PHYSICAL INSIGHT INTO FUEL MIXING ENHANCEMENT WITH BACKWARD-FACING STEP FOR SCRAMJET ENGINES VIA MULTI-OBJECTIVE DESIGN OPTIMIZATION

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Abstract

Fuel injection into crossflow behind a backwardfacing step is studied by means of multi-objective design optimization, aiming at fuel/air mixing for supersonic combustion of scramjet propulsion. A variety of injector configurations have been examined in the optimization process using evolutionary algorithms in conjunction with local search methods and surrogate modeling. Data mining has been performed by applying statistical techniques including variance-based sensitivity analysis to the surrogate models constructed with solutions from computational fluid dynamics. The injection angle and backward step height have been found to be the most influential design parameters on the mixing performance for the configurations considered in this study.

1 Introduction

Hypersonic air-breathing propulsion offers the potential for reliable and economical transport for access to space and high-speed atmospheric flight. In particular, scramjet (Supersonic Combustion Ramjet) propulsion is a promising technology that can enable efficient and flexible transport systems by removing the need to carry oxidizers and other limitations of conventional rocket engines. The last decade has seen remarkable milestones achieved by various flight exper-

iments including The University of Queensland's HyShot II in 2002[1, 2], the NASA X-43 vehicles in the Hyper-X program in 2004[3], and the Boeing X-51A WaveRider in 2010[4].

The scramjet mechanism critically depends on the sequential process - capture and compression of hypersonic airflow in the inlet, fuel injection into the air, supersonic combustion in the chamber, and expansion of combustion products through the nozzle for thrust. Fuel injection plays a major role in the flow process, responsible for efficient combustion and hence overall scramjet performance[5]. The airflow slows down from hypersonic to supersonic through the inlet, but further deceleration would lead to undesirable high static temperature and result in limited heat release due to excessive dissociation of nitrogen and oxygen gases[6]. The interactions between fuel and air including mixing, ignition and combustion occur at an extremely short timescale, rendering the development of efficient and reliable fuel injection systems of crucial importance.

The significance of fuel injection in airbreathing engines has brought about a considerable number of mixing techniques. Examples include: traverse/tangential injection through wall orifices[7, 8, 9], streamwise vortices with alternating wedges (hypermixers)[10, 11], shockenhanced mixing with alternative compression ramps and expansion troughs[12], and backward

transverse/inclined injection in the vicinity of a backward-facing step or a cavity[13, 14, 15, 16]. The last method, in particular, offers advantages in various aspects, in particular, self ignition and flame holding in the recirculation zone downstream of the step, where injected fuel is mixed with relatively slow airflow at high temperature.

A recent shock-tunnel experiment conducted by the authors observed strong interactions between recombination shock waves due to the reattachment of the separated shear layer and the inclined fuel jet adjacent to the reattachment point downstream of a backward-facing step (Fig. 1)[17]. The flow visualization via highspeed Schlieren suggested promising effects of the jet interactions on fuel/air mixing enhancement owing to the baroclinic torque induced by misaligned pressure gradient in conjunction with shear-induced Kelvin-Helmholtz vorticity. Former research efforts on fuel injection with a backward step have been made, with primary focus on the jet interactions and mixing characteristics for prefixed configurations[13, 14, 15, 16, 17], and no preceding research has studied geometric effects on the mixing performance systematically, to the knowledge of the authors.

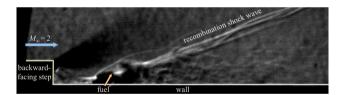


Fig. 1 Interactions of recombination shock waves with fuel injected into supersonic cross-flow behind a backward-facing step[17]

The present numerical study is undertaken to investigate the effects of the design parameters on the fuel/air mixing by means of multi-objective design optimization (MDO) using surrogate-assisted evolutionary algorithms coupled with computational fluid dynamics, which has been applied extensively to numerous optimization problems for scramjet engines[18, 19, 20]. The results from are examined by covariance-based sensitivity analysis using surrogate prediction to extract essential information on key design factors for this fuel mixing method. Flowfields

are visualized and scrutinized for representative configurations in comparison with the reference geometry in order to elucidate underlying flow physics that is responsible for the fuel behavior and mixing characteristics.

