Adjoint-based sensitivity analysis for a reacting jet in crossflow

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With current advances in computational resources, high-fidelity simulations of reactive flows are increasingly being used as predictive tools in various industrial applications. In order to accurately capture the combustion process, detailed/reduced chemical mechanisms are employed, which in turn rely on various model parameters. Therefore, it would be of great interest to quantify the sensitivities of the predictions with respect to the introduced models. Due to the high dimensionality of the parameter space, methods such as finite differences which rely on multiple forward simulations prove to be very costly, and adjoint-based techniques are a suitable alternative. The complex nature of the governing equations, however, renders an efficient strategy in finding the adjoint equations a challenging task. In this study, we employ the modular approach of Fosas de Pando *et al.* (2012) to build a discrete adjoint framework applied to a reacting jet in crossflow. The developed framework is then used to extract the sensitivity of the integrated heat release with respect to the existing combustion parameters. Analyzing the sensitivities in the three-dimensional domain provides insight toward the specific regions of the flow that are more susceptible to the choice of the model. Masking functions are also employed in order to isolate specific regions within the computational domain for analysis.

1. Introduction

Accurate numerical simulation of multiphysics and multiscale phenomena is critical for many industrial applications. Over the past decade, numerical simulations of complex flows have advanced remarkably. High-fidelity simulations of complex physical processes, including multiphase flows, combustion and acoustic problems, and turbulent and thermal flows, are now being used in design and performance analysis of engineering systems.

Simulations of reacting flows involve the use of detailed/reduced chemistry models in order to capture the chemical mechanisms occurring in the flow. This introduces chemistry model parameters that are not always known *a priori* with high precision. Therefore, it is of practical interest to determine the uncertainties in the simulations with respect to these governing parameters or initial conditions. As an added complication, the large number of these parameters causes a purely forward approach to become very expensive and almost infeasible. Therefore, we propose the use of adjoint-based algorithms in order to identify and quantify the underlying sensitivities. This adjoint framework bears a great advantage in a case such as this, where a large input space is analyzed, since a single forward and backward sweep provides all the sensitivity information.

The adjoint solution in effect provides gradient or sensitivity information about an

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optimization problem. Given a cost functional or optimization objective while the governing equations are satisfied. This gradient is computed in the form of algebraic expressions based on the problem's Lagrange multipliers or adjoint variables, which in turn is used in standard optimization algorithms that rely on Jacobian information, such as the conjugate-gradient family (Guégan *et al.* 2006). Once the gradient information is extracted from the simulation, it can be used in its own right: it can provide physical insight into highly sensitive regions in the flow, point towards weak links in complex feedback loops, identify robust flow features for model reduction, and many other applications. The gradient-based analysis of fluid models has recently been applied to flow problems. However, most of the applications have been limited to linear or linearized problems (Kim *et al.* 2006). Only recently, nonlinear problems have been tackled, within the context of finding initial conditions that optimally trigger transition to turbulence, the enhancement of mixing efficiency or thermoacoustic instabilities (Rabin *et al.* 2012; Foures *et al.* 2014; Juniper 2010). The extra effort that arises from the nonlinear problem has been rather limited in these applications; more complex simulations dealing with reactive flows constitute a far larger step in complexity (Magri *et al.* 2014; Lemke *et al.* 2014; Braman *et al.* 2015).

This study outlines the use of discrete adjoints for optimization and sensitivity analysis in the context of a reacting jet in crossflow. Section 2 briefly describes the mathematical formalism for the sensitivity analysis. Section 3 describes the numerical details for the application to a reacting jet in crossflow. The results are outlined in Section 4, where the optimal initial condition that yields the maximum heat release rate at some finite time T is derived. Using this initial condition, the sensitivity of the integral heat release with respect to the combustion model parameters is extracted. Concluding remarks are presented in Section 5.

