Multistability and Hysteresis in an edge-flame in the near-wake of a fuel injector using the Newton–Krylov method

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1.Abstract

In this work we enable the robust and free open source computational fluid dynamics OpenFOAM code, to successfully trace a complete solution branch, even past turning points. Here the so-called Generalized Minimal RESidual algorithm (GMRES) is implemented as a computational shell "wrapped" around OpenFOAM, in conjunction with a pseudo arc-length method for convergence on the unstable branch. In addition, to investigate the stability and the presence of static or dynamic bifurcations, the ten largest eigenvalues of the Jacobian matrix are calculated for each solution. The case study is the stabilization of an edge-flame in the near-wake of a fuel injector with a realistically computed flow.

2 Introduction

There has been recent interest in the dynamics and stability of edge-flames, primarily because of their relevance to the long studied problem of lifted diffusion flames [1,2]. Oscillating edge-flames have been observed in various experimental configurations consisting of initially non-premixed reactants, such as jet diffusion flames [3,4] and flame spread over liquid beds or candle flames in microgravity [5,6]. Kurdyumov and Matalon [7] have studied the dynamics of an edge-flame formed in the near wake of a mixing layer. However, unlike all earlier studies which were based on a constant-density model with a trivial flow, in [7] the velocity field near the tip of the separating plate is numerically computed based on the full Navier–Stokes equations.

Nonlinear analysis of critical conditions for the onset of the oscillating flames as well as their bifurcations is of fundamental importance for the understanding of the main physical and chemical mechanisms involved in diffusional–thermal instabilities. However, a complete characterization of the nonlinear dynamics of diffusion flames may only be obtained if bifurcations and stability of all regimes, static and periodic too, are systematically computed. The main numerical methods used for

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the analysis of regimes of dynamical systems are the parametric continuation algorithms. Basically, a parametric continuation algorithm consist in a predictor corrector strategy, the parameterization strategy and step-length control are important too in these algorithms to overcame the problems related to the singularity of Jacobi matrix and to efficiently run the code. Parametric continuation algorithms are usually easy to solve when the dynamical system is described by a small number of variables. For this purpose, such program packages as AUTO, CONTENT, and MATCONT are used. In these packages, the iterative Newton method for systems of nonlinear equations or its modifications are used as the main "solver". It is well known that the Jacobi matrix must be computed and a system of linear algebraic equations (SLAE) must be solved at each iteration of this method. In high-dimensional problems, finding the Jacobi matrix explicitly can be a computationally costly task. Moreover, the matrix sparseness, which is characteristic of high-dimensional problems, is not always efficiently taken into account. Therefore, the main obstacle for using the well-known bifurcation analysis and parametric continuation algorithms in high-dimensional problems such those involved is the difficulty of employing the Newton method and direct techniques of linear algebra. This is not a trivial task when the governing model equations is in the form of a system of partial differential equations, as it is for the models aiming at representing real flow configurations, that always include variable density combustion flows. One of the main difficulties comes from the computational effort required to compute the stable solutions in a parameter varying investigation. However this is not the only difficulty to face. A more fundamental issue regards the meaningfulness of the map of solutions determined with a simple brute force approach. Indeed, several other choices have to be made when such an approach is adopted, the first being the adoption of a proper parameter step size, often dictated by the need of making computational demands affordable. Actually, it is not possible to guarantee, apart from the accuracy of the detection of bifurcation points, the validity of the map, as, for instance, in the case of multiplicity of solutions, in which the jump from a solution branch to another can be determined by a not appropriate choice of the parameter step. To avoid such circumstances, a rigorous parametric continuation algorithm has to be adopted.