2 Approaches

2.1 Configurations and Conditions

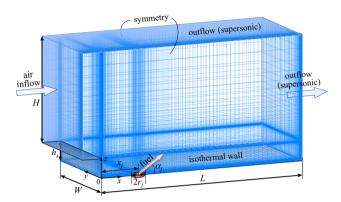


Fig. 2 Schematic of fuel injection into air crossflow downstream of a backward-facing step

The configuration considered in this study is schematically presented in Fig. 2, as per the settings experimental setups[17]. The flow conditions considered in this study are shown in Table 1 in terms of the Mach number (M), static and total pressures (p and p_0), and static and total temperatures (T and T_0), assuming sonic fuel injection into airflow incoming at Mach 2 with a dynamic pressure of 418 kPa and Reynolds number of 1.43×10^7 per unit length. Methane (CH₄) is used as fuel to be injected into crossflow of air, where both gases are assumed to be calorically perfect with a specific heat ratio γ of 1.32 and 1.4, respectively, in the present study. The fuel injection pressure p_i is adjusted according to the injector radius r_j to maintain the jet-to-freestream momentum flux ratio $J\left(\equiv \frac{(\rho V^2)_j}{(\rho V^2)_\infty}\right)$ at 1.43.

Table 1 Crossflow air and fuel injection conditions

	M	p [kPa]	p ₀ [kPa]	T [K]	<i>T</i> ₀ [K]
Air	2	150	1174	1100	1980
Fuel	1	910	7003	259	425

The floor is taken to be an isothermal wall, with the temperature maintained at 300 K for a

short test time in the impulse facility, as shown in Fig. 2, which displays the boundary conditions used in this paper. It also depicts the four design parameters, namely, the angle α_i , streamwise position x_i , and radius r_i of the fuel injector as well as the height of the backward-facing step h_s . The length (L, after the step), width (W), height (H) of the computational domain are fixed at 0.055 m, 0.02 m, 0.032 m, respectively, in concordance with the experimental setups[17]. The domain also include a 5 mm trailing-edge of the backward step at a height of h_s . Imposed at its entrance as an inflow is the profile of a turbulent boundary layer, which has grown over 30 mm from the leading edge of a flat plate, as per the experimental arrangement.

2.2 Computational Fluid Dynamics

Compressible flowfields in the presence of fuel injection are computed by utilizing a commercial solver CFD++ [22], which has been employed by the Australian hypersonics network for scramjet research due to its demonstrated fidelity in hypersonic aerodynamics[18, 19, 20]. An implicit algorithm with second-order spatial accuracy is used to solve the Navier-Stokes equations for viscous flowfields and convergence is accelerated by the multigrid technique. The boundary layer is taken to be fully turbulent and modeled by the two-equation SST k- ω RANS model. Steady flowfields are computed in the present study, which focuses on fuel/air mixing purely due to steady fluid dynamics and interactions, excluding effects of unsteady phenomena such as shear-induced vorticity motion.

Three-dimensional computational meshes are generated automatically by Glyph scripting on a commercial grid generator Pointwise[23] for the fuel injection configuration represented by the four design variables introduced in the former section. A fully structured mesh comprising 1,275,000 cells are generated for each configuration, based on the topology and mesh sensitivity study described in the preceding studies[20, 21]. The computational mesh is superimposed in Fig. 2 for the baseline geometry, which corresponds to the experimental model[17].

