Structure and Evolution of the Stabilization Point of a Lifted Reacting Jet

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Introduction

In this work we study the stabilization point of a lifted, reacting jet of nitrogen diluted methane in co-flowing air. The jet flow is acoustically forced so as to organize the large scale vortical structures. The validation of the numerical results is possible through a concurrent experimental investigation of a similar planar jet. The use of an acoustically forced planar jet allows for significant savings by the restriction of the computation to two dimensions; the model is otherwise applicable in three dimensions.

We base our study on the following parameters, which are derived from the experimental setup: a jet width of 1.16 cm, a mean jet velocity of 0.8 m/s, and a coflow velocity of 0.1 m/s. The acoustical forcing is studied at frequencies of 7.5 MHz and 90 MHz, which have been established experimentally as being characteristic of two broad behavioral modes.

Numerics

The governing equations used in the numerical method are the Navier-Stokes equations enhanced with multiple species transport and reaction equations, including variable transport and thermodynamic properties [1]. Several reasonable assumptions are made for simplification, including a low Mach number approximation for an open domain [2], the ideal gas law, the simplification of binary diffusion to the dominant diffusion into nitrogen, and the neglect of radiation and the Soret/Dufour effects. The model allows for the inclusion of arbitrary chemistry, with N species and M reactions governed by Arrhenius rates. In this work, however, we will restrict ourselves to five species and the single step, irreversible, global reaction: $\text{CH}_4 + 2\text{O}_2 \Rightarrow \text{CO}_2 + \text{H}_2\text{O}$ (with passive $\text{N}_2$).

This global chemistry is sufficient to establish the characteristics of the flow and the flame structure. To study more detailed events such as extinction phenomena, a more detailed mechanism is required [3]. The main difficulty in including detailed chemistry stems from the stiffness of the reaction terms, which can result in the need for greatly reduced time step; however, recent progress has been made here [4].

In proceeding with a numerical solution of these equations, the first issue that we must address is the large range of relevant length scales, from large scale flow features, on the order of centimeters, to the fine scale flame structures, in the sub-millimeter range. Consequently, we have chosen to implement the scheme on an adaptive mesh structure that allows us to resolve the flame structure within a domain large enough to incorporate the major flow features. The ability to increase the domain size without computational penalty also reduces the chance of corruption from imposed boundary conditions, in particular from the two boundaries parallel to the jet axis, which we treat as slip walls.

The use of adaptive mesh refinement (AMR) makes it difficult, however, to employ a fully Eulerian low Mach number scheme, which would involve a Poisson solution for the pressure. Furthermore, the solution
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of the Poisson problem also becomes limiting on a parallel machine (and the use of a parallel machine is required to provide the resolution we seek). So, instead, we have chosen to implement a Lagrangian method for the momentum and continuity equations and to couple this to an Eulerian solution of the energy and species equations on the adaptive mesh.

The fluid motion is tracked using a traditional vortex element method [5]. Such schemes are widely used because of their natural adaptivity and their ability to generate accurate flow dynamics with a minimum of computational effort. For maximal efficiency, we compute the Biot-Savart interactions using the Fast Multipole Method (FMM) [6]. Viscous diffusion is conveniently handled by employing a random walk method based on constant (room temperature) viscosity and imposing a correction to account for the variable viscosity in the heated jet.

Velocity boundary conditions are applied through the use of a boundary element method, which allows the potential flow within the domain to be easily computed from mixed conditions on the boundary [7]. In our case, we impose a known total normal velocity on the inflow, zero total normal velocity on the side “slip” walls, and a normal outflow velocity with constant potential as required for continuity. We have also been able to translate the resultant boundary element strengths into multipole expansion for direct inclusion in the FMM velocity computations, thereby making the cost of the potential flow computation transparent.