Recently, the so-called matrix-free iterative methods for solving systems of linear and nonlinear algebraic equations have become increasingly popular. In these methods, there is no need to compute and store a matrix; rather, only the result of multiplying this matrix by a vector is used; that is, a vector is computed. Jacobian-free Newton-Krylov (NK) methods represent one of the most promising approach in this contest, in particular NK method with the Generalized Minimal RESidual (GMRES) algorithm. The main drawback of NK-GMRES is the slow convergence of the GMRES algorithm. It is known that, usually, the convergence rate of GMRES considerably depends not only on the condition number of the SLAE's matrix but also on its whole spectrum (eigenvalues of the matrix). To overcome this difficulty, we take advantage of the approach based on the use of the results of the numerical integration of a system of ordinary differential equations (ODEs) on a short time interval. Using the integration results, we replace the original system of nonlinear algebraic equations by another system that has better (from the viewpoint of GMRES) spectral properties of the Jacobi matrix. In the case under examination, time integration acts as an efficient although unconventional preconditioning. In the present work, we study the NK-GMRES iteration as a computational "wrapper" around a legacy time-stepper. This wrapper enables the computation and continuation of fixed points of the time- map of the robust dynamical solver (i.e. steady states of the corresponding dynamical equations). It is useful, for purposes of discussion, to consider that the dynamical solver is available as an input-output black box (an executable) which cannot be modified. For the computations, we used the implementation nsoli.m of NK-GMRES developed for MATLAB (see [8] and references therein). For finding the leading eigenvalues of sparse matrices, we used the standard function eigs.m of the package MATLAB. In the present work, the GMRES algorithm is implemented as a computational shell "wrapped" around OpenFOAM, in conjunction with a pseudo arc-length method for convergence on the unstable branch. Such an algorithm is firstly validated for a simple case found in the literature. Then, it is applied to a problem describing an edge-flame in the near-wake of a fuel injector with a realistically computed flow. Preliminary results that address the need for a detailed bifurcation analysis will be presented.

2 Problem definition

The prototype problem adopted in this work is similar to the configuration already proposed by Kurdyumov and Matalon [7]. A semi-infinite plate separates two streams of fuel (pure methane) and oxidizer (air, represented by a mixture of oxygen and nitrogen in proportion of 0.23/0.77 by mass). Just before the edge, the plate is heated to provide a means of flame ignition. Aiming at representing accurately all the physical mechanisms involved, the plate has a finite thickness, and the flowing gas is a mixture of ideal gases. The main simplifications here adopted, to reduce the computational effort, are the assumption of a 2D symmetry, and the adoption of a one-step irreversible reaction for methane conversion:

$$CH_4 + 2O_2 \Rightarrow CO_2 + 2H_2O \qquad R_{CH_4} = A\exp(-T_a / T) Y_{CH_4}^a Y_{O_2}^b$$

The governing equations for the laminar reacting flow include the balance of mass, species, momentum and energy, written in the form:

$$\begin{aligned}
&\frac{\partial \rho}{\partial t} + \nabla\cdot\rho\mathbf{U} = 0 \\
&\frac{\partial}{\partial t}\rho Y_k + \nabla\cdot(\rho\mathbf{U}Y_k) = \nabla\cdot\left(\rho\alpha\nabla Y_k\right) + \rho R_k \qquad k = 1,\ldots,N_S - 1 \\
&\frac{\partial}{\partial t}\rho\mathbf{U} + \nabla\cdot(\rho\mathbf{U}\mathbf{U}) = -\nabla p + \nabla\cdot\sigma \\
&\frac{\partial}{\partial t}\rho h + \nabla\cdot(\rho\mathbf{U}h) = \frac{Dp}{Dt} + \nabla\cdot\left(\lambda\nabla T\right) + \sigma : \nabla\mathbf{U}
\end{aligned} \qquad (1)$$

being:

$$\sigma = 2\mu(T)\mathbf{S} - \frac{2}{3}\mu Tr(\mathbf{S})\mathbf{I} \qquad (2)$$

the deviator of the shear stress tensor and $\mathbf{S}$ the strain tensor, and with usual meaning for the main variables.

The extension of the domain is of particular importance as it has a great effect on the computed solution, as clearly discussed in [7]. We adopt dimensions comparable to those suggested in [7] if expressed adopting a similar non-dimensionalization. However, in the present case, all quantities are expressed in the dimensional form, as a choice of the parameters representing a real configuration is pursued. Domain geometry and dimensions are reported in Fig. 1.

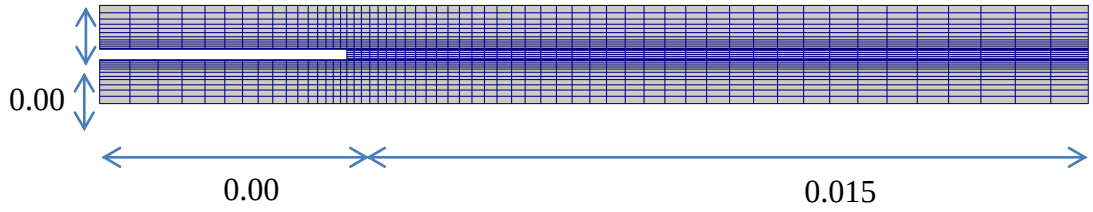

Figure 1. Computational domain and mesh (about 1500 cells). Dimensions are in m.

Inlet conditions are chosen to determine an almost stoichiometric feeding of fuel and oxidant, while the inlet temperature is fixed to ambient temperature for both streams, and the outlet pressure is fixed to ambient pressure.

