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# Boundary Conditions for Low Mach Number Reacting Flows

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*Abstract:* In this paper we explore the specification of time dependent boundary conditions for the simulation of low Mach number reacting flows. A new approach is presented which is derived from the method of characteristics and an application of a Mach number based double expansion. Through the double expansion, it is possible to identify and seperate inertial events from acoustic events. By controlling the inertial components of the flow, non-reflecting conditions for a wide variety of problems may be specified. The accuracy of the method is demonstrated using a curved stagnating flame, in which the reaction zone crosses the boundary.

*Key–Words:* Boundary conditions, turbulence, characteristics

## 1 Introduction

The specification of accurate boundary conditions for subsonic turbulent reacting flows remains an open problem. There is a considerable literature available for the specification of time dependent boundary conditions for cold flows; the same cannot be said for reacting flows, or for flows where a strong divergence does not emerge as a result of compressible flow physics. Broadly speaking, there are two categories available for the selection of time dependent boundary conditions; *global* and *local* methods. Global methods have a stronger theoretical underpinning, but are not easy to implement in either turbulent or reacting flows; in these cases the linearization used to produce the pseudodifferential operators used at the boundary may not be appropriate [1]. Local methods have seen considerable development in recent years and, although they were originally designed for the linearized Euler system [2, 3, 4, 5, 6], extensions to other flows have also been discussed. These extensions are largely based around the **N**avier-**S**tokes **C**haracteristic **B**oundary **C**onditions (NSCBC) and the **L**ocal **O**ne **D**imensional **I**nviscid (LODI) approaches developed by Poinsot et al. [7], and have sought to incorporate viscous and reacting effects [8, 9, 10, 11]. The limitations of characteristics-based boundary conditions for the simulation of turbulent flows have been examined by Colonius et al [12]. In their work the authors introduce a base flow, which is supposed to be 'near' to the actual flow evolution in some sense. Such a reference flow need not satisfy the Navier-Stokes equations, but is rather an artifact designed to improve the accuracy of the linearization used to develop the boundary conditions. Even disregarding the difficulties of specifying an appropriate base flow in complex geometries, the results they present are not significantly improved by this practise.

A framework for the well posedness of Navier-Stokes problems has been proposed by Strikwerda [13]. Dutt has built on this and produced an energy estimate that serves as a tool for the specification of the required boundary conditions [14]. In the latter case, a well posed boundary condition is expressed in terms of an entropy estimate. It is not immediately obvious how the standard non-reflecting treatment fits into the latter's framework; furthermore the resulting boundary conditions specified by Dutt, although well posed, are not always expressed in terms of easily definable physics.

In earlier work, we described an approach that maintains the spirit of the proposal by Colonius et al. in that the flow is linearized around a base state. For cold low Mach number inviscid flows, the base state is assumed to be solenoidal [15]. Dilatation arising from thermal conduction in low Mach number flows has been examined in a more recent work [16], and this paper further extends the analysis by examining boundary conditions for problems with significant enthalpy transport and chemical reaction effects. The boundary condition is tested using a curved flame, with a reaction zone that crosses the computational boundary.

In section 2, we review the linearized equations used to derive the boundary conditions. In section 3, we examine the extension of the treatment to reacting flows. Section 4 reviews the problem used to test the boundary conditions, and discusses the results obtained. Conclusions and avenues for future work are presented in section 5

## 2 Governing equations

For a boundary whose normal points in the $\widetilde{x}_\alpha$ direction, the NSCBC [7] approach decomposes the $\alpha-$direction flux term of the Navier-Stokes equations into

$$\begin{aligned} \frac{\partial}{\partial t}(\mathbf{U}) + & \quad \mathbf{S}_\alpha^{-1}\mathbf{L}_\alpha \frac{\partial}{\partial \widetilde{x}_\alpha}(\mathbf{U}) \\ + & \quad \sum_{\substack{i=1 \\ i\neq\alpha}}^{n} \mathbf{P}^{-1}(\mathbf{F}_i)_{\mathbf{U}} \frac{\partial}{\partial \widetilde{x}_i}(\mathbf{U}) \\ = & \quad \mathbf{P}^{-1}\mathbf{C}, \end{aligned} \tag{1}$$

