Design Optimization in Non-equilibrium Reacting Flows

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Abstract The objective of this study is to develop a reliable and efficient design tool that can be used in chemically reacting flows. The flow analysis is based on axisymmetric Euler and the finite rate reaction equations. These coupled equations are solved by using Newton's method. Both numerical and analytical methods are used to calculate Jacobian matrices. Sensitivities are evaluated by using adjoint method. The performance of the optimization method is demonstrated for a rocket motor nozzle design.

1 Introduction

The reliability of design methods depends on the accuracy of flow models used. In order to capture the chemically reacting and rotational flow physics, the finite-rate reaction and axisymmetric Euler equations are solved simultaneously. In gradient base design optimization, the derivatives of objective function with respect to design variables are needed. In literature, these derivatives are called sensitivities. The accurate and efficient calculation of sensitivities is important for the performance of design method. In design optimization, using implicit methods for flow analysis is advantageous because the evaluation of sensitivities is very efficient. In order to improve the efficiency of design method and to reduce the numerical stiffness that occurs in the solution of reaction equation, Newton's solution method is used. Newton's method needs the Jacobian matrix which is the derivative of residual vector with respect flow variable vector. Analytical or numerical methods can be used in the calculation of Jacobian matrices. The analytical method is more accurate and faster compare to the numerical method [4]. However, the implementation of numerical method is much easier; the analytical method requires code development. Direct differentiation or adjoint methods can be used to evaluate the sensitivities. Adjoint method has more advantageous because the Jacobian matrix is

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solved only once to evaluate the sensitivities of all design variables. In order to avoid solving large Jacobian matrix for each design variable the adjoint method is used.

2 Reacting Flow Solver

The formulation is based on the conservation equations of mass, momentum, energy and species concentrations for a chemically reacting system of N_s species

$$R(Q) = \frac{\partial E}{\partial x} + \frac{1}{y}\frac{\partial (y^n G)}{\partial y} - S = 0 \,, \tag{1}$$

where n = 0 for two dimensional and n = 1 for axisymmetric coordinates, respectively. The flow variable vector, Q, and convective flux vectors E and G in the x and y directions. The fluxes are computed by Van-Leer upwinding schemes, and the second order discretizations are implemented. The source term vector S, contains contributions from chemical reactions. The chemical reaction includes 8 species. They are CO_2, CO, OH, H, O_2, H_2, H_2O, O. The reactions considered are given in Table 1.

$$\mathrm{Q} = \begin{pmatrix} \rho_i \\ \rho u \\ \rho v \\ \rho E \end{pmatrix} \quad E = \begin{pmatrix} \rho_i u \\ P + \rho u^2 \\ \rho u v \\ \rho u H \end{pmatrix} \quad G = \begin{pmatrix} \rho_i v \\ \rho u v \\ P + \rho v^2 \\ \rho v H \end{pmatrix} \quad S = \begin{pmatrix} \dot{\omega}_i \\ 0 \\ 0 \\ 0 \end{pmatrix} \quad i = 1, 8 \tag{2}$$

In Newton's method, the change in flow variable vector at the nth iteration can be calculated as:

$$\left[\frac{\partial R}{\partial Q}\right]^n \Delta Q^n = -R\left(Q^n\right) \tag{3}$$

Jacobian matrices are evaluated with both analytical and numerical methods [3]. The sparse Jacobian matrix is LU factorized and solution is executed by using UMFPACK sparse matrix solver [1]. The boundary conditions are implemented implicitly.