2.3 Multi-Objective Design Optimization



Fig. 3 Optimization chain

In order to conduct a design optimization for the injector in a coupled MDO/CFD approach, a process chain is set up and implemented, consisting of mesh generation (pre-processing), CFD computation (evaluation), post-processing and optimization algorithms, as schematically shown in Figure 3. Design optimization is performed by applying evolutionary algorithms, in particular, the elitist non-dominated sorting genetic algorithm (NSGA-II)[24, 25]. It is a populationbased approach that evolves the candidate solutions in the population pool over generations, enabling global search. Simulated binary crossover and polynomial mutation are used as recombination operators at a given probability (1.0 and 0.1, respectively, in this study) with a specified distribution index (10 and 20, respectively).

Multiple surrogate models including response surface models, radial basis function networks, kriging and multilayer perceptrons, are employed to mitigate the computational cost by replacing the CFD evaluations[26], trained regularly (every 5 generations in this study). Once surrogate models become available, hybrid (memetic) optimization is performed by incorporating local search methods including pattern search and sequential quadratic programming combined with adaptive weighting into evolutionary algorithms[27, 28]. Covariance-based global sensitivity analysis[29, 30] is applied to the solution archive resulting from CFD evaluations so as to investigate the effects of the decision variables (input parameters) on the objective functions (objective functions).

2.4 Design Criteria

The performance of fuel injection is evaluated by quantifying the resultant flowfields with respect to multiple criteria. High total pressure recovery is a desired feature in fuel mixing so as to enable effective combustion and high thrust production. This objective is targeted by minimizing the total pressure loss defined as $\Delta p_0 \equiv 1 - \frac{\int_x p_0 dm}{\int_{x=0} p_0 dm}$. Fuel penetration into the crossflow is another important characteristic of fuel injection. This criterion is assessed by the penetration height defined as $h_p \equiv \max \left(z \mid_{c_{\text{CH}_4} > 0.1 c_{\text{CH}_4}^s}\right)$ at the exit, where c_{CH_4} and $c_{\text{CH}_4}^s$ are the fuel mass fraction and its stoichiometric value (0.0548), respectively. It evaluates the fuel remaining in the mainstream without being captured in the recirculation region behind the backward step.

The mixing efficiency is commonly used to evaluate the mixing ability of transverse fuel injection by examining the fuel massflow with respect to the stoichiometric ratio for the outflow, but it is not deemed as a suitable criterion for the current configuration, where the recirculation zone plays a major role in fuel mixing and flame holding (in case of ignition and combustion). The fuel massflow deficit is thus considered in this study, defined as $\Delta \dot{m}_f \equiv 1 - \frac{\int_x d\dot{m}_f}{\int_{x=0} d\dot{m}_f}$, where \dot{m}_f is the fuel massflow rate. The nondimensionalized streamwise circulation is employed as the last metric to account for the overall effects of streamwise vortices, which plays a primary role in the fuel/air mixing[5, 12]. It is defined as: $\Gamma \equiv \frac{1}{ud} \int_{x} |\omega_{x}| dA$, where ω_{x} is the streamwise vorticity, u the crossflow velocity and d the effective injector diameter (1330 m/s and 1 mm, respectively).

2.5 Optimization Problem

Multi-objective design optimization is performed with these parameters, aiming to minimize Δp_0 and maximize h_f simultaneously. The geometric parameters introduced in Section 2.1 are employed as the decision variables. The optimization problem statement of this study is expressed as:

minimize:
$$\Delta p_0$$
 $-h_f$ subject to: $30^\circ \le \alpha_j \le 90^\circ$ $0.005 \, \text{m} \le x_j \le 0.015 \, \text{m}$ $0.0003 \, \text{m} \le r_j \le 0.001 \, \text{m}$ $0.0025 \, \text{m} \le h_s \le 0.01 \, \text{m}$

3 Results

3.1 Design Optimization

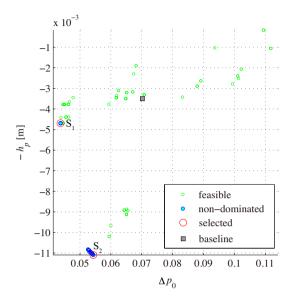


Fig. 4 Optimization results with CFD evaluations ($N = 12, 10^{\text{th}}$ generation)

An MDO coupled with CFD has been performed over 10 generations with a population size of N=12, primarily to obtain a minimal number of flow solutions that allows surrogate models to be trained for post analysis within the constraints of time and resources. The distribution of all individuals evaluated in the course of this run is displayed in Fig. 4, along with the non-dominated and representative configurations.