In equation 1, $\mathbf{L}_\alpha = \{L_1, L_2, \ldots, L_{N_s+4}\}^T$ is the vector of *amplitudes*, $\mathbf{U}$ is a vector of primitive variables, $\mathbf{P}$ is the transformation matrix relating primitive and conserved quantities, $\mathbf{F}_i$ is the flux vector, and $\mathbf{S}_\alpha$ is the matrix of left eigenvalues of $\mathbf{P}^{-1}(\mathbf{F}_\alpha)_{\mathbf{U}}$. For this study $\mathbf{U} = \{\rho, u, v, E, Y_1, ..., Y_{N_s}\}^T$. There is no summation over Greek indices. For two dimensional problems, the amplitude vector is associated with $N_s + 4$ eigenvalues: a left-going and a right-going 'acoustic' or non-linear amplitude [17] (propagating with speeds $u_i - a$ and $u_i + a$, respectively), and $N_s + 2$ degenerate eigenvectors with propagation speed $u_i$ representing convective transport. A non reflecting outflow is traditionally obtained by setting to zero all of those amplitudes that are incoming at the outflow [4].

We will assume in this paper that the domain is a two dimensional square, whose boundaries are aligned with the $x-$ and $y-$ axes. We will assume an inflow at $x = 0$ and and outflow at $x = X$. outflows will also be assumed at $y = 0$ and $y = Y$ where $X$ and $Y$ represent the size of the domain in appropriate physical units. If we introduce a low Mach number asymptotic expansion [18] into the definition of the amplitudes, coupled with a two scale decomposition to separate the *acoustic* length scales $\xi_i = Mx_i$ (where $M$ is the flow Mach number) from the *inertial* length scales $x_i$ [19], a new non-reflecting convective outflow boundary condition for equation set 1 at the $x = X$ boundary can be shown to be [15, 16]

$$L_1^x = L_4^x + (\gamma - 1) T \left( \frac{1}{a} \left( v\frac{\partial u}{\partial y} - u\frac{\partial u}{\partial x} \right) - \Delta^{(1)} \right), \tag{2}$$

while for the $y = 0$ boundary, we have

$$L_4^y = L_1^y - (\gamma - 1) T \left( \frac{1}{a} \left( u\frac{\partial v}{\partial x} - v\frac{\partial v}{\partial y} \right) + \Delta^{(1)} \right) \tag{3}$$

and the $y = Y$ boundary condition requires

$$L_1^y = L_4^y + (\gamma - 1) T \left( \frac{1}{a} \left( u\frac{\partial v}{\partial x} - v\frac{\partial v}{\partial y} \right) - \Delta^{(1)} \right) \tag{4}$$

In each of the preceding equations, $\Delta^{(1)}$ is an *acoustic divergence* and is defined as

$$\Delta^{(1)} = \frac{\partial u_i^{(0)}}{\partial \xi_i}.$$

The key challenge in the application of equations 2, 3 and 4 lies in the identification of the acoustic divergence.

## 3 Reacting flow treatment

We define $\Delta$ as the numerical divergence, calculated using some numerical scheme during the simulation. It is straightforward to show that for cold flows, $\Delta^{(1)} \equiv \Delta$. For reacting flows, there are effects that can produce a leading order divergence without compressibility effects; these are reaction, thermal conduction and mass diffusion. For these types of problem, $\Delta$ contains a non-negligible leading order contribution;

$$\Delta = \Delta^{(0)} + M\Delta^{(1)} + O\left(M^2\right), \tag{5}$$

where $\Delta^{(0)}$ is the *inertial divergence*—it is that component of the divergence that moves with the local entropy speed, and is defined as

$$\Delta^{(0)} = \frac{\partial u_i^{(0)}}{\partial x_i}.$$

An estimate for $\Delta^{(0)}$ for general flows is obtained from the pressure transport equation [20]. Using the same low Mach number/two scale decomposition as for the non-reacting case, it is straightforward to show that

$$\begin{aligned} \frac{\gamma p^{(0)}}{(\gamma - 1)}\Delta^{(0)} = & \nabla_x \cdot \left(\lambda \nabla_x T^{(0)}\right) \\ + & \sum_{\alpha=1}^{N_s} \left(\omega_\alpha^{(0)} + \nabla_x \cdot (\rho D_\alpha \nabla Y_\alpha)\right) \left(h_\alpha^{(0)} - \gamma e_\alpha^{(0)}\right) \\ + & \sum_{\alpha=1}^{N_s} \nabla_x \cdot \left(h_\alpha^{(0)} \rho D_\alpha \nabla_x Y_\alpha\right). \end{aligned} \tag{6}$$

$\nabla_x$ represents a spatial gradient with respect to the inertial length scales. The species mass fraction gradients are leading order effects alone; they can only affect the leading order density and temperature. This explains why they are not indexed in the same way as the other terms. $\Delta^{(0)} = 0$ is recovered in the limit of no chemical reaction and no gradients in composition or temperature. The one dimensional analogue of $\Delta^{(0)} = 0$ is the condition imposed to all orders by the standard non-reflecting boundary condition treatment [4], irrespective of the actual flow physics.

