Paper # 070LT-0278 **Topic: Laminar & Turbulent Flames**

8th US National Combustion Meeting
Organized by the Western States Section of the Combustion Institute
and hosted by the University of Utah
May 19-22, 2013.

An adjoint approach to understanding perturbation of flames

Kalen Braman[1] *Todd Oliver*[2] *Venkat Raman*[1]

[1]*Department of Aerospace Engineering and Engineering Mechanics,*
The University of Texas at Austin, Austin, TX 78712, USA

[2]*Institute for Computational Engineering and Sciences,*
The University of Texas at Austin, Austin, TX 78712, USA

Adjoints have been applied to the calculation of the sensitivity of a laminar hydrogen flame to changes in the upstream field variables. These changes are applied through the use of source term additions to the governing equations. Sensitivity to the variation of the source terms typically would require the repeated solution of the laminar flame. With the use of adjoints, only an additional adjoint solution is required to compute the sensitivity of the desired quantitiy of interest to changes in those variables. Here, the effects of changes to the content of several species in the flow on the NOx content of a downstream region are computed. Results show that the NOx levels are sensitive to H_2 and O_2 in the region flanking the fuel jet near the inlet and in the flame itself. Additionally, the NOx levels are sensitive to radicals in the flow flanking the region of high-temperature combustion products.

1 Introduction

Design and control of reliable combustion devices requires planning for every possible hazard. For example, in the case of gas turbine combustors, blow out of the flame may happen in extreme operating conditions. When such a difficulty occurs, an ignition source must be placed back into the flowfield of the combustor in order to reinitiate the flame. While this reignition may occur given a powerful ignition source in many locations within the combustor, it can occur faster and more efficiently in certain regions of the combustor. Those regions can be determined by knowledge of the sensitivity of reignition to the placement of an ignition source. This concept can be abstracted to a general idea. One can define key quantities, such as temperature profile at exit or the average NOx concetration as the primary targets of the simulation, and call them quantities of interest (QoIs). In this context, knowledge of the sensitivity of QoIs to changes of the combustor's conditions can lead to improved design and control.

Generally, the sensitivity of QoIs to parameters can be computed using one of two methods: forward sensitivity equations or adjoint equations. The relative advantage of the method depends on the nature of the simulations. Any combustion simulation will involve a host of model parameters (e.g., Arrhenius rate coefficients). Similarly, depending on the flow configuration, a number of QoIs may be necessary. The forward sensitivity method of solution is best suited to situations which involve small numbers of parameters and multiple QoIs since each parameter adds an additional partial differential equation to be solved. An alternative method for sensitivity determination uses the adjoint method. This method is well suited to applications that involve few QoIs and many parameters since each QoI, not each parameter, adds additional equations to be solved.

Adjoint methods have been used in several aerospace-related applications including aerodynamic shape optimization, flow control, and acoustic noise reduction. Optimization of airfoil and aerodynamic shapes has been the focus of many studies [1–6]. These applications used adjoint methods to optimize shape parameters and improve certain aspects of performance, such as drag. Airfoil optimization has been carried out both using continuous adjoint derivations, in which the adjoint equations are derived and then discretized, and using discrete adjoint equations, in which the adjoint equations are derived from the already-discretized governing equations [7]. In the realm of flow control, adjoints have been used to reduce drag over bodies and in channels [8, 9]. Further applications of adjoints have aimed at the reduction of acoustic production [10, 11] in unsteady Direct Numerical Simulation (DNS) and Large Eddy Simulation (LES). Adjoint methods have also been used in the realm of chemical kinetics as it relates to atmospheric pollution. Sensitivity of output variables to kinetics parameters has been derived and implemented for the adjoint method alongside the direct decoupled method [12], and subsequently been applied to air pollution models [13, 14].

Here, the continuous adjoint equations are derived for steady incompressible variable density laminar combustion. The adjoints are then used to calculate the sensitivity of a laminar flame to changes in the upstream field variables. Any number of changes may affect the chosen QoIs in the combustor. Here, we consider the situation where small changes to local scalar values could be introduced. In a practical configuration, this could be the result of a spark ignition source placed in the flow. Typically, the flow would need to be solved repetitively with the perturbed values in order to determine the effects of local scalar changes on QoIs in the flame. With the use of adjoints, no additional flow solve is necessary for each scalar value perturbation. Only an additional solution of the adjoint equations for each specified QoI is required in order to give the sensitivity of that QoI to the perturbations. In this way the effect of changes to the state of the flow within the combustor have been determined for NOx concentrations.

2 Computational Methodology

Computation of the sensitivity of the QoIs to perturbations of upstream properties is desired. The determination of the sensitivities requires the steady state solution of the primal problem, which is the laminar reacting flow, and the subsequent solution of the dual problem, which is the set of adjoint equations. From these solutions the sensitivity of important quantities in the flame can be calculated. The following three sections detail the primal problem, the dual problem, and the calculation of the sensitivity of a QoI to perturbations.

2.1 Primal Problem

The primal problem consists of steady-state laminar incompressible variable density reacting flow. Reactions are handled with a multistep kinetics approach for laminar reactions. As a result, a reacting scalar for each chemical species will be carried in the flow.

The primal problem is governed by the incompressible variable density Navier-Stokes (NS), reactive scalar, and enthalpy equations which can be written in the following form:

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u_i}{\partial x_i} = 0$$

$$\frac{\partial \rho u_j}{\partial t} + \frac{\partial \rho u_i u_j}{\partial x_i} + \frac{\partial p}{\partial x_i}\delta_{ij} - \frac{\partial}{\partial x_i}\left(\mu \frac{\partial u_j}{\partial x_i}\right) = 0$$

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial \rho u_i Y_k}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\rho D_k \frac{\partial Y_k}{\partial x_i}\right) = \rho S_k$$

$$\frac{\partial \rho h_s}{\partial t} + \frac{\partial \rho u_i h_s}{\partial x_i} - \frac{\partial}{\partial x_i}\left(\rho \alpha \frac{\partial h_s}{\partial x_i}\right) = \rho S_{hs}$$

where u_i is the velocity, p is the pressure, Y_k is the mass fraction for species k, D_k is the diffusivity for species k, S_k is the source term for species k, h_s is the sensible enthalpy, α is the thermal diffusivity, and S_{hs} is the chemical source term for enthalpy. Since a steady state solution is desired, the primal problem is evolved in time until the flame solution reaches steady state.

