Effects of Buoyancy and Forcing on Transitioning and Turbulent Lifted Flames

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Introduction

The objectives of this paper are two-fold. First, a numerical scheme for the simulation of a buoyant, reacting jet is presented with special attention given to boundary conditions. In the absence of coflow, a jet flame is particularly sensitive to boundary conditions enforced upon the computational domain. However, careful consideration of proper boundary conditions can minimize their effect upon the overall simulation.

Second, results of some preliminary simulations are presented over a range of Froude and Damköhler numbers. This range was chosen so as to produce lifted flames in both normal gravity and microgravity environments.

Numerical Method

A low Mach number approximation [1] is applied to the Navier-Stokes equations and the resulting system is solved numerically using a predictor-corrector method similar to that described by Najm et al. [2]. This predictor-corrector scheme handles large density ratios necessary to study buoyancy effects. A one-step, reversible, Arrhenius-type reaction is used to model the chemistry. Also, the numerical method is adapted for numerical solution on a variable spaced, staggered, cylindrical mesh, with a computational domain as shown in Figure 1. For more details about this numerical method, please refer to [3].

Boundary Conditions

Inlet

The inlet condition corresponds to a jet issuing from a small orifice in a wall. The velocity is specified at all points using a "top-hat" profile constructed from a tanh function as suggested by Michalke [4].

Lateral

As a jet flow develops, it entrains ambient fluid from its surroundings. In the absence of coflow, a closed lateral boundary condition encourages recirculation by preventing entrainment across the lateral boundary. Recirculation of heat and species can have a significant effect upon a reacting system. In order to allow entrainment across the lateral boundary, a modification of the traction-free boundary condition discussed by Boersma et al. [5] is

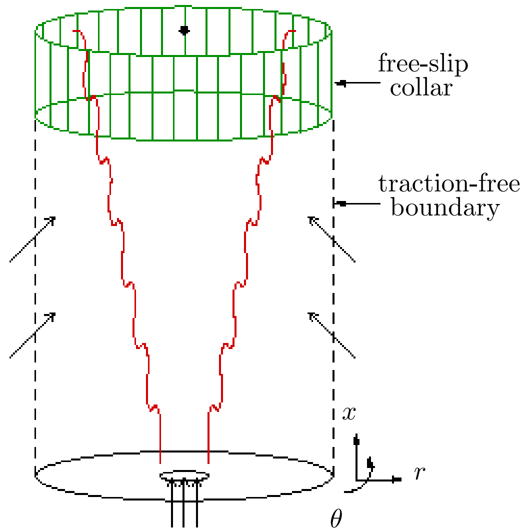

Figure 1. Diagram of the computational domain with a traction-free lateral boundary condition and a free-slip collar around the outlet.

employed. This condition specifies that

$$\boldsymbol{\tau} \cdot \hat{\boldsymbol{n}} = \mathbf{0}, \tag{1}$$

where $\hat{\boldsymbol{n}}$ is the unit outward normal vector at the lateral boundary. The left hand side of (1) is proportional to the force due to viscosity exerted on a small surface element of the boundary.

Outlet

At the outlet of the domain a convective boundary condition was employed of the form:

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + U_{max} \frac{\partial \rho \boldsymbol{u}}{\partial x} = 0 \tag{2}$$

The convective speed U_{max} was chosen to be the maximum measured velocity in the plane of the outlet [6]. This choice was found to be representative of the small central portion of the domain containing the jet with which the simulation is primarily concerned. Therefore, it exerts the least amount of unphysical influence upon the region of interest.

Mass Conservation

Mass conservation was preserved by correcting ρu_x at the outlet. The amount of excess mass flux j across the outlet was determined by a control volume analysis of the form:

$$j = \int \int \int \frac{\partial \rho}{\partial t} dV + \int \int \rho \boldsymbol{u} \cdot \boldsymbol{n} dS \tag{3}$$

The outlet mass flux was corrected by uniformly subtracting j/A from ρu_x, where A is the cross sectional area of the outlet.

Free-slip Collar

Physically, the outlet mass flux correction is equivalent to introducing a uniform pressure gradient in the x direction across the entire outlet, so that Eqn. (2) can be written:

$$\frac{\partial \rho \boldsymbol{u}}{\partial t} + U_{max}\frac{\partial \rho \boldsymbol{u}}{\partial x} + \frac{\partial p_c}{\partial x} = 0 \tag{4}$$

Note that the addition of a corrective pressure gradient is not consistent with the traction free boundary condition at the edge of the domain. It was found that the introduction of a free-slip "collar" around the outlet (see Figure 1) significantly improves numerical stability by decoupling the convective outflow and the lateral traction-free boundary conditions.

