimensional flames the extra dimension will certainly bring some new difficulties in both modeling and solution procedures. Furthermore, problems originally not so critical for one-dimensional cases emerge and become obvious obstacles for two-dimensional simulations, such as, the strategy for local refinement, size of the discretized system and algorithm's efficiency. Often used discretization methods for one-dimensional flames, e.g., finite difference method, if not completely unsuitable, show some obvious weakness. New avenues have to be considered and explored. Among many different approaches, the finite element method seems to possess many useful and promising features. In the present work, a new strategy is developed to handle local grid refinement for FEM. Specifically, a new set of special elements have been introduced to deal with the irregular nodes generated in the local refinement process. Furthermore, an effective criterion (based on local continuity) for local refinement has been developed for the two-dimensional combustion problems. In the next section, only the special elements will be briefly explained.

Special elements

Shown in Figs. 1 and 2 are the special quadrilateral elements for linear and quadratic cases, respectively. The new elements are especially designed for solving many practical combustion problems involving, e.g., moving flame fronts, complex boundaries or moving inter-phase boundaries.

The corresponding interpolation functions for the special bilinear elements in Fig.1 in natural coordinates ξ and η can be written as,

$$\Phi_1 = \frac{(1-\xi)(1-\eta)}{2(1-\xi_m)},$$



Figure 1: Normal (a) and special bilinear quadrilateral elements of first (b), second (c) and third (d) kind for a 1-irregular mesh. The numbers indicate local node number; solid circles indicate corner nodes and solid squares the extra nodes for the corresponding irregular corner nodes; circles mark the location of the irregular nodes.



Figure 2: Normal (a) and special quadratic quadrilateral elements of first (b), second (c) and third (d) kind.

$$\Phi_{2} = -\frac{1 + \xi_{m} - \eta_{m} + 3\xi_{m}\eta_{m} - (1 + \xi_{m} + 3\eta_{m} - \xi_{m}\eta_{m})\xi}{4(1 - \xi_{m})(1 + \eta_{m})} - \frac{(1 - 3\xi_{m} - \eta_{m} - \xi_{m}\eta_{m})\eta + (3 - \xi_{m} + \eta_{m} + \xi_{m}\eta_{m})\xi\eta}{4(1 - \xi_{m})(1 + \eta_{m})},$$

$$\Phi_{3} = \frac{(1 + \xi)(1 + \eta)}{2(1 + \eta_{m})},$$

$$\Phi_{4} = \frac{(1 - \xi)(1 + \eta)}{4},$$
(1)

where parameters ξ_m and η_m indicate the different kinds of bilinear elements used and their values also depend on the degree of irregularity of the elements. Geometrically, ξ_m and η_m are the characteristic distance between irregular node's replacement and the center of the special element. More details can be found in [1].

Similarly, the interpolation functions for the special quadratic elements in Fig.2 can be written as,

$$\Phi_{1} = -\frac{(1-\xi)(1-\eta)(1+\xi+\eta+\xi_{m}\eta)}{4(1+\xi_{m})},$$

$$\Phi_{2} = \frac{(1+\xi)(1-\eta)(1+\xi_{m}\eta_{m}-\xi-\eta_{m}\xi+\eta-\xi_{m}\eta)}{4(1-\xi_{m})(1+\eta_{m})},$$

$$\Phi_{3} = -\frac{(1+\xi)(1-\xi+\eta_{m}\xi-\eta)(1+\eta)}{4(1-\eta_{m})},$$

$$\Phi_{4} = \frac{(1-\xi)(1+\xi-\eta)(1+\eta)}{4},$$

$$\Phi_{5} = \frac{(1-\xi^{2})(1-\eta)}{2(1-\xi_{m}^{2})},$$

$$\Phi_{6} = \frac{(1+\xi)(1-\eta^{2})}{2(1-\eta_{m}^{2})},$$

$$\Phi_{7} = \frac{(1-\xi^{2})(1+\eta)}{2},$$

$$\Phi_{8} = \frac{(1-\xi)(1-\eta^{2})}{2}.$$
(2)

Using these new elements, the discretization has been performed on the governing equations with primitive variables, including full Navier-Stokes equations, species conservation equations and energy equation. Variable multi-component properties and transport models [2] have been employed. To satisfy Babuska–Brezzi condition, pressure is discretized on bilinear elements and other quantities on quadratic elements, respectively. Though the new concept has been successfully used to solve incompressible flow and simple combustion problems [1], in the current work, however, some further test cases have been carried with emphasis on CDR systems. Simple reaction models like one-global chemistry as well as more complex reduced mechanisms have been employed to treat the chemical source terms in species and energy equations.

Numerical Results

The full governing equations for reactive flows are highly nonlinear and stiff because of convection and chemical reaction terms. In the present work, the SIMPLE algorithm [3] has been implemented to handle the nonlinear system. Stream-line upwinding scheme [4] is also used to improve the accuracy and the stability. The numerical simulations in the current work are carried out with a research code FESTAL v.2.0 (Finite Element System for Turbulent And Laminar Phenomena) developed by the author.

Because of the space limitations, only a test case for a burner-stabilized flame is shown here. Though it is physically more of a one-dimensional case, it is however suitable to test the functionality of the two-dimensional code. Shown in Fig. 3 are the numerical results of a laminar premixed methane-air flame with a 4-step reduced mechanism [5] for the burner-stabilized flame. It can be seen that with the self-adaptive method (based on local discontinuity, i.e., the discontinuity of dependent variable at inter-element) the finer elements, including normal and special ones, are deployed in the reaction zone and the region with higher acceleration (near the burner mouth at x = 0). Finer elements are also



Figure 3: Non-dimensional velocity, non-dimensional temperature and mass-fractions of species calculated with a 4-step reduced mechanism for premixed flame of CH_4 -air in a burner-stabilized geometry. The mesh consists of 393 nodes in 116 elements.

located at down stream boundary because a finite-sized domain is employed to simplify the physical problem originally in a half infinity domain. The special elements perform effectively in catching the localized physical and chemical phenomena in the whole computational domain without using a great number of nodes and elements.

Final Remarks

The special elements perform quite satisfactorily for the full governing equations for the two-dimensional combustion problems which possess strong nonlinear and stiff features. Combined with the self-adaptive strategy based on local discontinuity, the localized physical and chemical occurrences in the domain of interest have been well reproduced in an effective manner.

The main focus of the current work is on the functionality and the effectiveness rather than the efficiency. Further research work will be needed to explore the potential from efficiency aspect.

References

- W. Wang, Special quadratic quadrilateral finite elements for local refinement with irregular nodes, Accepted by Comput. Meths. Appl. Mech. Engrg. (1999).
- [2] A. Ern and V. Giovangigli, Fast and accurate multicomponent transport property evaluation, J. Comput. Phys. (1995).
- [3] S. V. Patankar, Numerical Heat Transfer and Fluid Flow, McGraw-Hill International Book Company, 1981.
- [4] A. N. Brooks and T. J. R. Hughes, Stream-line upwind/Petrov-Galerkin formulation for convection dominated flow with particular emphasis on the incompressible Navier-Stokes equations, Comput. Meths. Appl. Mech. Engrg. 32 (1982) 199-259.
- [5] N. Peters, Numerical and asymptotic analysis of systematically reduced reaction schemes for hydrocarbon flames, in Lecture Notes in Physics, pages 90–109, Springer-Verlag, 1985.