When solving the above equations in practical applications, often the Poisson equation for pressure is solved in place of continuity. The Poisson equation can be written in the following manner:

$$\frac{\partial^2 p}{\partial x_i \partial x_i} + \rho \frac{\partial}{\partial x_j}\left[\frac{\partial u_i u_j}{\partial x_i}\right] = 0.$$

In this application to a two-dimensional flame, boundary conditions must be set on the four boundaries of the rectangular domain. The four boundaries are an inflow boundary, an outflow boundary, and two open lateral boundaries. The inflow boundary includes a core fuel flow as well as a coflow. The boundary conditions for that inflow are set as a specified value (Dirichlet condition) for u, v, and Y_k, while the boundary condition for pressure is set as a zero-gradient condition. The lateral boundaries involve two types of boundary condition. Zero-gradient boundary conditions are set for u, v, and Y_k, and a Dirichlet condition is used for pressure. The outflow boundary uses a non-reflective open condition. This outflow involves zero-gradient boundary conditions for all variables save pressure, which is set as a Dirichlet condition.

2.2 Dual Problem

The dual problem involves the solution of the adjoint equtions for a specific QoI. Starting with the defined QoI, the adjoint equations can be derived through the use of Lagrange multipliers. This derivation is detailed in Appendix A. The result of this derivation is the following set of adjoint equations corresponding to incompressible steady state reacting flow:

$$2u\frac{\partial \varphi_u}{\partial x} + v\frac{\partial \varphi_v}{\partial x} + Y_k\frac{\partial \varphi_{Y_k}}{\partial x} + h_s\frac{\partial \varphi_{hs}}{\partial x} + v\frac{\partial \varphi_u}{\partial y} + \frac{\partial}{\partial x_j}\left(\nu \frac{\partial \varphi_u}{\partial x_j}\right) = -\frac{\partial Q}{\partial \rho u}$$

$$u\frac{\partial \varphi_v}{\partial x} + u\frac{\varphi_u}{\partial y} + 2v\frac{\partial \varphi_v}{\partial y} + Y_k\frac{\partial \varphi_{Y_k}}{\partial y} + h_s\frac{\partial \varphi_{hs}}{\partial y} + \frac{\partial}{\partial x_j}\left(\nu \frac{\partial \varphi_v}{\partial x_j}\right) = -\frac{\partial Q}{\partial \rho v}$$

$$\frac{\partial \varphi_u}{\partial x} + \frac{\partial \varphi_v}{\partial y} + \frac{\partial}{\partial x_j}\bigg(- \frac{\partial \varphi_p}{\partial x_j}\bigg) = -\frac{\partial Q}{\partial p}$$

$$u\frac{\partial \varphi_{Y_k}}{\partial x} + v\frac{\partial \varphi_{Y_k}}{\partial y} + \frac{\partial}{\partial x_j}\bigg(D_k\frac{\partial \varphi_{Yk}}{\partial x_j}\bigg) = -\bigg(\frac{\partial \rho S_l}{\partial \rho Y_k}\varphi_{Yl} + \frac{\partial \rho S_{hs}}{\partial \rho Y_k}\varphi_{hs}\bigg) - \frac{\partial Q}{\partial \rho Y_k}$$

$$u\frac{\partial \varphi_{hs}}{\partial x} + v\frac{\partial \varphi_{hs}}{\partial y} + \frac{\partial}{\partial x_j}\bigg(\alpha\frac{\partial \varphi_{hs}}{\partial x_j}\bigg) - \frac{\partial \nu}{\partial \rho h_s}\bigg(\frac{\partial \rho u}{\partial x_i}\frac{\partial \varphi_u}{\partial x_i} + \frac{\partial \rho v}{\partial x_i}\frac{\partial \varphi_v}{\partial x_i}\bigg)$$
$$+\frac{\partial D_k}{\partial \rho h_s}\frac{\partial \rho Y_k}{\partial x_i}\frac{\partial \varphi_{Yk}}{\partial x_i} + \frac{\partial \alpha}{\partial \rho h_s}\frac{\partial \rho h_s}{\partial x_i}\frac{\partial \varphi_{hs}}{\partial x_i} = -\bigg(\frac{\partial \rho S_k}{\partial \rho h_s}\varphi_{Yk} + \frac{\partial \rho S_{hs}}{\partial \rho h_s}\varphi_{hs}\bigg) - \frac{\partial Q}{\partial \rho h_s}$$

In the above adjoint equations, φ refers to the adjoint variables with the subscript denoting the corresponding primal variable and Q refers to the chosen QoI.

2.3 Sensitivity to perturbations

A QoI Q can be selected which is impacted through the governing equations by flowfield properties. Perturbations to the properties can be effected by adding an additional term to the governing equations which acts as a source. For example if the QoI could be affected by OH radicals in the flow, then a source for OH can be introduced upstream of the flame. The added source term can be treated as a parameter in the governing equations. Considering the species mass fraction equation for species k, an additional source term can be introduced which will be labeled ϕ_k, as written in the following equation:

$$\frac{\partial \rho u_i Y_k}{\partial x_i} - \frac{\partial}{\partial x_j}\bigg[\rho D_k \frac{\partial Y_k}{\partial x_j}\bigg] = \rho S_k + \phi_k. \tag{1}$$

The adjoint solution permits calculation of sensitivities of a QoI to changes in the governing equations such as addition of the above source term. In general the sensitivity of a QoI Q to a source parameter ϕ is written as

$$\frac{dQ(\boldsymbol{U}(\boldsymbol{\phi}))}{d\boldsymbol{\phi}} = \frac{\partial Q}{\partial \boldsymbol{\phi}} + \frac{\partial Q}{\partial \boldsymbol{U}}\frac{\partial \boldsymbol{U}}{\partial \boldsymbol{\phi}}.$$

In the cases where Q has no explicit dependence on $\boldsymbol{\phi}$, $\frac{\partial Q}{\partial \boldsymbol{\phi}} = 0$, and therefore

$$\frac{dQ(\boldsymbol{U}(\boldsymbol{\phi}))}{d\boldsymbol{\phi}} = \frac{\partial Q}{\partial \boldsymbol{U}}\frac{\partial \boldsymbol{U}}{\partial \boldsymbol{\phi}}. \tag{2}$$

The full set of governing equations can be written in discrete residual form as the following

$$\boldsymbol{R}(\boldsymbol{U},\boldsymbol{\phi}) = \frac{\partial \boldsymbol{F}_i(\boldsymbol{U})}{\partial x_i} - \frac{\partial \boldsymbol{G}_i(\boldsymbol{U})}{\partial x_i} - \rho \boldsymbol{S}(\boldsymbol{U}) - \boldsymbol{\phi} = \boldsymbol{0}, \tag{3}$$

for which $\boldsymbol{U}$ is the vector of independent variables, $\boldsymbol{F}_i$ is the flux term vector in the ith direction, $\boldsymbol{G}$ is the viscous term vector in the ith direction, $\boldsymbol{S}$ is the source term vector, and $\boldsymbol{\phi}$ is the parameterized source term vector, each term with values at each discrete location.