Results and Discussion

Sixteen axisymmetric simulations were performed with Damköhler numbers varying in increments of 100.0 from 600.0 to 900.0 and inverse Froude number varying in increments of 0.1 from 0.0 (non-buoyant) to 0.3 (highly buoyant). A mesh of 256 by 512 grid points was used with spatial resolution such that in the region of the flame $\Delta r \approx 0.03$ and $\Delta x \approx 0.04$. A time step of $\Delta t = 0.002$ was used. Initially, the flame was piloted by the introduction of a region of high temperature at the edge of the nozzle. Then, at non-dimensional time 16.0, the pilot was turned off, allowing the flame to lift.

Figure 2 shows contours of density of four resulting lifted flames taken at time $t = 192.0$ corresponding to the four different Froude numbers tested and a Damköhler number of 800.0. It is immediately apparent that in the case of $Fr = 3.33$, the flow is much more complicated than in the non-buoyant case. Although the flow is unforced at the inlet, the buoyant cases develop an instability in the convection layer at the outer edge of the flame. Note that in this region, the baroclinic torque has the same sign as the vorticity generation due to viscous shear. The initial source of this instability may be numerical noise associated with roundoff as well as rather high frequency, small fluctuations in pressure at the outflow boundary.

Although the non-buoyant momentum-dominated jet is expected to be unstable, it is evident from Figure 2 that the instability is not manifested. Although there is always numerical noise associated with computations performed on a discrete computer, this noise is very low level (on the order of 10^{-6} for single precision arithmetic) compared to the main flow, so that these instabilities are not triggered. However, the instabilities generated by buoyancy seem to be very sensitive to low level excitation. Bahadori et al. [7] note that even slightly buoyant flames, with Froude numbers in excess of 40.0, show significant differences from non-buoyant flames. This seems reasonable in light of the fact that in a laboratory setting low-level noise is usually several orders of magnitude greater than that introduced by a computer simulation. Also, the fact that the flow is constrained to be axisymmetric in the computer simulations may help stabilize the flow for moderate Froude numbers where unstable flow is observed experimentally. Buoyant instabilities are often highly three dimensional and this may play a key role in the transition to turbulence for lifted flames.

Conclusions

From numerical experiments, it was found that a convective outflow boundary condition with a choice of U_{max} for the convective wind speed, and a traction-free lateral boundary

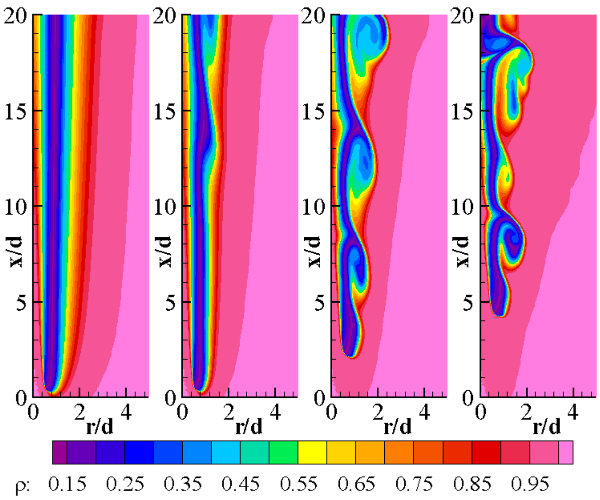

Figure 2. Density field of lifted flames at time 192 with Damköhler number 800. From left to right, the Froude number in each plot is ∞, 10.0, 5.0, and 3.33 respectively.

condition yielded the best performance for the jet flow. The addition of a free-slip collar around the outlet provided the decoupling necessary for these conditions to function together.

It was also observed that the effects of buoyancy tend to destabilize the jet flow. However, for moderate Froude numbers, the computer simulated flames appeared to be weakly unstable whereas corresponding flames in the laboratory exhibited stronger instabilities.

Acknowledgments

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References

1. P. A. McMurtry, Direct numerical simulations of a reacting mixing layer with chemical heat release, Ph.D. thesis, University of Washington (1987).
2. H. N. Najm, P. S. Wyckoff, O. M. Knio, A semi-implicit numerical scheme for reacting flow. i. stiff chemistry, *Journal of Computational Physics* **143** (1998) 381–402.
3. J. W. Nichols, J. J. Riley, Effects of buoyancy and forcing on transitioning and turbulent lifted flames, in: *Proceedings of the Third Joint Meeting of the U.S. Sections of the Combustion Institute*, The Combustion Institute, Chicago, 2003.
4. A. Michalke, Survey on jet instability theory, *Progress in Aerospace Sciences* **21** (1984) 159–199.
5. B. J. Boersma, G. Brethouwer, F. T. M. Nieuwstadt, A numerical investigation on the effect of the inflow conditions on the self-similar region of a round jet, *Physics of Fluids* **10** (4) (1998) 899–909.
6. C. D. Pierce, P. Moin, Progress-variable approach for large-eddy simulation of turbulent combustion, Tech. rep., Stanford University (2001).
7. U. Hegde, L. Zhou, M. Y. Bahadori, The transition to turbulence of microgravity gas jet diffusion flames, *Combustion Science and Technology* **102** (1994) 95–113.