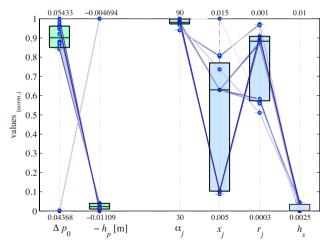


Fig. 5 Distributions of performance and design parameters with CFD evaluations

The correlations of the performance and de-

sign parameters (objective functions and decision variables) are shown as a parallel coordinate plot in Fig. 5 for all non-dominated solutions evaluated with CFD. A trade-off tendency between total pressure saving and fuel penetration is suggested by the fact that lines connecting corresponding values of Δp_0 and $-h_f$ intersect near the center point within their ranges. The lines for the decision variables indicate that the non-dominated configurations are commonly characterized by large injection angle (α_j) and low height of the backward step (h_s) close to their upper and lower bounds, respectively, whereas they are less decisive on the injector location (x_j) and radius (r_j) , as seen by scattered distributions.

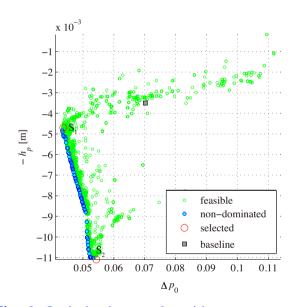


Fig. 6 Optimization results with surrogate prediction ($N = 60, 50^{\text{th}}$ generation)

An additional full-scale MDO has been performed over 50 generations with a population size of N=60, using estimation from surrogate models with the best accuracy in lieu of CFD simulations (the mean square error for the prediction of Δp_0 and h_f is 2.67% and 8.16%, respectively, with the kriging model). The resultant distribution plotted in Fig. 6 indicates the presence of a well-defined Pareto optimal front comprising the non-dominated individuals.

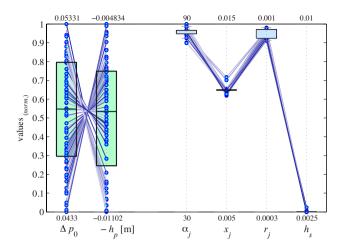


Fig. 7 Distributions of performance and design parameters with surrogate prediction

Figure 7 displays the correspondence between the objective functions and decision variables in the form of a parallel coordinate plot for all non-dominated individuals from surrogate prediction. A counteracting nature of the total pressure and fuel penetration is evident with the intersecting lines. A bundle of lines linking the decision variables suggest that the non-dominated configurations are associated with unique combinations of these variables about $\alpha_j \approx 90^\circ$, $x_j \approx 11.5$ mm, $r_j \approx 1$ mm, and $h_s \approx 2.5$ mm, in contrast to the MDO results from CFD (Fig. 5), where x_j and r_j were more flexible.

3.2 Data Reduction

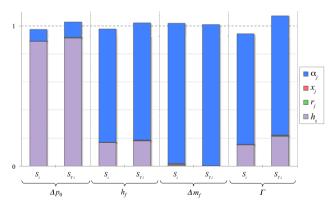


Fig. 8 Sensitivity indices

Statistical techniques have been applied to the optimization results so as to extract useful knowledge effectively. Figure 8 displays the sensitivity indices obtained with surrogate prediction for

10,000 sample data points. The first-order (S_i) and total-effect (S_{T_i}) indices from the input parameters $(\alpha_j, x_j, r_j, \text{ and } h_s)$ are plotted for the output parameters, *i.e.*, objective functions (Δp_0) and h_f and additional design criteria, that is, the fuel massflow deficit Δm_f and streamwise circulation Γ (for which the best prediction is given by the kriging with m.s.e. of 3.03% and 4.40%, respectively). It is seen that all output parameters are predominantly influenced by two parameters, namely, the injection angle α_j and backward step height h_s , with minor or negligible influence of the other two parameters (x_i) and (x_i) .