The final form of the boundary conditions are the same as those given by equations 2, 3 and 4, with the acoustic divergence estimated as (in dimensional quantities)

$$\frac{\gamma p}{(\gamma-1)}\Delta^{(1)} \simeq \frac{\gamma p}{(\gamma-1)}\Delta - \nabla\cdot(\lambda\nabla T) + \sum_{\alpha=1}^{N_s}\left(\omega_\alpha + \nabla\cdot(\rho D_\alpha \nabla Y_\alpha)\right)(h_\alpha - \gamma e_\alpha) + \sum_{\alpha=1}^{N_s}\nabla\cdot(h_\alpha \rho D_\alpha \nabla Y_\alpha).$$

Where we understand that the spatial gradients are now just those calculated numerically. This approach is similar to that derived in [15] for cold flows, and differs only in the expression for $\Delta^{(0)}$.

# 4 Test problem and results

We have tested the boundary conditions via the simulation of a curved and strained flame. This configuration is particularly challenging, as the flame front crosses the boundary at an angle and previous treatments have encountered some difficulties in accommodating the flame at the boundary without introducing large pressure transients [11]. The flame has a single step chemistry, with the simplified reaction mechanism

$$Reactants \rightarrow Products.$$

The thermochemical state of the fluid is characterized by a normalized product mass fraction, commonly referred to as a *reaction progress variable* and denoted $c$. The reaction rate is given by

$$\omega = \rho B^*(1-c)\exp\left(\frac{-\beta(1-c)}{1-\alpha(1-c)}\right),$$

where $B^* = 285 \times 10^3 s^{-1}$, the Zeldovitch number $\beta = 6$, and $\alpha = 0.8$ (corresponding to a heat release of 4). This leads to a product temperature of $1500K$. Molecular transport is handled by the joint assumptions of constant unit Lewis number and a constant Prandtl number $(= 0.71)$. The thermal conductivity is given by [21]

$$\lambda = 2.58 \times 10^5 c_p,$$

where the temperature dependence of $\lambda$ has been suppressed. $B^*$ has been set such that the resulting laminar flame speed is $0.6m/s$.

The initial conditions are estimated using potential flow theory. A point source is placed far to the right of the outflow, and a planar flow is assumed at $x = -\infty$. By controlling the strength and position of the source, flames with different curvatures and strain rates can be simulated. As the flow is not inviscid, both reaction and transport effects cause the solution to move rapidly away from the initial conditions via the production of a large transient pressure field. The transient leaves through the non-reflecting boundaries. Non-reflective convective outflows are specified on the spanwise boundaries. 'Fixed' conditions are specified on the $x-$boundaries, by which we understand that the *inertial* component of the velocity does not change on these boundaries—they are, however, still non-reflecting. The code used to test the new boundary conditions has been described in our earlier work. The accuracy and validity of the approach has been established using an asymptotic flame solution, and is reported elsewhere [22].

## 4.1 Viscous conditions

For this study, we have tried a number of viscous boundary conditions. Of the those tested, we found that the most successful in terms of long term stability were

$$\frac{\partial(\tau_{xx})}{\partial x} = 0 \text{ (on } x - \text{boundaries)}$$
$$\frac{\partial(\tau_{xy})}{\partial y} = 0 \text{ (on } y - \text{boundaries).}$$

It is interesting to examine the long term effects of viscous condition specification on flow solutions that are nominally stationary (such as the strained, curved flame studied in this paper). We have found that if the normal stresses are set to zero in both directions, then there is a long term wind up in the flow velocities at the corner of the domain; this has been traced back to the effective vorticity transport equation implicitly solved during the simulation. By choosing an inconsistent set of viscous conditions conditions for the momentum equations, it appears that the boundary conditions act as a vorticity sourceterm in the domain corners. Similar problems have been seen for reacting flows, where an over specification of viscous conditions at the boundary can lead to ill behaved solutions [11]. For the case described here, the sourceterm produced by incompatible viscous conditions is only $O\left(M^2\right)$, and the simulation can proceed for a long integration time before a problem emerges. The vorticity wind-up does not produce a spurious pressure field; increments in the pressure field driven by the vorticity sourceterm are propagated out of the domain by the acoustic wave treatment discussed in this paper. Future work will seek to remedy the spurious vorticity production, while simultaneously meeting the generalized energy estimates of Dutt [14] required for very long term stability.