4 Numerical Technique and Results

After discretizing in space, the governing equations (1) are reduced to a set of ordinary differential equations:

$$\frac{du}{dt} = f(u, p) \quad u \in \mathbb{R}^n, p \in \mathbb{R} \tag{2}$$

where the vector *u* represents the state variables at each node of the grid including the boundary nodes and *p* a scalar parameter. The main numerical methods used for the analysis of regimes of dynamical systems are the parametric continuation algorithms. They are used to find solutions to systems of nonlinear algebraic equations:

$$0 = f(u^*, p^*) \tag{3}$$

for various values of the "bifurcation" parameter *p*. Moreover, it is possible to define the stability and bifurcations of the detected regime by calculating the eigenvalues of the Jacobi matrix $J_f(u^*, p^*)$.

Our purpose is to replace (3) by another equation so as to considerably improve the convergence of NK-GMRES. Using the initial values u_0, a numerical method for (2) (a dynamic solver) finds the new values of the variables at a given time τ>0; the dynamical solver will be denoted by the integral operator $\Phi_\tau(u_0, p)$. Basically, the problem of finding the regime solutions (3) can be recast as follows:

$$\Psi(u, p) = u - \Phi_\tau(u, p) = 0 \tag{4}$$

Indeed, if a stationary solution u* is specified as the initial condition in the Cauchy problem for system (2), this solution does not change after the integration with time; therefore, $u^* = \Phi_T(u^*, p)$ is also a solution to (4).

In other words, we construct a computational structure that designs and combines several calls to an existing time-stepper, effectively turning it into a fixed point solver for the reformulated problem where Φ_τ is the result of the integration of the system (2) whit initial condition *u* and for a time τ. Moreover, eigenvalues λ_i of the Jacobian J_f and the eigenvalues μ_i of the Jacobian J_Ψ are related by the following equation:

$$\mu_i = 1 - \exp(-\lambda_i \tau) \tag{5}$$

Note that J_Ψ can be found using numerical differentiation when small perturbations of each component of the vector variables are given as the initial values. Therefore, the use of time steps enables one to find the eigenvalues λ of J_f for determining the stability of the stationary solutions u* also in the case when the function $f(u^*, p^*)$ is not known explicitly.

At a first glance, solving the original equations of form (2) seems to be a simpler problem from the computational point of view than the integration of the system of ODEs with respect to time and the solution of Eq. (3). However, it turns out that the situation drastically changes when high-dimensional problems are solved using NK-GMRES, where the spectra of the of the Jacobi matrices J_f and J_Ψ can be significantly different. In particular the eigenvalues of the reformulated problem can be clustered to 1 by an appropriate choice of the time horizon τ. Clustering the eigenvalues is known to be beneficial for the GRMES performance. Moreover, a practical advantage of this approach is that the time stepper can be considered as a black box or even an executable file. This procedure has been tested on the well-known Brusselator model (e.g.[9]) and all of the features of the bifurcation behavior reported in [9] are reproduced by the continuation algorithm above discussed.

Here we discuss preliminary results obtained by choosing the temperature of the plate surface as continuation parameter. In particular, this parameter has been step changed in the range [293 - 600]. Figure 2 reports the coexisting stable regimes as the temperature of the plate surface is changed. The stable regimes have been calculated by numerical integration of the dynamical system for a long time. Solutions for several values of this parameter have been computed, with increments of 10 K. Each

solution has been computed by restarting the simulation from the last time of the previous solution and covering a time span of 0.1 s, previously estimated as being long enough to reach steady state conditions. However, in some regions of the parameter space, specifically close to the ignition point, it has been necessary to reduce the step size, down to 2 K, to obtain convergence.
Then a new set of runs has been performed by reducing the plate temperature with steps of 10 K. The typical hysteresis of the extinction branch arises, making it impossible to actually obtain the extinction of the flame. At Tp = 380, a different behavior is detected, indicating the birth of a branch of oscillating solutions.