Further data mining has been performed, with particular focus on the impact of these two dominant design parameters. Figures 9-12 display the variations of the output parameters in response to these two input parameters. The colored dots represent the values from all CFD solutions, whereas the floor contours are based on surface fitting of surrogate-predicted points via linear least squares with 10%-span robust bi-square weighting (the R-squared values are shown in the captions).

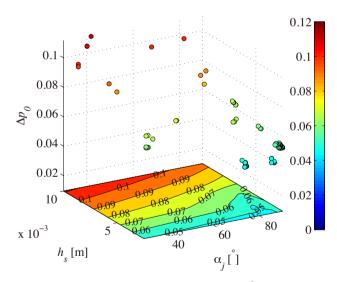


Fig. 9 Total pressure loss variation ($R^2 = 0.977$)

In Fig. 9, Δp_0 increases almost linearly as the step height h_s increases. The injection angle α_j has rather minor influence, but it is interesting to note that larger total pressure is incurred at lower injection angles, opposite to the tendency commonly observed in transverse injection studies[31]. This may partly be due to the fact that a higher injection angle causes a larger

amount of fuel with a higher total pressure (as seen in Table 1) carried downstream to the exit, which effectively compensates the total pressure loss from a stronger bow shock.

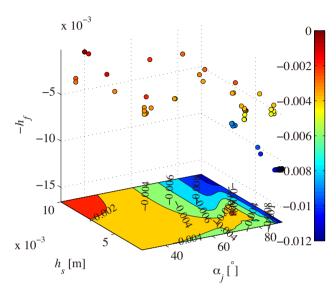


Fig. 10 Fuel penetration height variation ($R^2 = 0.944$)

On the other hand, higher fuel penetration h_f at the exit is achieved with higher injection angles (Fig. 10). The contour suggests that large step heights tend to be associated with greater fuel penetration on the whole, but this trend is somewhat blurred near the lower bound of the injection angle ($\alpha_j \approx 30^\circ$) as well as the lower height limit ($h_s \approx 2.5$ mm).

Figure 11 indicates substantial changes in the fuel massflow deficit with the increase in both injection angle and backward step height. It suggests that the portion of the fuel poured into in the recirculation zone decreases at higher injection angles and that the injection angle exerts influence on the pooled fuel amount over a wider range with higher backward steps. It is notable that most fuel remains in the recirculation zone $(\Delta \dot{m}_f \approx 1)$, with little influence of the injection angle (except high angles $\alpha_j \approx 90^\circ$) at low step heights $(h_s \approx 2.5 \text{ mm})$.

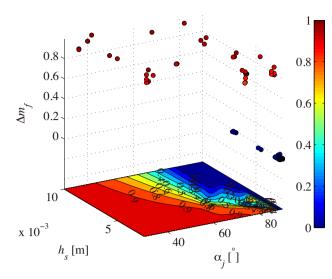


Fig. 11 Fuel massflow deficit variation ($R^2 = 0.848$)

Figure 12 shows considerable dependency of the streamwise circulation on the two design parameters. In particular, Γ increases drastically in the vicinity of normal injection ($\alpha_j \approx 90^\circ$). It grows further with larger backward step heights, associated with enhanced generation of streamwise vortices, while there is a little ambiguity near the lower bound ($h_s \approx 2.5 \text{ mm}$) especially at high injection angles ($\alpha_i \approx 90^\circ$).