### 4.2 Results

A square domain of side approximately 1mm is used, with 128 grid points used in each spatial direction. The flame structure is deliberately over-resolved in order to ensure that any spurious waves produced are a result of the boundary conditions and not under-resolution of the flame structure. Figure 1 shows the velocity vectors associated with the curved flame front. We observe that the flame crosses the boundary with no apparent ill effects. The curvature appears to produce a lensing effect which, in turn, will increase the curvature of the flame over time in the absence of other influences. The lensing is also responsible for the entrainment behaviour of the spanwise boundaries—these act as part inflow and part outflow. The boundary conditions appear well able to handle this behaviour.

The pressure field associated with the solution is given in figure 2. The flow is accelerated by the pressure gradient imposed through the streamwise boundary conditions until it reaches the reaction zone, whereupon the gradient flattens due to the heat release. We note that the pressure field exhibits none of the spurious effects associated with other characteristics based approaches, and that the dynamic pressure range (about $5N/m^2$) is consistent with that estimated from the velocity field using

$$\Delta p \sim \frac{1}{2}\Delta\left(\rho\mathbf{u}\cdot\mathbf{u}\right).$$

A solution cannot be obtained for this configuration using the LODI/NSCBC approach of Poinsot et al. [7].

No asymptotic solutions for the curved flame configuration are available for benchmarking. Nevertheless, we may compare the curved flame structure to an analytic one dimensional solution [23], and assess whether the differences between the two are consistent with the effects driven by the local flow field. Figure 3 compares the progress variable profile of both flame structures along the centre line of the domain. The first curve is that obtained from the numerical solution, and contains transverse strain components as well as curvature. The second curve is the asymptotic solution. The flame in the curved, strained case is thinner than the one dimensional solution. This can be explained by comparing the normal strain rate ($= \partial u/\partial x$) encountered by the flame along the centre line of the solution. In figure 4, the curved flame is associated with a double peaked positive normal strain rate, the maximum magnitude of which is significantly less than that associated with the one dimensional flame profile. In the unstrained case, the higher normal strain rate acts to stretch the flame, and so produce the observed thicker flame profile.

## 5 Conclusions

In this paper, we have presented a method designed to prescribe time dependent boundary conditions. The new method is quite general, and can be applied to multidimensional flows both with and without chemical reaction. The scheme is based on a linearization of the solution about an appropriately defined base flow. This base flow is solenoidal in cold, low Mach number flows, but is non-zero in the presence of reaction and transport effects. The resulting formulation allows non-reflecting boundary conditions for a wide class of flows to be applied. The behaviour of the new approach shows a significant improvement over other methods.

The method is based on the calculation of the numerical divergence, and on the separation of inertial and acoustic effects. Consequently, the approach relies heavily on the numerical discretization schemes employed in the simulation. Future work will examine more thoroughly the interplay between the numerical schemes and the boundary conditions, in particular examining the treatment of corners (which often have to contend with doubly poor numerical approximations). Additionally, more analysis will be undertaken to verify that the proposed boundary conditions are stable, using the energy estimates of Dutt [14]; the current simulations have shown themselves to be stable over very long simulation times (of the order of tens of thousands of time steps), but additional theoretical work is still required to prove very long term stability.