2. Mathematical description

The sensitivity information with respect to the model parameters can be computed using the adjoint framework. In this section we outline the mathematical formalism to extract these sensitivities. The forward/direct equation constitutes the evolution of the state variables, $\mathbf{q}(t)$, forward in time defined by

$$\frac{d\mathbf{q}}{dt} = \left.\frac{\partial \mathbf{F}}{\partial \mathbf{q}}\right|_{\bar{\mathbf{q}}} \mathbf{q} = f(\mathbf{q}, \mathbf{g}), \quad \mathbf{q}(0) = \mathbf{q}_0, \tag{2.1}$$

where $\mathbf{F}$ is the discrete nonlinear equation that governs the state variables, $\mathbf{g}$ represents a set of model parameters, $\mathbf{q}_0$ is the initial condition, and $\bar{\mathbf{q}}$ is the base solution about which the governing equations are linearized. Since the quantity of interest is integrated in time, the objective functional J can be defined as

$$J(\mathbf{q}) = \phi(\mathbf{q}(T)) + \int_0^T \psi(\mathbf{q}(t))dt, \tag{2.2}$$

where ϕ is the contribution from the terminal state and ψ accounts for the path taken to reach this terminal state. Using this objective functional, we can form the Lagrange functional L as

$$L(\mathbf{q}, \mathbf{g}, \boldsymbol{\eta}, \xi) = J(\mathbf{q}) - \int_0^T \boldsymbol{\eta} \cdot \left(\frac{d\mathbf{q}}{dt} - f(\mathbf{q}, \mathbf{g})\right) dt - \xi(\mathbf{q}(0) - \mathbf{q}_0), \tag{2.3}$$

where we introduce $\boldsymbol{\eta}$ and ξ as Lagrange multipliers. Since, in this project, the focus lies in optimizing the integral heat release of the reactive flow, the term $\phi(\mathbf{q}(T))$ in the description of the objective functional can be neglected, and $\psi(\mathbf{q}(t)) = \langle \mathbf{b} \cdot \mathbf{q}(t), \mathbf{b} \cdot \mathbf{q}(t) \rangle$, where $\mathbf{b} \cdot \mathbf{q}(t)$ results in the linearized heat release rate. The inner product is defined as $\langle \mathbf{u}, \mathbf{v} \rangle = \mathbf{v}^\top \mathbf{D} \mathbf{u}$, where $\mathbf{D}$ represents a symmetric positive-definite mass matrix that accounts for the volume integral of the discretized domain. Setting the variation of the Lagrange functional with respect to the state variables to zero leads to the adjoint equation defined by

$$-\frac{d\boldsymbol{\eta}}{dt} = \left(\frac{\partial f}{\partial \mathbf{q}}\right)^\top \boldsymbol{\eta} + 2\mathbf{M}\mathbf{q}(t), \quad \boldsymbol{\eta}(T) = 0, \tag{2.4}$$

where $\mathbf{M} = \mathbf{b}^\top \mathbf{D} \mathbf{b}$. Hence, the equation governing the evolution of the adjoint variable is forced by the solution of the direct system, $\mathbf{q}$. This implies that $\mathbf{q}$ needs to be stored and used when solving the adjoint equations for each time step, even if the direct equations are linear. From a numerical point of view, large storage capabilities are required to store the whole time history of $\mathbf{q}(t)$. One possible solution is to use a checkpointing algorithm, in which the solution is stored at strategically chosen time locations. The forward problem is solved in between the stored time intervals, and the adjoint equation is solved backward in time (Griewank *et al.* 2000; Wang *et al.* 2009).

