

Self-Adaptive Numerical Simulations of Laminar Two-Dimensional Flames

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Abstract

In this paper we present a numerical model for two-dimensional reactive low-Mach-number gaseous flows based on the fundamental conservation equations in primitive variables. The chemical reaction is modeled by the standard flamesheet approximation, alternatively by detailed reaction mechanisms. The equations are discretized by a finite-element method on a triangulized grid using the well known Taylor-Hood elements. A fully operative local adaptive mesh-refinement procedure is used. The formulation is found to be of an effectiveness and robustness, which is comparable to that known from one-dimensional cases.

Introduction

For various reasons, the study of laminar flames is of particular interest. From a physical point of view, such flames are free of the complex physics-chemistry interactions inherent in turbulent flames and hence they lend themselves to isolated basic study of either fluid mechanics or chemistry. From a numerical point of view, laminar flames provide more stringent test cases than turbulent ones, a fact which is mainly due to the nonlinearity and stiffness of the chemical reaction terms. Whilst the numerical simulation of one-dimensional laminar flames – these comprise both truly one-dimensional flames¹ and two-dimensional flames that after a similarity transformation can be treated like one-dimensional ones² – can be viewed as being standard, the numerical simulation of, for instance, truly two-dimensional flames is not. Successful simulations of such flames exist but still substantial efforts are required, and being made, to develop truly efficient, generally robust and under a wide variety of conditions reliable solution algorithms.

Numerical Approach

In the present work, mixtures of ideal gases flowing at low Mach numbers are considered. Thus, the governing equations solved here are the conservation equations for overall mass, species mass, momentum and energy with the usual neglects resulting from the low Mach number assumption together with the usual auxiliary relationships such as thermal and caloric ideal-gas equations of state. The material laws are the commonly adopted laws for Newtonian fluids. In particular, Fick's law of diffusion in terms of a mole fraction gradient is used together with detailed models of the various required thermodynamic and molecular data. For details the Appendix of [1] should be consulted.

The governing equations are formulated for cartesian rectangular coordinates and, alternatively cylindrical coordinates. For the latter, axial symmetry is assumed. Thus, a broad class of two-dimensional geometries can be handled. The conservation equations are discretized using a finite-element method. To this end, the computational domain is triangularized. In the present paper, Taylor-Hood elements are chosen and hence the so-called BB-condition is satisfied. The formulation developed herein is such that numerical integration over individual triangles is used.

¹ For instance, freely propagating or burner-stabilized premixed flames.

² For instance, flames in counterflow geometries or tubular flames.

Specifically, here a 7-point Gaussian integration formula is applied hence ensuring exact integrals of polynomials of up to 5th order. An iterative approach to the solution of the governing equations is sought in which the convective terms in the momentum or Navier-Stokes equations are linearized. As a consequence, a linear system is to be solved repeatedly.

The simulations are carried out on unstructured grids with a fully operative local adaptive mesh-refinement procedure. The adaptive gridding is based on a ‘red-green colouring scheme’. The basic refinement of a triangle is ‘red’; ‘green’ refinement serves to remove possibly existing hanging nodes and – in this sense – to *close* a triangulation. On a given triangulation, once a final solution of the steady equations or a solution of the unsteady equations after a specified number of timesteps has been obtained, in a first step, this solution is examined according to certain criteria to establish where the mesh should be refined or could be coarsened. In a second step, all green refinements from a previous triangulation closure are reverted. In a third step, local red mesh refinement and coarsening is carried out and, in a fourth and last step, mesh closure is achieved by green refinement. If the new mesh differs from the old one, the solution is interpolated onto the new mesh on which it serves as initial data for further computations. The efficiency and robustness of the overall algorithm is confirmed by numerically simulating a variety of testcases. Two examples are presented in the following.

Selected Results

Methane-Air Diffusion Flame

Shown in Fig. 1 are selected results for an axisymmetric methan-air diffusion flame simulated using the standard flamesheet model.