Table 1 Chemistry models for simulation

Reactions	
$OH + CO \Leftrightarrow H + CO_2$	$H_2 + O \Leftrightarrow H + OH$
$CO + O_2 \Leftrightarrow CO_2 + O$	$H_2O + O \Leftrightarrow 2OH$
$O_2 + H \Leftrightarrow O + OH$	$H_2 + OH \Leftrightarrow 2O + H$

3 Design Optimization

In adjoint method, the Lagrangian function, L, is defined as:

$$L = F\left(Q\left(D_i\right), X\left(D_i\right), D_i\right) + \Lambda^T \underbrace{R\left(Q\left(D_i\right), X\left(D_i\right), D_i\right)}_{=0} \tag{4}$$

where F is the objective function, D_i is the ith component of design variable vector, X is the coordinate vector of grid points, and Λ is the adjoint variable vector. Differentiating above equation with respect to design variable gives:

$$\frac{dL}{dD_i} = \frac{\partial F}{\partial X}\cdot\left(\frac{dX}{dD_i}\right) + \frac{\partial F}{\partial D_i} + \Lambda^T\left\{\left[\frac{\partial R}{\partial X}\right]\left(\frac{dX}{dD_i}\right) + \frac{\partial R}{\partial D_i}\right\} + \left\{\underbrace{\left[\frac{\partial R}{\partial Q}\right]^T\Lambda + \left(\frac{\partial F}{\partial Q}\right)^T}_{0}\right\}\left(\frac{dQ}{dD_i}\right) \tag{5}$$

The unknown vector, $\frac{dQ}{dD_i}$, can be eliminated by choosing Λ as:

$$\left[\frac{\partial R}{\partial Q}\right]^T\Lambda = -\left(\frac{\partial T}{\partial Q}\right)^T \tag{6}$$

The remaining terms in Eq. (5) can be used to calculate sensitivities

$$\frac{dL}{dD_i} = \frac{\partial F}{\partial X}\left(\frac{dX}{dD_i}\right) + \frac{\partial F}{\partial D_i} + \Lambda^T\left\{\left[\frac{\partial R}{\partial X}\right]\left(\frac{dX}{dD_i}\right) + \frac{\partial R}{\partial D_i}\right\} \tag{7}$$

4 Results

The goal of the present design is to generate a nozzle geometry that produces the maximum thrust at a specified combustion chamber condition. Hence, the objective function is defined as:

$$F = \int_{A_{exit}} \left(\rho u^2 + p\right) dA \tag{8}$$

The initial baseline nozzle has a conical geometry with an area ratio of 6.1 [6]. The inlet flow condition is given in Table 2. At the inlet section, the mass fraction of

Table 2 Nozzle inlet flow conditions

	T_t = 3,000 K	P_t = 17 MPa	
Y_{H_2O} = 0.390	Y_{CO_2} = 0.211	Y_{CO} = 0.289	Y_{H_2} = 0.012
Y_{OH} = 0.054	Y_{O_2} = 0.029	Y_O = 0.01	Y_H = 0.00021

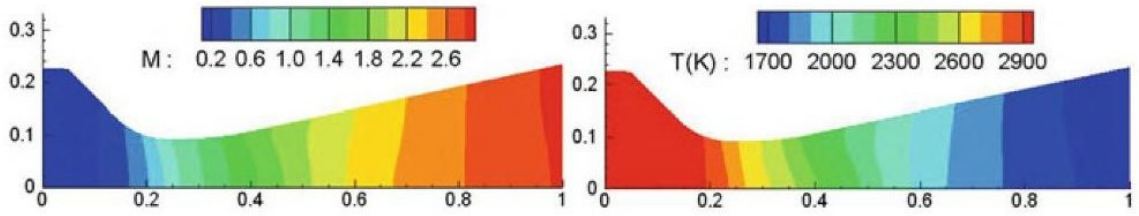

Fig. 1 Distributions of Mach number and temperature in the baseline nozzle configuration

species is evaluated by assuming equilibrium condition in the combustion chamber with specified pressure and temperature.

First, Euler and chemical reaction equations are solved around the baseline geometry. Since the analytical Jacobians of reaction equations are not available, Jacobians are evaluated numerically. As shown in Fig. 1, Mach number increases and temperature decreases in axial direction. Figure 2 shows the mass fractions contours of H_2, H_2O, CO, CO_2, O and OH. As expected, the mass fractions of H_2O and CO_2 increase, and the mass fractions of other species decrease in axial direction. Next, design optimization is performed by using Euler equations. The numerical optimization of the present study employs a commercial optimization package [5]. A total of ten Hicks-Henne functions are used to change nozzle geometry starting from throat to exit [2]. The throat and exit areas are fixed. Jacobians are evaluated analytically.