Next, considering the discrete version of the adjoint derivation as follows,

$$\frac{\partial Q}{\partial \boldsymbol{U}}\delta \boldsymbol{U} - \boldsymbol{\varphi}^T \frac{\partial \boldsymbol{R}}{\partial \boldsymbol{U}}\delta \boldsymbol{U} = 0,$$

the adjoint variable can be written in the form

$$\boldsymbol{\varphi}^T = \frac{\partial Q}{\partial \boldsymbol{U}} \left(\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{U}} \right)^{-1}.$$

With the governing equations in the form of (3), the following relation is derived,

$$\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{U}} \frac{\partial \boldsymbol{U}}{\partial \boldsymbol{\phi}} + \frac{\partial \boldsymbol{R}}{\partial \boldsymbol{\phi}} = 0,$$

which then leads to

$$\frac{\partial \boldsymbol{U}}{\partial \boldsymbol{\phi}} = - \left(\frac{\partial \boldsymbol{R}}{\partial \boldsymbol{U}} \right)^{-1} \frac{\partial \boldsymbol{R}}{\partial \boldsymbol{\phi}}.$$

Combining the above relations with (2) leads to the following expression for the sensitivity

$$\frac{dQ}{d\boldsymbol{\phi}} = -\boldsymbol{\varphi}^T \frac{\partial \boldsymbol{R}}{\partial \boldsymbol{\phi}}, \tag{4}$$

where the adjoint variable vector $\boldsymbol{\varphi}$ is substituted from the adjoint PDE solution.

The solution to the governing equations (3) can proceed with the parameterized source term set to zero; however, the sensitivity to that source term nonetheless can be calculated.

Considering only a single source term ϕ_k, (4) reduces to

$$\frac{dQ}{d\phi_k} = -\boldsymbol{\varphi}^T \frac{\partial \boldsymbol{R}}{\partial \phi_k},$$

where $\frac{\partial \boldsymbol{R}}{\partial \phi_k}$ is non-zero only for the Y_k equation. Thus, the sensitivity equation simplifies to

$$\frac{dQ}{d\phi_k} = \sum_{i^*} \varphi_k, \tag{5}$$

where i^* refers to those discrete locations in the domain to which the ϕ_k source term has been applied.

3 Results

A laminar hydrogen diffusion flame simulation and its corresponding adjoint solution have been developed to demonstrate the capabilities of the adjoint method. The flame includes a jet of pure hydrogen with a coflow of air. Figure 1 shows a schematic of the domain of the simulation with the inlet sections labeled. Table 1 lists the inlet flow properties. For this application a detailed kinetics model for hydrogen with NOx formation [15] has been used. This model includes 32 species and 172 reactions. The next two sections will include first a brief description of the flame simulation results and second a description of the sensitivity results calculated using the adjoint solution.

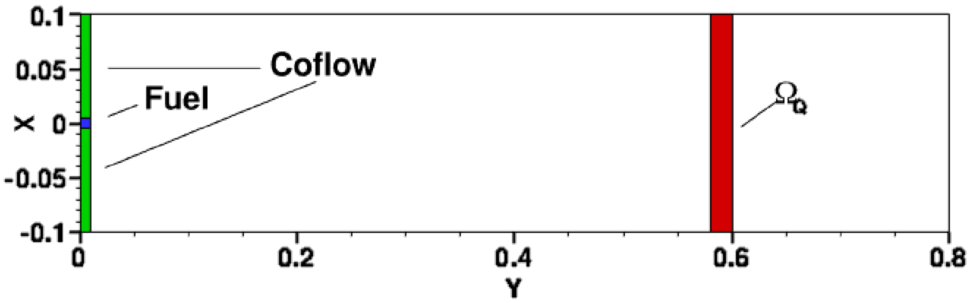


Figure 1: Simulation domain

Table 1: Inlet flow properties

Property \Stream	Fuel stream	Coflow stream
Temperature (K)	293.0	293.0
Y_{H_2}	1.0	0.0
Y_{O_2}	0.0	0.232
Y_{N_2}	0.0	0.768
U (m/s)	0.05	0.25

3.1 Laminar flame simulation results

Figure 2 displays the temperature field from the solution of the primal problem. The peak flame temperature reaches 2214K along the centerline at 0.099m downstream of the inlet. The NOx mass fraction fields are plotted in Fig. 3. Nitric oxide peaks in the region just downstream of peak temperature. Although its peak value decreases as the flow cools downstream, NO remains in the flow. Nitrogen dioxide peaks in the downstream area of the flow at the edge of the hot combustion products. Here, the NO formed in the higher temperature regions combines with the cool coflow and reacts to form NO_2.

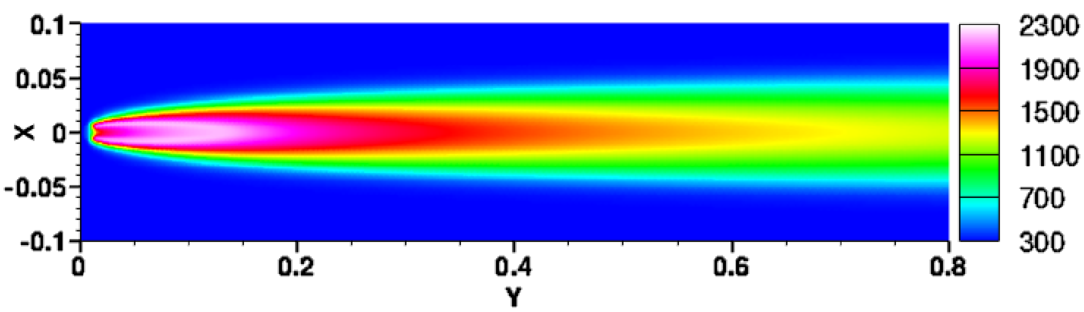
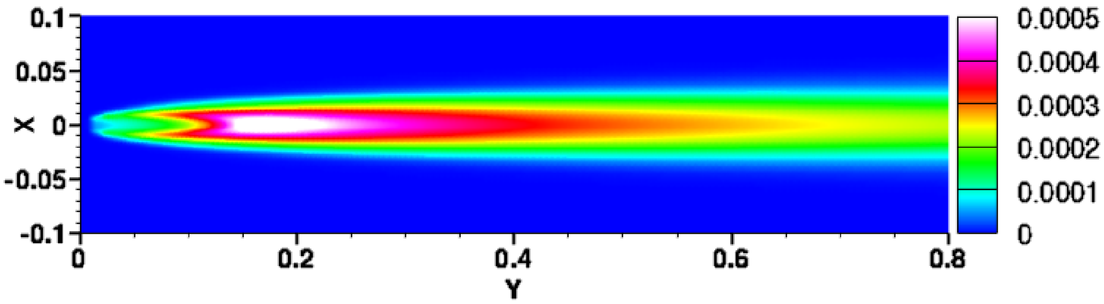
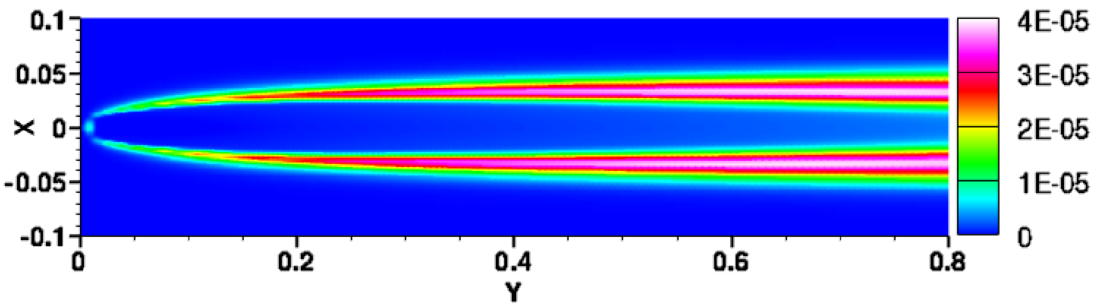