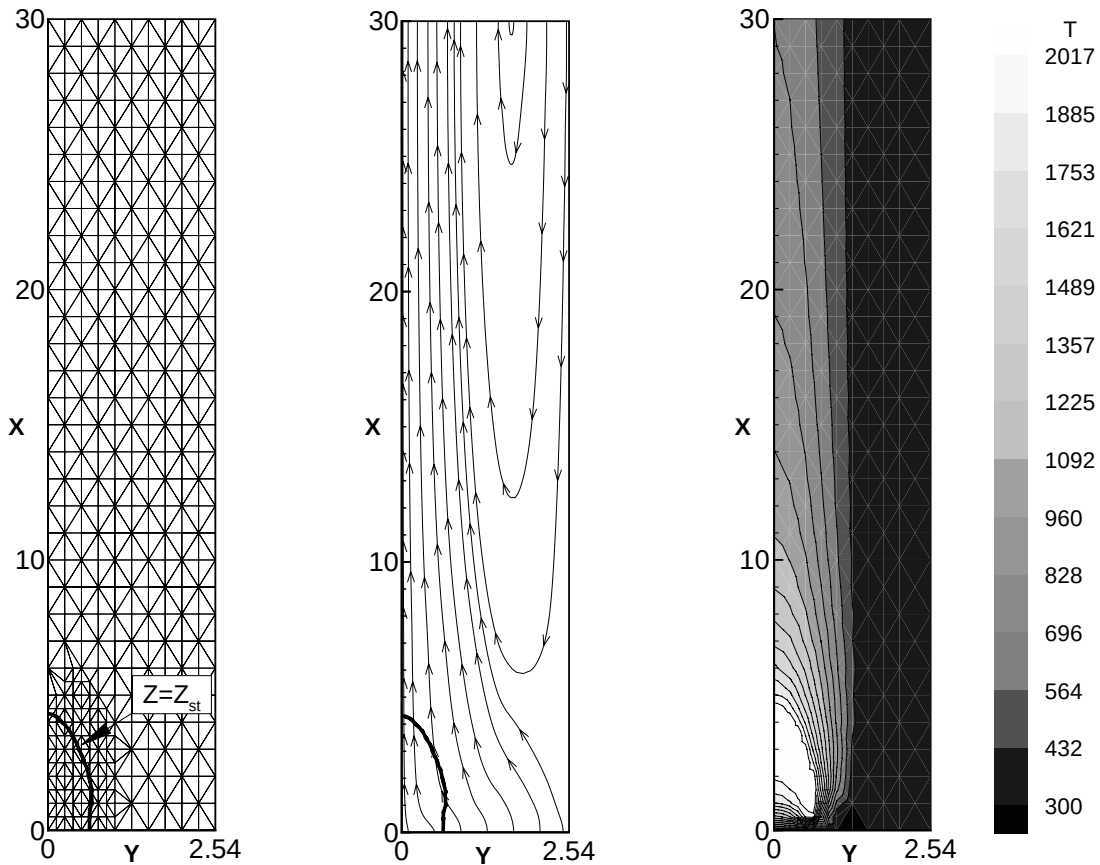


Figure 1: Results of diffusion flame computation using the flamesheet model, left: Computational mesh; middle: Streamline plot, right: Temperature contour plot, the coordinates, x and y , are in cm; the temperature T is in K.

Specifically, the results for the flame investigated originally experimentally and numerically by MITCHELL ET AL. [2] are shown. Thus, for details of stoichiometry, geometry, physical boundary conditions etc., ref. [2] should be consulted. The left picture in Fig. 1 shows the computational grid after adaptive refinement. The middle picture shows selected streamlines thereby providing information on the velocity field. The solid line in the left and middle picture represents the location of the flamesheet. The right picture shows a contour plot of the temperature.

Ozone Flame

As a further example, shown in Fig. 2, are the profiles of temperature and O -atoms for a burner-stabilized ozone flame.

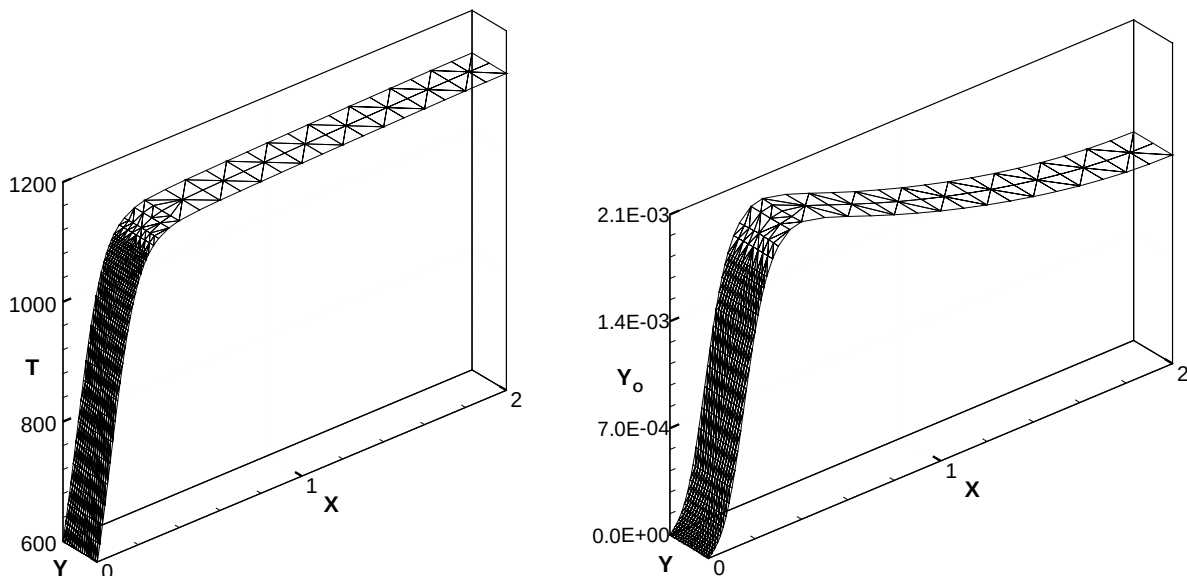


Figure 2: Profiles of temperature T and O -atoms for a burner-stabilized ozone flame; x is in mm, T in K.

The mesh, as obtained after three self-adaptive refinements, is superimposed on the profiles. The flame was simulated using a detailed mechanism consisting of 6 elementary reactions between the species O_3 , O_2 and O , see e.g. [3].

Conclusions

The numerical model presented here for reactive low-Mach-number gaseous flows is based on the fundamental conservation equations in primitive variables discretized by a finite-element method on a triangulized grid. In summary, the two-dimensional finite-element formulation presented here is found to be of an effectiveness (measured in terms of the required number of iterations) and robustness (measured in terms of the required quality of the initial guess), which is comparable to that known from one-dimensional combustion codes.

References

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- [3] B. Rogg, I. S. Wichmann. Approach to Asymptotic Analysis of the Ozone Decomposition Flame. *Combustion and Flame*, 62:271–293, 1995.