The Design is completed in three iterations and thirteen function calls. Last, the designed nozzle is analyzed by using Euler and reaction equations. Table 3 compares

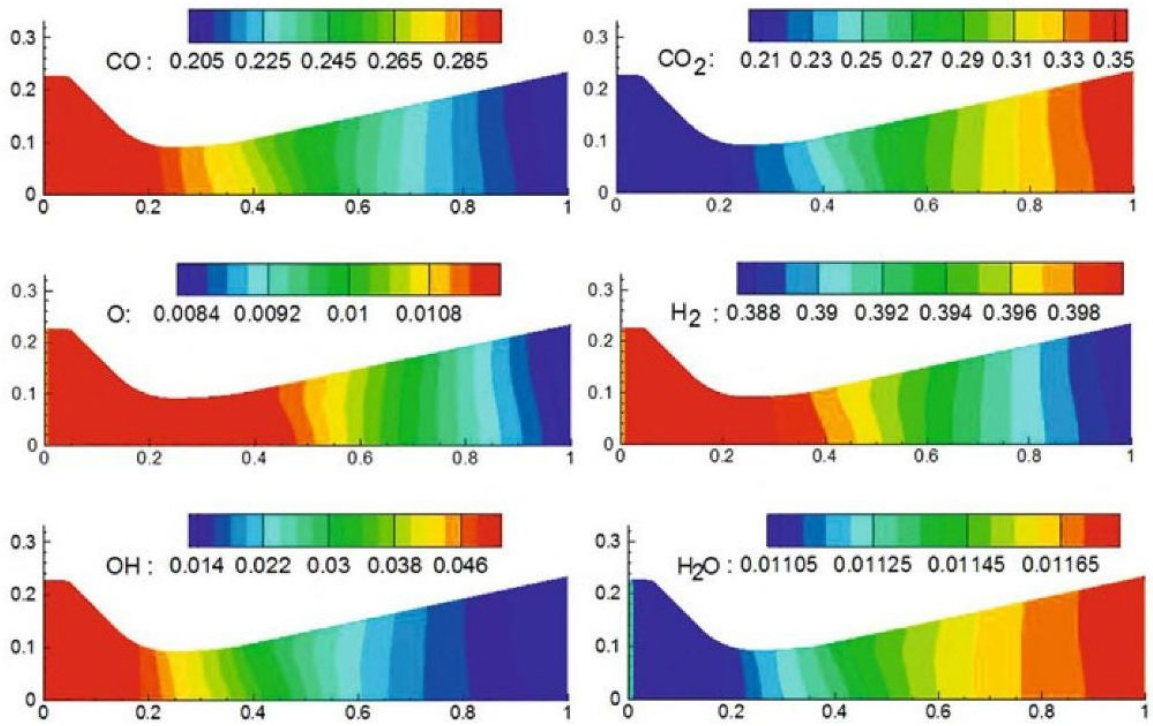

Fig. 2 Distributions of mass fractions of CO, CO_2, O, H_2, OH and H_2O in the baseline nozzle configuration

Table 3 The results of two nozzles

	Baseline	Optimized
Expansion ration	6.45	6.45
Nozzle throat diameter (m)	0.021	0.021
Vacuum thrust (kN)	87.08	89.31

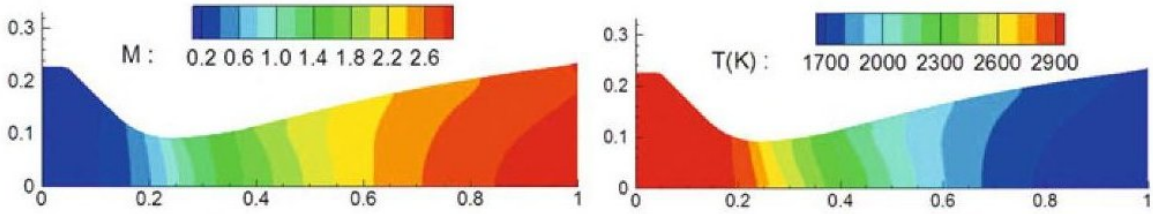

Fig. 3 Distributions of Mach number and temperature in the optimized nozzle configuration