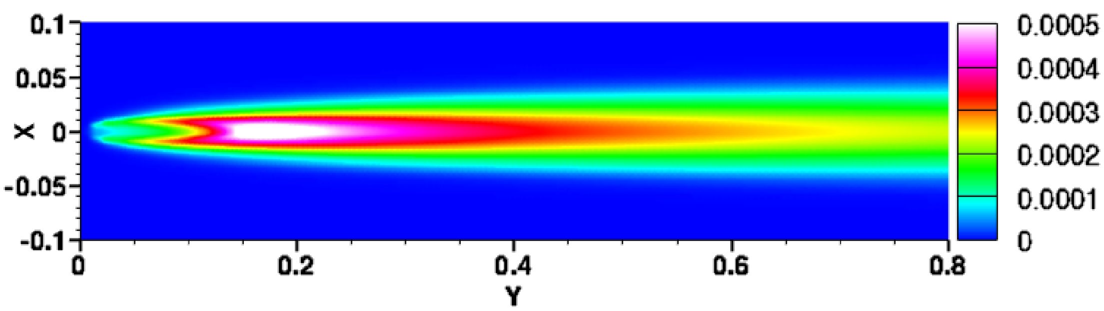
Figure 2: Temperature (K)



(a) Y_{NO}



(b) Y_{NO_2}



(c) Y_{NOx}

Figure 3: NOx fields

3.2 Laminar flame sensitivity results

Although control of ignition can be a goal of adjoint-based sensitivity methods, control of pollutant emissions from combustion devices also is desired. The study of the sensitivity of pollutants to the state of the flow inside the combustor is a step towards that control. Combustion pollution includes such chemicals as unburned hydrocarbons, carbon monoxide, carbon dioxide, and NOx. NOx for instance contributes to the formation of acid rain and smog. Determination and minimization of the level of pollutant output is a driving factor in the development of simulation techniques used in the combustor design cycle. Here the sensitivity of NOx levels in a laminar flame are considered.

For this reason, NOx concentration is used as the QoI for the analyses below. The QoI thus can be written in the following manner:

$$Q = \int_{\Omega_Q} \rho(Y_{\mathrm{NO}} + Y_{\mathrm{NO_2}}), \tag{6}$$

where Ω_Q refers to the region over which the NOx has been calculated. Figure 1 shows Ω_Q, the rectangular region downstream of the flame in which the NOx has been calculated. The region occupies the full width of the domain and extends from 0.58m to 0.6m.

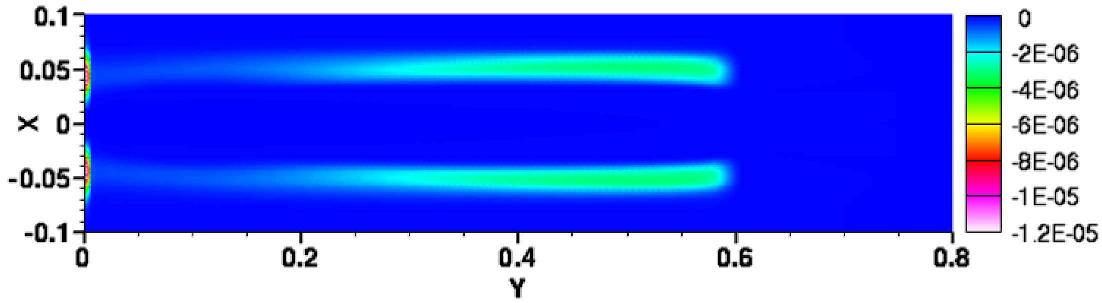
From (5) values for the sensitivity of NOx concentrations can be calculated for source additions to different variables. The source additions can be applied anywhere within the domain. Since the sensitivity value is a summation of the adjoint solution over the source-applied region, plots of the adjoint variables themselves depict where the source additions most affect the QoI.

Figure 4 shows the adjoint variable solutions for Y_{OH}, Y_{O}, and Y_{N}. The adjoint solutions for OH and O indicate regions near the inlet 0.04m to either side of the core fuel jet where the NOx concentration is sensitive for which increases to Y_{OH} and Y_O decrease the QoI. These regions continue downstream with a lower magnitude flanking either side of the high temperature combustion products. Additionally for O, two small rgions of sensitivity exist immediately to either side of the fuel jet in which increases to Y_O will increase NOx. For Y_N a region of high sensitivity exists near the inlet for the majority of the span of the domain. Continuing downstream, a lower sensitivity region encompasses the region of higher temperature combustion products.