Finally, the equation defining the final sensitivities is obtained by finding the variation of the Lagrange functional with respect to the modal parameters,

$$\frac{\delta L}{\delta \mathbf{g}} = \frac{\partial \phi}{\partial \mathbf{g}} + \int_0^T \left[\frac{\partial \psi}{\partial \mathbf{g}} + \left(\frac{\partial f}{\partial \mathbf{g}}\right)^\top \boldsymbol{\eta}\right] dt, \tag{2.5}$$

$$= \int_0^T \left(\frac{\partial f}{\partial \mathbf{g}}\right)^\top \boldsymbol{\eta} \, dt. \tag{2.6}$$

This equation can be written in differential form with the introduction of an auxiliary variable $\mathbf{s}$

$$-\frac{d\mathbf{s}}{dt} = \left(\frac{\partial f}{\partial \mathbf{g}}\right)^\top \boldsymbol{\eta}, \quad \mathbf{s}(T) = 0. \tag{2.7}$$

Introducing this variable allows the sensitivity equation to be solved simultaneously with the adjoint equation. The algorithm can be summarized as follows;

(i) Given an initial condition $\mathbf{q}_0$, solve the direct problem forward in time,

(ii) Solve the adjoint equation (Eq. 2.4) and the sensitivity equation (Eq. 2.7) backward in time to get $\boldsymbol{\eta}(0)$ and $\mathbf{s}(0)$,

(iii) The final sensitivity is given by $\mathbf{s}(0)$.

3. Numerical approach

Direct numerical simulation is performed using a modified version of the solver developed by Nagarajan *et al.* (2003) and Sayadi *et al.* (2013), where the compressible Navier-Stokes equations, including reactions, are solved. An explicit third-order Runge-Kutta scheme is used for time stepping. The spatial discretization is on a structured curvilinear grid with staggered variables in space.

3.1. *Chemistry*

We employ operator splitting to solve the reacting part of the governing equations. The stiff source terms, related to the chemistry, are integrated in time using a fifth-order backward differentiation method (Brown *et al.* 1989). The chemistry is modeled using a simple one-step combustion model with lean chemistry approximations (Blanchard *et al.* 2015).

The combustion source terms, that is, the fuel mass depletion rate $\dot{\omega}_f$ and reaction heat release rate $\dot{\omega}_T$, in the non-dimensional form are,

$$\dot{\omega}_f = \text{Da}\,\rho Y_f \exp\left(-\frac{\text{Ze}}{T}\right),$$

$$\dot{\omega}_T = \text{Ce}\,\dot{\omega}_f,$$

where Da is the Damköhler number, Ze is the Zeldovich number and Ce is the heat release parameter. For this study we have chosen $\text{Da} = 10$, $\text{Ze} = 5$ and $\text{Ce} = 10$. So the state variables and governing parameters for this study are

$$\mathbf{q} = [\rho \quad \rho u_1 \quad \rho u_2 \quad \rho u_3 \quad E \quad \rho Y_f]^\top,$$

$$\mathbf{g} = [\text{Da} \quad \text{Ze} \quad \text{Ce}]^\top,$$

where ρ is the density, u_i is the velocity in the i-th direction, E is the total energy and Y_f is the mass fraction of the fuel.

3.2. *Base flow computation*

The base flow solution $\bar{\mathbf{q}}$ is taken as the steady state solution of the nonlinear governing equations. We employ selective frequency damping (SFD) (Akervik *et al.* 2006) to obtain the base flow by solving the following system of equations until convergence is achieved,

$$\frac{d\mathbf{q}}{dt} = f(\mathbf{q}, \mathbf{g}) - \chi(\mathbf{q} - \bar{\mathbf{q}}), \tag{3.1}$$

$$\frac{d\bar{\mathbf{q}}}{dt} = \frac{(\mathbf{q} - \bar{\mathbf{q}})}{\Delta}. \tag{3.2}$$

Here, χ and Δ are user-defined filter parameters that control the filter width and cutoff frequency of the filter.