The Eulerian scheme for the energy and species equations incorporates a second order Godunov method for the convective terms and an explicit, second order central difference method for the diffusive terms. These provide second order spatial accuracy throughout regions of uniform mesh size. Spatial and temporal interpolation is used to transition from coarse to fine mesh solutions [8]. The use of AMR largely restricts the choice of method for diffusion, however, and with the global chemical mechanism, we find our time step limited by the stability requirement for the explicit handling of diffusion. For detailed chemistry, the stiffness of the reaction term becomes the dominant stability limitation. The only restriction on the convective scheme is via the CFL number, which is generally satisfied long before the other stability requirements.

The coupling of the Lagrangian and Eulerian schemes requires, in one direction, that the velocity be computed on the adaptive grid using the Lagrangian elements and the FMM for efficiency. In the other direction, the adaptive mesh must provide for the generation of baroclinic vorticity (due to both flow acceleration and buoyancy), the temperature dependence of viscous diffusion, and the volume expansion due to heat release and transfer. This last, dilatational, effect is modeled through the use of discrete expansion sources, created at adaptive mesh cell centers. Because vorticity is being generated throughout the domain during every time step we must carefully manage the number of vortex elements. To some extent this can be done through traditional vorticity redistribution schemes [9, 10], but we have also had to develop methods to distribute created vorticity directly onto existing elements.

We also allow for a larger Lagrangian than Eulerian time step, so that relatively slow flow dynamics do not have to be computed at the higher rates imposed by the reaction. Within each global predictor-corrector Lagrangian time step, two AMR update passes are made, the first (predictor) pass being strictly first order and the second (corrector) being a second order pass composed of a sub-sequence of predictor-corrector steps. This coupling produces an overall second order temporal accuracy.

Results

We initialize the problem uniformly along the direction of the jet axis, with the velocity field given by the inflow jet velocity profile and the temperature and chemical profiles matched to a one dimensional Chemkin solution for an opposed jet diffusion flame. After initialization, we see a quick transition to a lifted jet mode, with the cold fuel and oxidizer streams mixing in the first centimeter downstream before igniting.
Without acoustical forcing, and after the initial settling, the location and character of the stabilization point remains steady and within the region of laminar flow near the jet exit. At this point we see a fully developed and clearly marked triple flame structure, with premixed flames extending well into both the fuel and oxidizer streams and with a diffusion flame trailing behind along the stoichiometric mixture contour. The triple flame structure can clearly be seen in the heat release profile, with each of the branches being sharply defined, and with the two partially premixed branches showing a much higher peak heat release than the diffusion branch (Figure 1a). All figures show a $2.0 \times 2.5 \text{cm}^2$ region of the computation, with the lower left corner being the center of the jet outlet; the computation domain itself is $40 \times 20 \text{cm}^2$.

It is not possible to discern the triple flame structure from the temperature profile, however, as can be seen in Figure 1c. This fact largely explains the lack of experimental identification of triple flames in lifted jets using Rayleigh temperature measurements.

Figure 1: Heat Release after 150 ms with various contours superposed:

(a) Mixture Fraction  (b) Vorticity  (c) Temperature

The acoustical forcing of the jet produces significant behavioral effects. First, the stabilization point is drawn inward (toward the jet center) and downward as the large vortex structure approaches (see Figure 2a). The stabilization point is then lifted further downstream and with the passage of the structure, and eventually settles back to its quiescent location. More extreme dynamics can be seen in the fuel side branch of the premixed flame. This branch is stretched far downstream in the wake of the vortex pair, even to the point that a local extinction occurs along its midsection (Figure 2b). A detached flame island then continues downstream until it burns out (Figure 2c).

Similar extinction events have been seen in the experimental investigation, with islands of detached flame drifting downstream on the fuel side of the main diffusion flame structure. Further comparisons to experimental data are in progress.

The future inclusion of detailed chemistry in these computations should allow for improved analysis of localized events such as the extinction seen here. Also of interest will be the numerical investigation of the effectiveness of traditional flame markers such as OH and CH in the identification of the triple flame structure.
Figure 2: Evolution of Stabilization Point (Heat Release and Vorticity):

(a) after 180 ms  
(b) after 194 ms  
(c) after 210 ms

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References