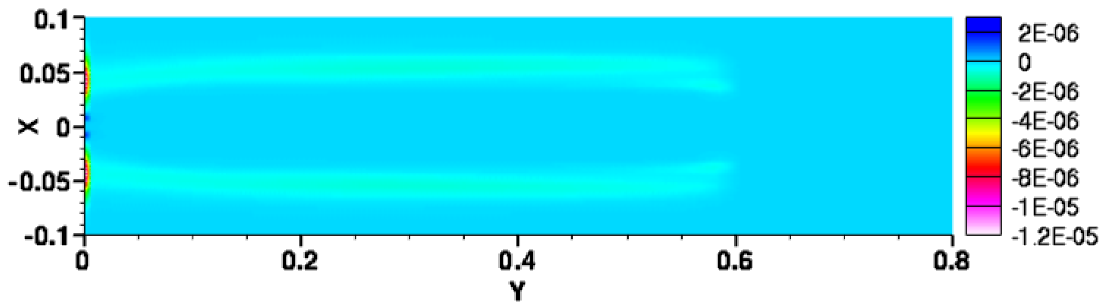
The adjoint variable solutions for $Y_{\mathrm{H_2}}$, $Y_{\mathrm{O_2}}$, and $Y_{\mathrm{N_2}}$ are displayed in Fig. 5. The regions near the inlet of the domain and just outside of the fuel jet show the greatest sensitivity. Additionally, the region of the flame itself shows sensitivity to H_2, O_2, and N_2. For H_2 increases to its source decrease the QoI, while for O_2 and N_2 increases increase the QoI.

4 Conclusions

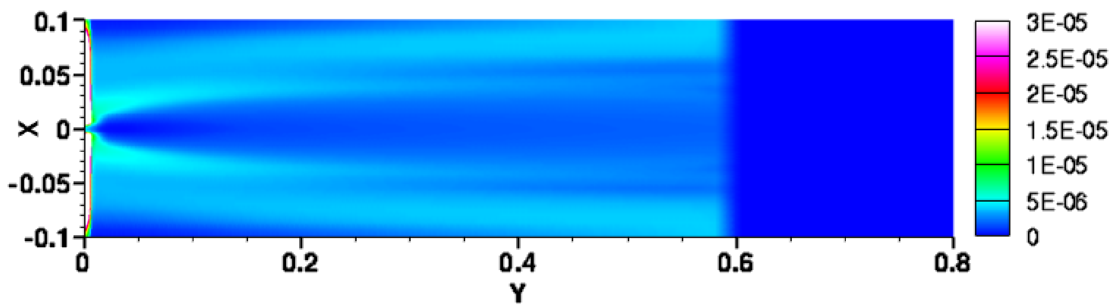
The adjoint equations have been derived for steady state laminar variable density reacting flow. A laminar hydrogen flame simulation has been developed to demonstrate the capabilities of the adjoint method in determining sensitivity of the NOx production of the flame to perturbations of the state variables via source terms. The adjoint solutions show that the NOx levels are sensitive to H_2 and O_2 in the region of the flame itself and near the inlet where they would be transported into the flame. Additionally, the NOx levels are sensitive to addition of radicals in the region bordering



(a) φ_{OH}

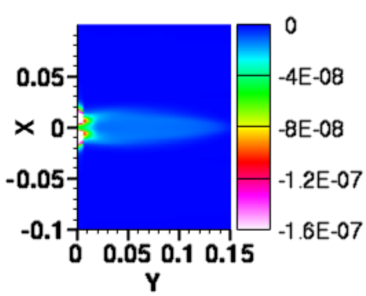


(b) φ_{O}

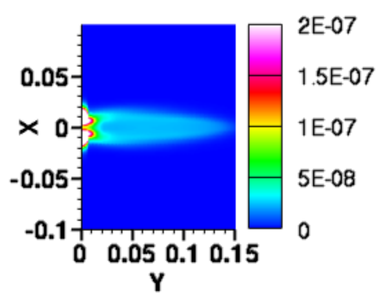


(c) φ_{N}

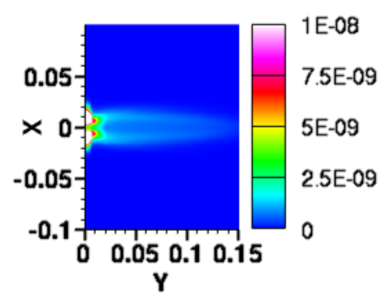
Figure 4: Adjoint variable fields for OH, O, and N



(a) $\varphi_{\mathrm{H_2}}$



(b) $\varphi_{\mathrm{O_2}}$



(c) $\varphi_{\mathrm{N_2}}$

Figure 5: Adjoint variable fields for H_2, O_2, and N_2

the hot combustion products, and again at the inlet where they would be transported into those regions.

Acknowledgments

This research has been financially supported by the DOE PSAAP center at the University of Texas.

A Appendix

The adjoint equations are derived starting from the steady-state governing equations for the primal problem. To facilitate the derivation, the NS, reactive scalar, and enthalpy equations can be written compactly in the following form:

$$\frac{\partial F_i}{\partial x_i} - \frac{\partial G_i}{\partial x_i} = S,$$

for which

$$U = [\rho u, \rho v, p, \rho Y_k, \rho h_s]^T$$
$$F_i = [\rho u_i u + p\delta_{i1}, \rho u_i v + p\delta_{i2}, 0, \rho u_i Y_k, \rho u_i h_s]^T$$
$$G_i = \left[\mu\frac{\partial u}{\partial x_i}, \mu\frac{\partial v}{\partial x_i}, -\frac{\partial p}{\partial x_i}, \rho D_k\frac{\partial Y_k}{\partial x_i}, \rho\alpha\frac{\partial h_s}{\partial x_i}\right]^T$$
$$S = \left[0, 0, \rho\frac{\partial}{\partial x_j}\left[\frac{\partial \bar{u}_i\bar{u}_j}{\partial x_i}\right], \rho S_k, \rho S_{hs}\right]^T,$$

where U is the state vector, F_i is the inviscid flux vector in the ith direction, G_i is the viscous flux vector in the ith direction, and S is the source term vector. For later substitution in the dual problem, G_i can be written as $K_{ij}\dfrac{\partial U}{\partial x_j}$.

A.1 Adjoint derivation

The dual problem involves a specific quantity of interest (QoI). In this derivation, the QoI $\mathcal{J}$ will be the domain-wide integral of a scalar function. Here, the scalar function J will depend only upon the state variable for simplicity:

$$\mathcal{J}(U) \equiv \int_\Omega J(U).$$

The dual problem requires the Lagrangian $\mathcal{L}$ which is defined as

$$\mathcal{L}(U,\varphi) \equiv \mathcal{J}(U) - \int_\Omega \varphi^T\left(\frac{\partial F_i}{\partial x_i} - \frac{\partial G_i}{\partial x_i} - S\right),$$

where φ is the Lagrange multiplier as well as the adjoint state.