3.3. *Adjoint-based framework*

The derivation of adjoint equations can be carried out in two ways. In the continuous approach, a variational principle is applied to the unconstrained optimization problem and adjoint equations are derived by setting first variations with respect to all dependent variables to zero, leading to the governing equations for the adjoint variables with appropriate boundary conditions and initial conditions. The resulting set of equations is then discretized and implemented. This process is very cumbersome and error prone, especially for sophisticated systems with elaborate objective functions. Alternatively, the spatially discretized equations can be fed into an automatic-differentiation (AD) software to produce the associated adjoint code. This process, although simple to implement, often leads to overly inflated and thus very inefficient and ultimately impractical code. As an alternative, we employ the approach outlined in Fosas de Pando *et al.* (2012). The discrete adjoint operators are obtained by taking the transconjugate of the discretized direct operator. This approach has been used in Fosas de Pando *et al.* (2012) to improve

airfoil shape design in aeroacoustic applications and in Blanchard *et al.* (2015) it was recently applied to an axi-symmetric M-flame where the inverse problem was solved for a frequency response analysis of the flame to acoustic waves.

4. Application to a reacting jet in crossflow

We consider a transverse jet entering a crossflow boundary layer with a free-stream Mach number $Ma = 0.2$. The jet to free-stream velocity ratio is $R = 3$, resulting in a Mach number of 0.6 at the jet inlet. The reference Reynolds number, based on the distance from the leading edge of the plate x_{ref}, is $Re_{ref} = 10^4$. All distances are non-dimensionalized by this reference length such that $x/x_{ref} = Re_x/10^4$. The inlet of the computational domain is at $x_{inlet} = 0.7$ measured from the leading edge of the plate and the jet is located at the distance of $x_{jet} = 0.92$. The jet diameter is $D = 0.0495$. The domain lengths in the streamwise, wall-normal and spanwise directions are 1.2, 0.4 and 0.5, respectively. In this study, we chose the Prandtl number to be 0.7 and the Lewis number is set to be unity.

The velocity profile at the inlet of the jet is prescribed using an inhomogeneous boundary condition, through wall-normal velocity at the plate (Bagheri *et al.* 2009). Due to a compressible framework, we also impose a temperature profile at the jet inlet that satisfies pipe Poiseuille flow distribution. Isothermal wall boundary conditions are prescribed everywhere else on the plate. Periodic boundary conditions are used along the spanwise and streamwise directions. To account for the spatially growing boundary layer in a streamwise periodic domain, we reshape and re-scale the profile at the end of the domain into a similarity solution of a laminar compressible boundary layer at the inflow. Sponges are used at all the boundaries except for the wall boundary at the location of the plate to ensure nonreflective inflow and outflow.

4.1. *Optimal initial condition*

The initial condition used to perform the sensitivity analysis is chosen to be the optimal initial perturbation, resulting in the maximum rate of heat release at terminal time T. This terminal time is chosen to be one-third of the flow through time, defined by the free-stream velocity, which allows for the perturbations to travel from their place of origin, close to the inlet of the jet, to the counter-rotating vortex pair in the base flow. The optimal initial condition is extracted using the adjoint-based framework and consists of perturbations around the base state. Figure 1 shows the vortical structures in the instantaneous and base flow fields. The counter-rotating vortex pair (CVP) is observed in the base flow and it develops, as expected, along the jet trajectory shown in the instantaneous flow field. Figure 1(b) shows the optimal initial condition (green), the optimal solution at time T (blue) superimposed on the base flow (red) visualized through Q criterion (Chakraborty *et al.* 2005) iso-surfaces. The perturbations which originate near the wall, in the shear layer upstream of the jet inflow, are convected downstream along the jet trajectory. The perturbations grow in amplitude and surround the CVP of the base flow as they are convected. The steepest descent approach described in Gunzburger (2003) is employed to extract the optimal solution at time T.