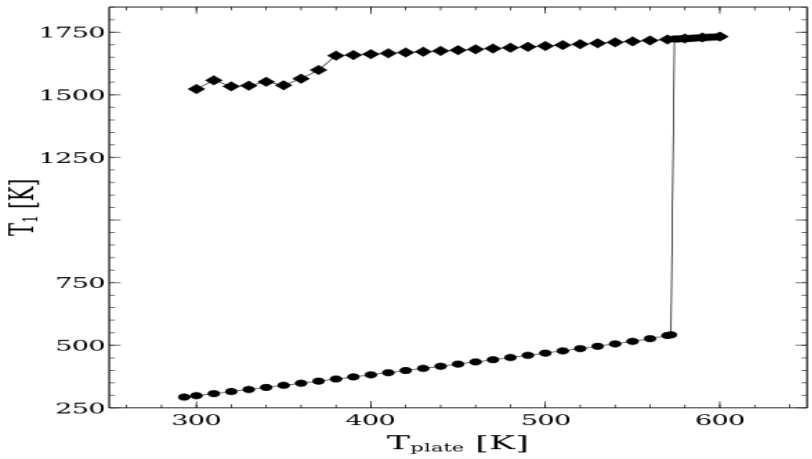

Figure 2. Typical hysteretic behavior representing the ignition and extinction of the system. The T1 temperature is reported as a function of the temperature of the plate surface.

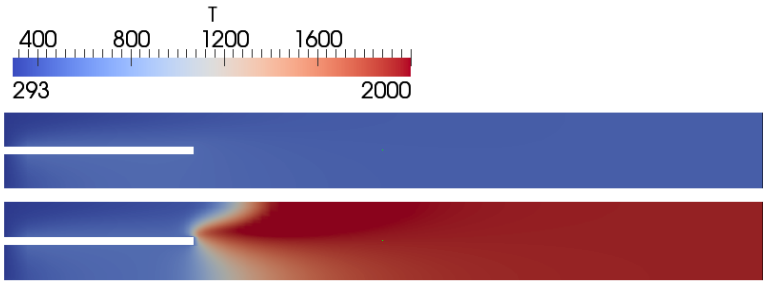

Figure 3. Temperature field in K at Tp = 550 K for the solutions along the ignition branch (top) and extinction branch (bottom).

In Figure 3 typical coexisting ignited and non-ignited regimes are represented. In particular the temperature field computed for Tp = 550 along the two branches of solutions are compared. In this case, the heating due to the contact of the gas stream with the hot plate is not enough to ensure the ignition of the mixture within the residence time the mixture spends in the domain, when all the mixture is cold. Preheating from the already burned mixture is strong enough to ensure a stable and steady condition of the flame. If the plate temperature is further reduced below 384 K, this mechanism is not sufficient to guarantee steady ignited conditions.

Figure 4 reports the comparison of the solution computed during the entire simulation in terms of the probe temperature T1, both along the extinction branch at Tp = 380, before the Hopf bifurcation, and Tp = 370, just inside the oscillating region of the parameter range, respectively. This comparison clearly illustrates that the two oscillating solutions at Tp=370 K, nominally corresponding to the same condition, look different and are strongly sensitive to the initial conditions.

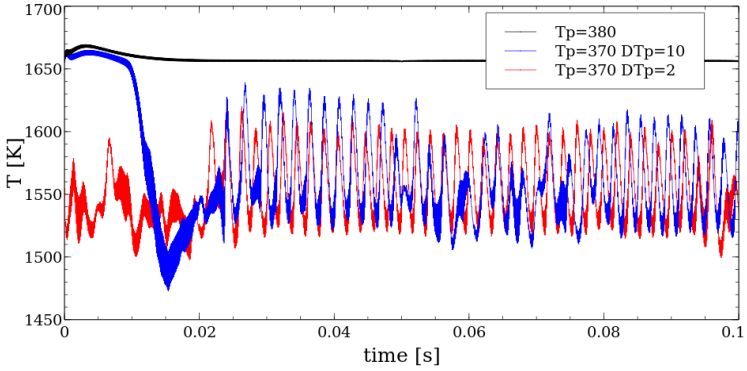

Figure 4. T1 temperatures vs time recorded during the computation of solution on the extinction branch at Tp=380 K, black line, and Tp=370 K, blue line with a single jump of 10 K from Tp=380 K, red line as the result of subsequent computations for Tp progressively reduced by 2 K jumps from 380 K.

5. Conclusions

We used the concept of time-stepper to analyze the dynamics of an edge-flame in the near-wake of a fuel injector with a realistically computed flow. More specifically, we were able to construct the full bifurcation diagrams including the branches of limit cycles choosing the temperature of the plate surface as bifurcation parameter. In particular, we systematically computed the stability and the bifurcation of regime solutions for different values of the bifurcation parameter. The main advantage of using the proposed approach over more conventional methods – used in most of the bifurcation analysis packages – is that the explicit calculation and storage of the system's Jacobian is not required: what is needed are matrix–vector multiplications which can be extracted by calling the time-stepper from appropriately perturbed initial conditions.

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