The adjoint equations are derived under perturbation of the Lagrangian with perturbation V. With $\mathcal{L}$ stationary to variations in V, the adjoint equations can be developed from the following:

$$\mathcal{L}'[U](V,\varphi) = 0, \tag{7}$$

where $\mathcal{L}'[U]$ refers to the Frechet derivative of $\mathcal{L}$ taken at U. $\mathcal{L}$ can be broken down into different terms corresponding to the compact form of the RANS equations as follows:

$$\mathcal{L}(U,\varphi) \equiv \mathcal{L}_{QoI}(U,\varphi) - \left[\mathcal{L}_{inv}(U,\varphi) - \mathcal{L}_{visc}(U,\varphi) - \mathcal{L}_{src}(U,\varphi)\right].$$

Applying the same term break down to (7), $\mathcal{L}'$ is written

$$\mathcal{L}'_{QoI}[U](V,\varphi) = \mathcal{L}'_{inv}[U](V,\varphi) - \mathcal{L}'_{visc}[U](V,\varphi) - \mathcal{L}'_{src}[U](V,\varphi). \tag{8}$$

A.1.1 Inviscid flux

The inviscid flux portion of the Lagrangian equation is given by

$$\begin{aligned}\mathcal{L}_{inv}(U+V,\varphi) &= \int_\Omega \varphi^T \frac{\partial F_i(U+V)}{\partial x_i} \\ &= \int_\Omega \varphi^T \frac{\partial F_i(U)}{\partial x_i} + \int_\Omega \varphi^T \frac{\partial F_i'[U](V)}{\partial x_i} + H.O.T. \\ &= \mathcal{L}_{inv}(U,\varphi) + \int_{\partial\Omega} \varphi^T F_i'[U](V) n_i - \int_\Omega \frac{\partial \varphi^T}{\partial x_i} F_i'[U](V) + H.O.T.,\end{aligned}$$

where $F_i'[U]$ is the Frechet derivative of the flux in the ith direction taken at U, which is the Jacobian of F_i evaluated at U. Additionally, since $\frac{\partial \varphi^T}{\partial x_i} F_i'[U](V)$ is a scalar, the following relation applies:

$$\frac{\partial \varphi}{\partial x_i}^T F_i'[U](V) = \left(\frac{\partial \varphi}{\partial x_i}^T F_i'[U](V) \right)^T = V^T F_i'[U]^T \frac{\partial \varphi}{\partial x_i}.$$

Ultimately, the inviscid flux contribution is written as

$$\mathcal{L}_{inv}'[U](V,\varphi) = \int_{\partial\Omega} \varphi^T F_i'[U](V) n_i - \int_\Omega V^T F_i'[U]^T \frac{\partial \varphi}{\partial x_i}.$$

A.1.2 Viscous flux

The viscous portion of the Lagrangian equation is given by

$$\begin{aligned}\mathcal{L}_{visc}(U+V,\varphi) &= \int_\Omega \varphi^T \frac{\partial}{\partial x_i}\left(K_{ij}(U+V) \frac{\partial (U+V)}{\partial x_j} \right) \\ &= \int_\Omega \varphi^T \frac{\partial}{\partial x_i}\left(K_{ij}(U) \frac{\partial U}{\partial x_j} + K_{ij}'[U](V) \frac{\partial U}{\partial x_j} + K_{ij}(U) \frac{\partial V}{\partial x_j} \right) + H.O.T. \\ &= \mathcal{L}_{visc}(U,\varphi) + \underbrace{\int_\Omega \varphi^T \frac{\partial}{\partial x_i}\left(K_{ij}'[U](V) \frac{\partial U}{\partial x_j} \right)}_{\text{Term I}} \\ &+ \underbrace{\int_\Omega \varphi^T \frac{\partial}{\partial x_i}\left(K_{ij}(U) \frac{\partial V}{\partial x_j} \right)}_{\text{Term II}} + H.O.T.\end{aligned}$$

Integrating by parts the first term of the viscous flux gives

$$\begin{aligned}&\int_\Omega \varphi^T \frac{\partial}{\partial x_i}\left(K_{ij}'[U](V) \frac{\partial U}{\partial x_j} \right) = \\ &\quad \int_{\partial\Omega} \varphi^T K_{ij}'[U](V) \frac{\partial U}{\partial x_j} n_i - \int_\Omega \frac{\partial \varphi}{\partial x_i}^T \left(K_{ij}'[U](V) \frac{\partial U}{\partial x_j} \right),\end{aligned}$$

for which the interior term can be rewritten as

$$\int_\Omega \frac{\partial \varphi}{\partial x_i}^T \left(K'_{ij}[U](V) \frac{\partial U}{\partial x_j} \right) = \int_\Omega V^T R,$$

where R is a vector such that

$$R_\alpha = \left(K'_{ij}[U_\alpha] \frac{\partial U}{\partial x_j} \right)^T \frac{\partial \varphi}{\partial x_i}$$

Integrating by parts the second term of the viscous flux gives

$$\int_\Omega \varphi^T \frac{\partial}{\partial x_i} \left(K_{ij}(U) \frac{\partial V}{\partial x_j} \right) = \int_{\partial\Omega} \varphi^T K_{ij}(U) \frac{\partial V}{\partial x_j} n_i - \int_{\partial\Omega} V^T K_{ij}(U)^T \frac{\partial \varphi}{\partial x_i} n_j + \int_\Omega V^T \frac{\partial}{\partial x_j} \left(K_{ij}(U)^T \frac{\partial \varphi}{\partial x_i} \right).$$

Finally, the viscous term can be written

$$\begin{aligned} \mathcal{L}'_{visc}[U](V,\varphi) &= \int_{\partial\Omega} \varphi^T K'_{ij}[U](V) \frac{\partial U}{\partial x_j} n_i - \int_\Omega V^T R \\ &+ \int_{\partial\Omega} \varphi^T K_{ij}(U) \frac{\partial V}{\partial x_j} n_i - \int_{\partial\Omega} V^T K_{ij}(U)^T \frac{\partial \varphi}{\partial x_i} n_j + \int_\Omega V^T \frac{\partial}{\partial x_j} \left(K_{ij}(U)^T \frac{\partial \varphi}{\partial x_i} \right). \end{aligned}$$

A.1.3 Source term

The source term portion of the Lagrangian is given by

$$\begin{aligned} \mathcal{L}_{src}(U+V,\varphi) &= \int_\Omega \varphi^T S(U+V) \\ &= \int_\Omega \varphi^T S(U) + \int_\Omega \varphi^T S'[U](V) + H.O.T., \end{aligned}$$

leading to the following

$$\mathcal{L}'_{src}[U](V,\varphi) = \int_\Omega V^T S'[U]^T \varphi.$$

A.1.4 QoI term

The QoI portion of the Lagrangian is given by

$$\begin{aligned} \mathcal{L}_{QoI}(U+V,\varphi) &= \int_\Omega J(U+V) \\ &= \int_\Omega J(U) + J'[U](V), \end{aligned}$$

which leads to

$$\mathcal{L}'_{QoI}[U](V,\varphi) = \int_\Omega V^T J'[U]^T.$$

A.2 Adjoint Equations

To arrive at the adjoint equations, the contributions to $\mathcal{L}'$ can be split into interior and boundary condition terms, as follows:

$$\mathcal{L}'[U](V,\varphi) = \mathcal{L}'_{interior}[U](V,\varphi) + \mathcal{L}'_{BC}[U](V,\varphi).$$