4.2. *Sensitivities with respect to the terminal heat release*

As a first step, the sensitivities of the rate of heat release at terminal time T are extracted with respect to the combustion parameters. This setup simplifies Eq.(2.4) by removing the last term on the right-hand side and, hence, the need for a checkpointing strategy.
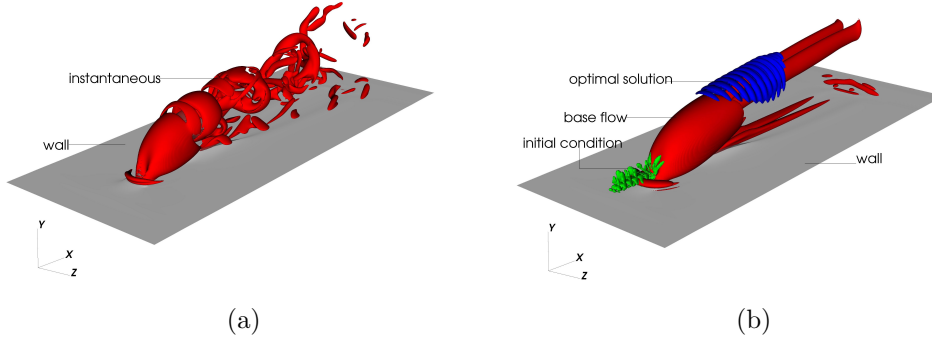
(a)   (b)

FIGURE 1: The red iso-surfaces of Q criterion indicate vortical sturctures in the (a) instantaneous and (b) base flow fields. The green and blue iso-surfaces show the initial condition and optimal solution at time T, respectively. Gray contours depict a streamwise velocity contour of the mean flow close to the wall.
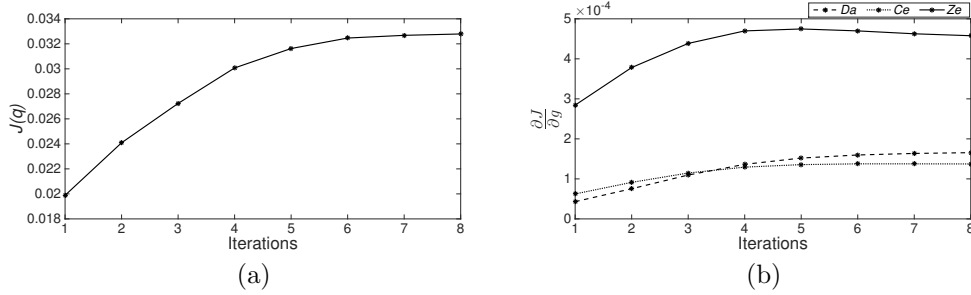

(a)   (b)

FIGURE 2: Convergence of (a) the rate of heat release at time T and (b) its sensitivities with respect to the combustion parameters.

Figure 2 shows the convergence of the terminal heat release rate and its sensitivities with increasing iterations of the steepest descent algorithm. The quantity of interest increases monotonically with each iteration until it reaches near convergence. The sensitivities also simultaneously reach a steady value. This confirms that the adjoint equation is well posed and initialized solely by the terminal state.

The relative parametric sensitivity of the terminal rate of heat release is shown in Figure 3. It is clear that the Zeldovich number, Ze, is the most influential combustion parameter. The sensitivities with respect to the heat release parameter, Ce, and the Damköhler number Da are almost the same and lower than that of Ze. This is because Ze influences the heat release rate exponentially, whereas Da and Ce have only a linear effect. The sensitivity with respect to all the parameters is positive, which means that an increase in these parameters results in an increase in the rate of heat release at terminal time T.
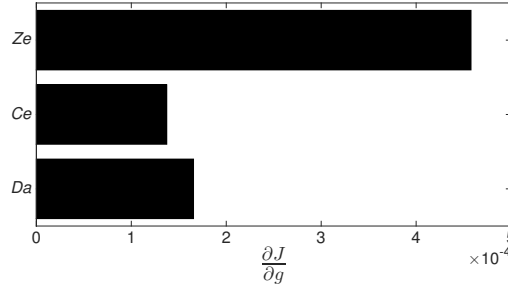
FIGURE 3: Relative sensitivity of the rate of heat release at time T with respect to the combustion model parameters.
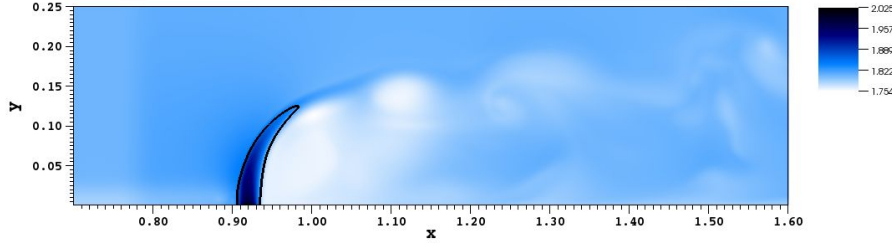