the thrust of baseline and optimized nozzles. Approximately 2.6·of thrust increase is achieved in the optimized nozzle. Figure 3 shows the distribution of Mach number and temperature in optimized nozzle. As shown in figures, the design optimization produced a bell shape nozzle. Figure 4 shows the distribution of mass fraction of species. As in the baseline nozzle the mass fractions of H_2O and CO_2 increase, and the mass fractions of other species decrease in axial direction.

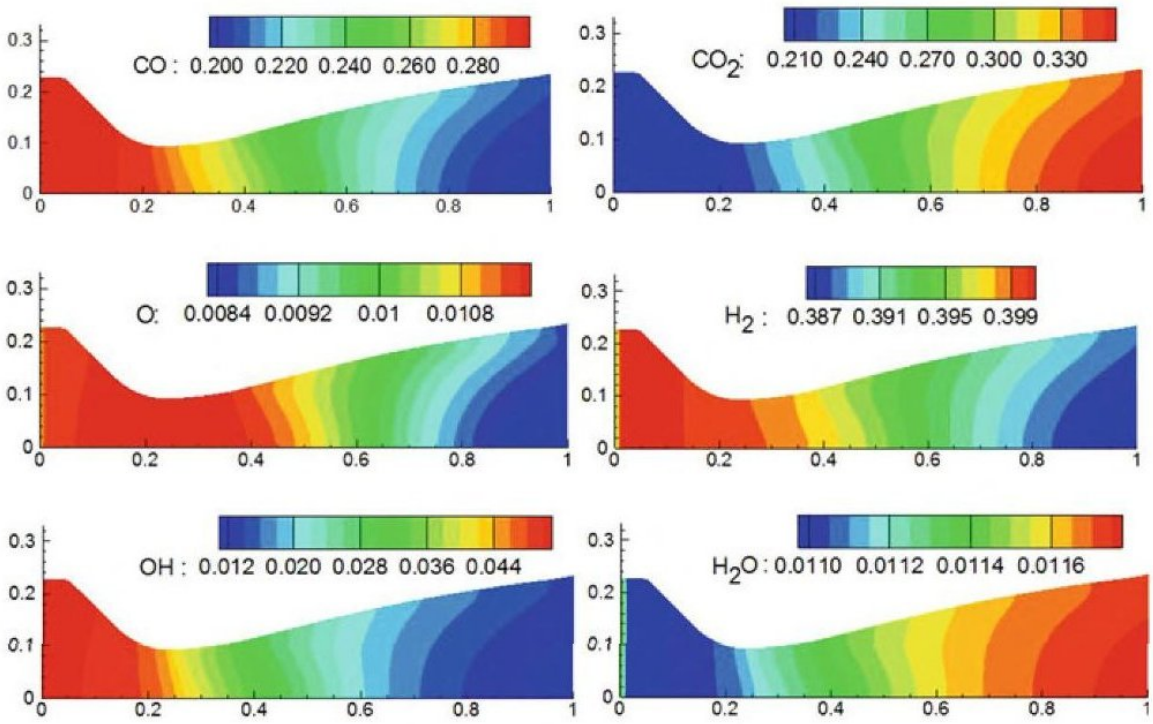

Fig. 4 Distributions of mass fractions of CO, CO_2, O, H_2, OH and H_2O in the optimized nozzle configuration

5 Conclusion

The presented design optimization method improves the performance of rocket nozzle in chemically reacting flows. Newton's solution method provides accurate and efficient sensitivity calculations. The present design optimization method employs Euler equations. The improvements in objective functions are calculated by solving Euler and chemical reaction equations for the baseline and the optimized geometries. A small improvement is achieved in thrust. A larger increase in thrust can be achieved by solving Euler and reaction equations during design optimization. Solving Euler and reaction equation with analytical Jacobian may also improve the performance of the solver.

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