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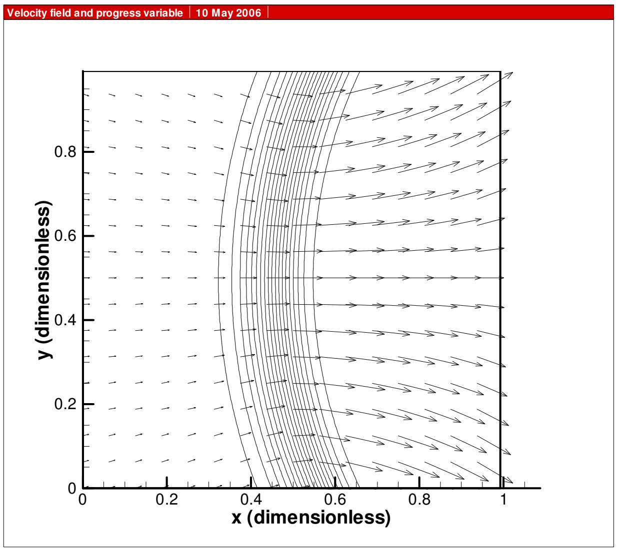


Figure 1: Velocity field associated with curved reaction front.

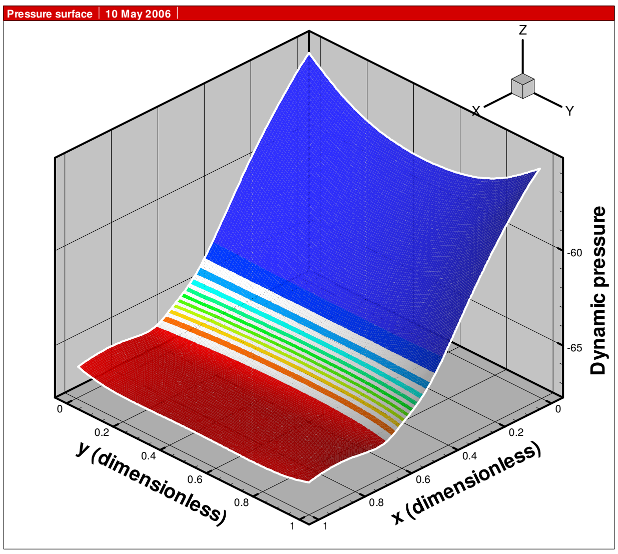


Figure 2: Pressure surface coloured by progress variable. Contours striped to clarify flame structure.

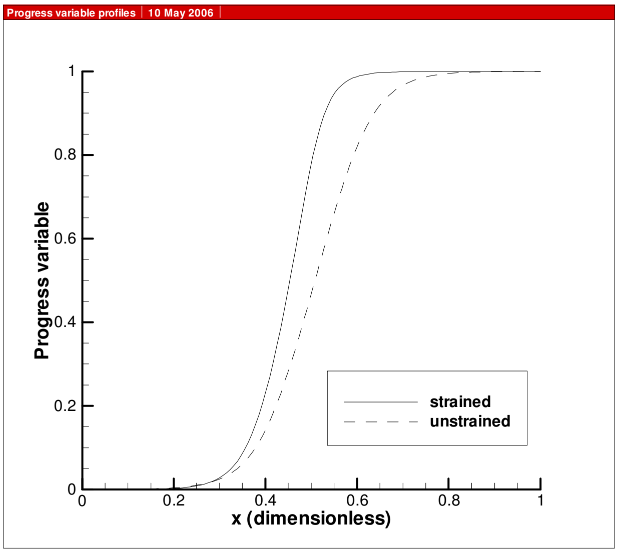


Figure 3: Comparison of progress variable profiles in cases with and without transverse strain

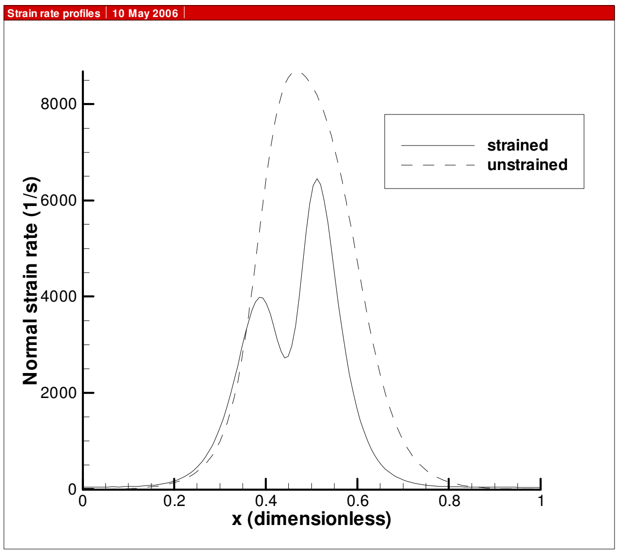


Figure 4: Comparison of normal strain rates for one dimensional flame structure and curved flame structure.