FIGURE 4: The colors represent total energy E for an instantaneous reacting jet in a crossflow flow field on the symmetry plane. The black line shows the contour for the reaction rate threshold used for the masking function.

4.3. *Sensitivities with respect to the integral heat release*

Here, the sensitivity of the integral heat release with respect to the combustion parameters are extracted. The objective functional is calculated within a time horizon $[0, T]$, and due to the presence of a time integral, the adjoint equation is driven at each time step by the solution of the forward problem, making the use of a checkpointing algorithm necessary. To this end, we use REVOLVE (Griewank *et al.* 2000), a checkpointing algorithm that employs a binomial strategy that is provably optimal, i.e., minimizes the amount of re-computations of the forward solution for a given number of checkpoints. In order to characterize the dependence of the extracted sensitivities on the domain under consideration, a masking function is introduced that excludes (masks) certain regions of the computational domain. For the purpose of this study, since the interest lies in the sensitivities of the reactive process to the combustion model parameters, the masking function, W, is designed to isolate the contribution of the reactions from the hydrodynamic effects,

$$W(x, y, z) = \begin{cases} 0 & \dot{\omega}_f < K, \\ 1 & \text{otherwise} \end{cases}$$

where, K is some pre-defined threshold for the reaction rate of the base flow, and $(x, y, z) \in \Omega$, where Ω denotes the physical domain. In the discretized framework, this function translates to a diagonal matrix operation with the diagonal elements either 0
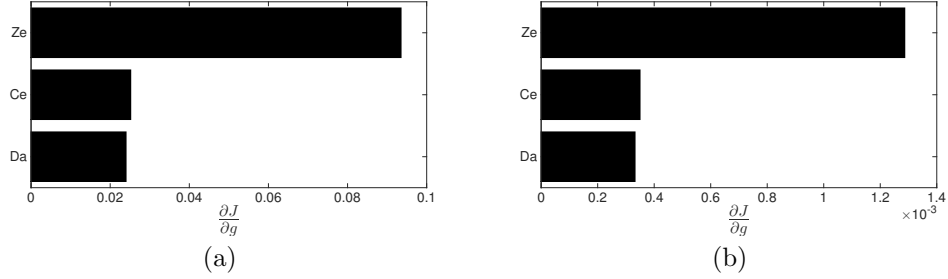
(a)   (b)

FIGURE 5: Relative sensitivity of the integral heat release for time period $[0, T]$ with (a) the entire computational domain and (b) a masked domain with respect to combustion model parameters.
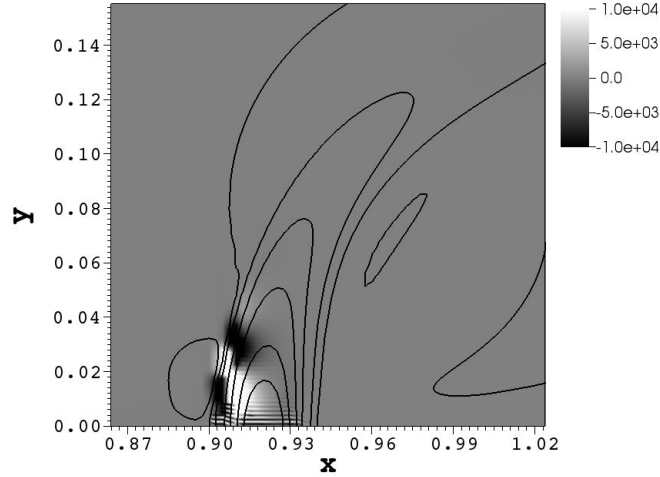