A.2.1 Interior

Selecting perturbations V that lead to both V and $\dfrac{\partial V}{\partial x_i}$ approaching zero in the neighborhood of all boundaries leads to the following equation:

$$\mathcal{L}'_{interior}[U](V,\varphi) = \int_\Omega V^T J'[U]^T - \int_\Omega V^T \Bigg[-F_i'[U]^T \frac{\partial \varphi}{\partial x_i} - \frac{\partial}{\partial x_j}\left(K_{ij}(U)^T \frac{\partial \varphi}{\partial x_i}\right) + R - S'[U]^T \varphi \Bigg]$$

This is zero according to (7). Since V in this application may be selected arbitrarily, the above equation may be reduced to the adjoint equations as follows:

$$J'[U]^T = -F_i'[U]^T \frac{\partial \varphi}{\partial x_i} - \frac{\partial}{\partial x_j}\left(K_{ij}(U)^T \frac{\partial \varphi}{\partial x_i}\right) + R - S'[U]^T \varphi.$$

This equation can also be written as

$$F_i'[U]^T \frac{\partial \varphi}{\partial x_i} + \frac{\partial}{\partial x_j}\left(K_{ij}(U)^T \frac{\partial \varphi}{\partial x_i}\right) - R = -S'[U]^T \varphi - J'[U]^T.$$

Substituting F_i, K_{ij}, and S gives the final form of the adjoint equations as follows:

$$2u\frac{\partial \varphi_u}{\partial x} + v\frac{\partial \varphi_v}{\partial x} + Y_k\frac{\partial \varphi_{Y_k}}{\partial x} + h_s\frac{\partial \varphi_{hs}}{\partial x} + v\frac{\partial \varphi_u}{\partial y} + \frac{\partial}{\partial x_j}\left(\nu\frac{\partial \varphi_u}{\partial x_j}\right) = -\frac{\partial J}{\partial \rho u}$$

$$u\frac{\partial \varphi_v}{\partial x} + u\frac{\varphi_u}{\partial y} + 2v\frac{\partial \varphi_v}{\partial y} + Y_k\frac{\partial \varphi_{Y_k}}{\partial y} + h_s\frac{\partial \varphi_{hs}}{\partial y} + \frac{\partial}{\partial x_j}\left(\nu\frac{\partial \varphi_v}{\partial x_j}\right) = -\frac{\partial J}{\partial \rho v}$$

$$\frac{\partial \varphi_u}{\partial x} + \frac{\partial \varphi_v}{\partial y} + \frac{\partial}{\partial x_j}\left(-\frac{\partial \varphi_p}{\partial x_j}\right) = -\frac{\partial J}{\partial p}$$

$$u\frac{\partial \varphi_{Y_k}}{\partial x} + v\frac{\partial \varphi_{Y_k}}{\partial y} + \frac{\partial}{\partial x_j}\left(D_k\frac{\partial \varphi_{Yk}}{\partial x_j}\right) = -\left(\frac{\partial \rho S_l}{\partial \rho Y_k}\varphi_{Yl} + \frac{\partial \rho S_{hs}}{\partial \rho Y_k}\varphi_{hs}\right) - \frac{\partial J}{\partial \rho Y_k}$$

$$\begin{aligned} u\frac{\partial \varphi_{hs}}{\partial x} + v\frac{\partial \varphi_{hs}}{\partial y} + \frac{\partial}{\partial x_j}\left(\alpha\frac{\partial \varphi_{hs}}{\partial x_j}\right) - \frac{\partial \nu}{\partial \rho h_s}\left(\frac{\partial \rho u}{\partial x_i}\frac{\partial \varphi_u}{\partial x_i} + \frac{\partial \rho v}{\partial x_i}\frac{\partial \varphi_v}{\partial x_i}\right) \\ + \frac{\partial D_k}{\partial \rho h_s}\frac{\partial \rho Y_k}{\partial x_i}\frac{\partial \varphi_{Yk}}{\partial x_i} + \frac{\partial \alpha}{\partial \rho h_s}\frac{\partial \rho h_s}{\partial x_i}\frac{\partial \varphi_{hs}}{\partial x_i} = -\left(\frac{\partial \rho S_k}{\partial \rho h_s}\varphi_{Yk} + \frac{\partial \rho S_{hs}}{\partial \rho h_s}\varphi_{hs}\right) - \frac{\partial J}{\partial \rho h_s}\end{aligned}$$

A.2.2 Boundary Conditions

$$\mathcal{L}'_{BC}[U](V,\varphi) = \int_{\partial\Omega} \left(\varphi^T \left[F'_i[U](V) - K'_{ij}[U](V)\frac{\partial U}{\partial x_j} - K_{ij}(U)\frac{\partial V}{\partial x_j} \right] n_i + V^T K_{ij}(U)^T \frac{\partial \varphi}{\partial x_i} n_j + V^T J'_{\partial\Omega}[U]^T \right) = \tag{9}$$

Combining the boundary conditions at the inflow leads to the following equation for the boundary conditions for the adjoint variables:

$$\left(\varphi_u V_p - \varphi_u \nu \frac{\partial V_u}{\partial x} - \varphi_v \nu \frac{\partial V_v}{\partial x} - \varphi_{Y_k} D_k \frac{\partial V_{Y_k}}{\partial x} - \varphi_{hs} \alpha \frac{\partial V_{hs}}{\partial x} - V_p \frac{\partial \varphi_p}{\partial x} \right) n_x = 0$$