FIGURE 6: Black and white contours show positive and negative sensitivity of the integral heat release with respect to the Zeldovich number Ze. Black lines are wall-normal velocity contours of the base flow, representing the shear layer upstream and downstream of the jet inlet.

or 1, depending on whether the reaction rate is above or below the threshold. Figure 4 shows the contour for the reaction rate threshold along with the total energy E for an instantaneous flow field in a reacting jet in crossflow. The region inside the black contour, which includes the jet inlet, is considered when computing the quantity of interest while the domain outside the black contour is masked.

The relative sensitivities shown in Figure 5 suggest that, in the case of a one-step chemistry model employed in this study, and for both the masked and unmasked quantities of interest, the Zeldovich number is potentially the largest source of uncertainty compared to the Damköhler number and the heat release parameter. This trend matches the previous case of the terminal heat release rate. Masking the hydrodynamic effects leads to a decrease in the sensitivity of the integral heat release.

The advantage of using an adjoint-based algorithm for defining the sensitivities is that, independent of the size of the parameter space, all sensitivities are extracted with a single forward and backward sweep of the algorithm. Therefore, it would be beneficial to consider each parameter as a scalar field that varies in all spatial directions and study the sensitivities of the quantity of interest with respect to each parameter locally. This approach would help identify regions in the physical domain that are more susceptible to the uncertainty in the model parameters. These results are shown in Figure 6 for the integrated heat release as the quantity of interest. Based on this figure, the most susceptible region lies in the shear layer upstream of the jet, close to the wall. This is the same region where the initial perturbation is also located.

Since the sensitivity to different parameters is an integral of different linear combinations of the adjoint solution, the location of the sensitivity is similar for all the parameters as shown in Figure 6. The local sensitivities for the masked quantity of interest, using the same masking function as described above, also show similar behavior. However, the value of the sensitivity is lower due to the masking of the hydrodynamic effects.

5. Conclusion

In this study we introduced a versatile discrete adjoint framework for the calculation of parametric sensitivities and optimization of reacting flows. A Lagrangian approach is employed to derive the sensitivity and adjoint equations for a given objective functional. Gradient information is used to find the optimal initial condition, yielding maximum rate of heat release at terminal time. Sensitivity with respect to the combustion model parameters gives details about the response behavior of the system with this initial condition, as these parameters are varied.

The sensitivity of two objective functionals is computed: the rate of heat release at terminal time and the integral heat release for the entire time period. Both objective functionals were most sensitive with respect to the Zeldovich number. Sensitivities toward variation in the Damköhler number and the heat release parameter were lower. We employ a masking function in the integral heat release study to exclude the effects of hydrodynamics and isolate the combustion effects. We find that although the trend across different parameters is retained, the sensitivities are lower for the masked objective functional. Finally, we exploit the computational efficiency of adjoint methods by finding field sensitivities of the integral heat release with respect to the combustion parameters. The regions most susceptible to the uncertainty in the model parameters lie in the shear layer upstream of the jet, close to the wall.

The methods used in this study are readily applicable to more realistic combustion models with considerably more governing parameters. Access to the gradient information is essential in a number of parameter-dependent studies. The sensitivity information can be used not only to quantify the uncertainty but also to develop better reduced-order chemistry models. In future work, we will examine more detailed combustion models and also consider nonlinear governing equations.

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