Considering that any V_p and any $\frac{\partial V_u}{\partial x}$, $\frac{\partial V_v}{\partial x}$, and $\frac{\partial V_{Y_k}}{\partial x}$ are admissible, the above boundary condition equation leads to the following boundary conditions for the adjoint variables:

$$\varphi_u = 0,$$

$$\varphi_v = 0,$$

$$\frac{\partial \varphi_p}{\partial x} = 0, \text{ and}$$

$$\varphi_{Y_k} = 0.$$

$$\varphi_{hs} = 0.$$

Combining the boundary conditions at the lateral boundaries leads to the following equation:

$$\begin{aligned}
&(\varphi_u v)V_u + (\varphi_u u + \varphi_v 2v + \varphi_{Y_k} Y_k + \varphi_{hs} h_s)V_v + (\varphi_{Y_k} v)V_{Y_k} \\
&\quad + (\varphi_{hs} v + \varphi_u \frac{\partial \nu}{\partial \rho h_s}\frac{\partial u}{\partial y} + \varphi_v \frac{\partial \nu}{\partial \rho h_s}\frac{\partial v}{\partial y} + \varphi_{Yk}\frac{\partial D_k}{\partial \rho h_s}\frac{\partial Y_k}{\partial y} + \varphi_{hs}\frac{\partial \alpha}{\partial \rho h_s}\frac{\partial h_s}{\partial y})V_{hs} + \varphi_p \frac{\partial V_p}{\partial y} n_y \\
&\quad + \left(V_u \nu \frac{\partial \varphi_u}{\partial y} + V_v \nu \frac{\partial \varphi_v}{\partial y} + V_{Y_k} D_k \frac{\partial \varphi_{Y_k}}{\partial y} + V_{hs} \alpha \frac{\partial \varphi_{hs}}{\partial y} \right) = 0.
\end{aligned}$$

Considering that any V_u, V_v, and V_{Y_k} and any $\frac{\partial V_p}{\partial y}$ are admissible, the above boundary condition equation leads to the following boundary conditions for the adjoint variables:

$$v\varphi_u + \nu \frac{\partial \varphi_u}{\partial y} = 0$$

$$u\varphi_u + 2v\varphi_v + Y_k \varphi_{Y_k} + h_s \varphi_{hs} + \nu \frac{\partial \varphi_v}{\partial y} = 0$$

$$\varphi_p = 0$$

$$v\varphi_{Y_k} + D_k \frac{\partial \varphi_{Y_k}}{\partial y} = 0$$

$$v\varphi_{hs} + \alpha \frac{\partial \varphi_{hs}}{\partial y} = 0$$

Finally, combining the boundary conditions at the outflow boundaries leads to the following equation:

$$
\begin{aligned}
&(\varphi_u 2u + \varphi_v v + \varphi_{Y_k} Y_k + \varphi_{hs} h_s)V_u + (\varphi_v u)V_v + (\varphi_{Y_k} u)V_{Y_k} \\
&\quad +(\varphi_{hs} u + \varphi_u \frac{\partial \nu}{\partial \rho h_s}\frac{\partial u}{\partial x} + \varphi_v \frac{\partial \nu}{\partial \rho h_s}\frac{\partial v}{\partial x} + \varphi_{Yk}\frac{\partial D_k}{\partial \rho h_s}\frac{\partial Y_k}{\partial x} + \varphi_{hs}\frac{\partial \alpha}{\partial \rho h_s}\frac{\partial h_s}{\partial x})V_{hs} + \varphi_p \frac{\partial V_p}{\partial x} n_x \\
&\quad + \left(V_u \nu \frac{\partial \varphi_u}{\partial x} + V_v \nu \frac{\partial \varphi_v}{\partial x} + V_{Y_k} D_k \frac{\partial \varphi_{Y_k}}{\partial x} + V_{hs}\alpha \frac{\partial \varphi_{hs}}{\partial x} \right) = 0.
\end{aligned}
$$

Considering that any V_u, V_v, and V_{Y_k} and any $\frac{\partial V_p}{\partial y}$ are admissible, the above boundary condition equation leads to the following boundary conditions for the adjoint variables:

$$2u\varphi_u + v\varphi_v + Y_k\varphi_{Y_k} + h_s\varphi_{hs} + \nu\frac{\partial \varphi_u}{\partial x} = 0$$

$$
\begin{aligned}
u\varphi_v + \nu \frac{\partial \varphi_v}{\partial x} &= 0 \\
\varphi_p &= 0 \\
u\varphi_{Y_k} + D_k \frac{\partial \varphi_{Y_k}}{\partial x} &= 0 \\
u\varphi_{hs} + \alpha \frac{\partial \varphi_{hs}}{\partial x} &= 0.
\end{aligned}
$$

References

[1] A. Jameson. *Journal of Scientific Computing*, 3 (1988) 233–260.

[2] O. Baysal and M. E. Eleshaky. In *29th Aerospace Sciences Meeting and Exhibit*, number AIAA 92-0471. American Institute of Aeronautics and Astronautics, 1991.

[3] A. Jameson, N. Pierce, and L. Martinelli. In *35th Aerospace Sciences Meeting and Exhibit*, number AIAA 97-0101. American Institute of Aeronautics and Astronautics, 1997.

[4] J. Reuther, J.J. Alonso, M.J. Rimlinger, and A. Jameson. *Computers & Fluids*, 28 (1999) 675 – 700.

[5] M.B. Giles and N.A. Pierce. *Flow, Turbulence and Combustion*, 65 (2000) 393–415.

[6] S. Kim, J.J. Alonso, and A. Jameson. In *40th Aerospace Sciences Meeting and Exhibit*, number AIAA 2002-0844. American Institute of Aeronautics and Astronautics, 2002.

[7] S.K. Nadarajah and A. Jameson. In *38th Aerospace Sciences Meeting and Exhibit*, number AIAA 2000-0667. American Institute of Aeronautics and Astronautics, 2000.

[8] M.D. Gunzburger, L. Hou, and T.P. Svobodny. *SIAM J. Control Optim.*, 30 (1992) 167–181.

[9] T.R. Bewly, P. Moin, and R. Temam. *Journal of Fluid Mechanics*, 447 (2001) 179–225.

[10] M. Wei and J. B. Freund. *Journal of Fluid Mechanics*, 546 (2005) 123.

[11] J. Freund, J. Kim, and D. Bodony. Adjoint-based optimal control of a mach 1.3 turbulent jet for noise reduction. In *49th AIAA Aerospace Sciences Meeting including the New Horizons Forum and Aerospace Exposition*. American Institute of Aeronautics and Astronautics, 2011.

[12] A. Sandu, D.N. Daescu, and G. R. Carmichael. *Atmospheric Environment*, 37 (2003) 5083–5096.

[13] A. Sandu, D. N. Daescu, G. R. Carmichael, and T. Chai. *Journal of Computational Physics*, 204 (2005) 222 – 252.

[14] A. Sandu and L. Zhang. *Journal of Computational Physics*, 227 (2008) 5949 – 5983.

[15] E. Ranzi, A. Frassoldati, R. Grana, A. Cuoci, T. Faravelli, A.P. Kelley, and C.K. Law. *Progress in Energy and Combustion Science*, 38 (2012) 468 – 501.