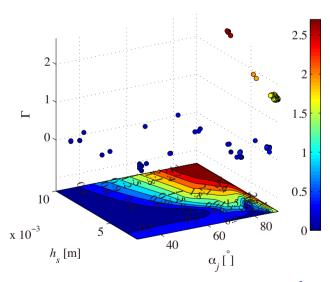


Fig. 12 Streamwise circulation variation ($R^2 = 0.841$)

In order to probe into the tendencies observed above, two individuals among all solutions evaluated with CFD are selected to represent the superior individuals with respect to the two objective functions, denoted as S_1 and S_2 , as plotted

in Figs. 4 and 6. The design parameters of these geometries are shown in Table 2 and compared in Fig. 13, along with the output parameters.

Table 2 Design parameters of baseline and selected configurations

	_			
	α_j [°]	x_j [mm]	r_j [mm]	h_s [mm]
baseline	60.0	10.0	1.00	5.00
S_1	86.4	13.0	0.98	2.50
S_2	88.7	11.3	0.91	2.85

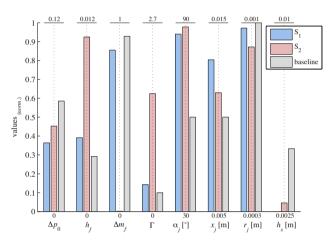
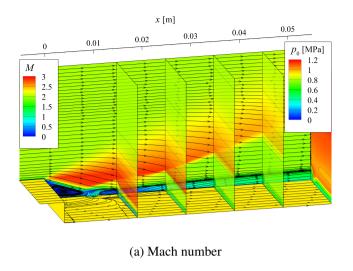
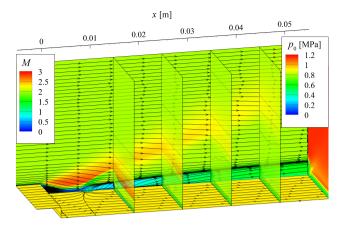


Fig. 13 Comparison of performance and design parameters for representative configurations

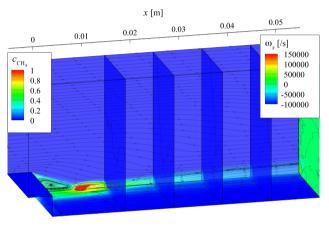
3.3 Flowfields

The flowfields associated with the baseline and selected configurations are plotted in Figs. 14-16. The first image of each figure set displays the Mach number distributions on the symmetry plane (y = 0 m) and cross sections with an equal interval of 0.05 m, except on the exit plane $(x = 0.055 \,\mathrm{m})$, where the total pressure distribution is plotted instead for the evaluation of the total pressure recovery. Streamlines are plotted on the symmetry plane, based on the velocity components (u and w), while those plotted on the floor are based on the surface shear stress (τ_x and τ_{z}). The second image shows the distributions of the fuel mass fraction on the symmetry and floor planes as well as equally-spaced streamwise stations, except at the exit plane, where the streamwise vorticity is plotted instead to allow the examination of the streamwise circulation.





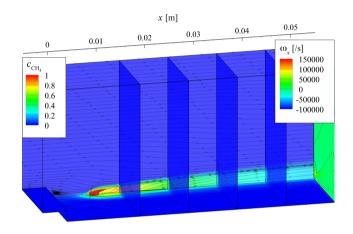
(a) Mach number



(b) fuel mass fraction

Fig. 14 Flowfields of baseline configuration

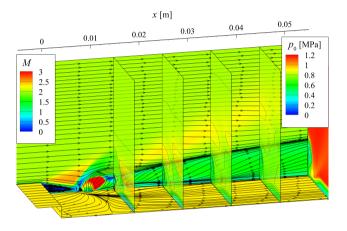
Figure 14 shows the flowfield due to the baseline configuration, corresponding to the Schlieren visualization in Fig. 1 from a shock-tunnel experiment[17]. The Mach number distribution and streamlines plotted on the symmetry plane in Figure 14 (a) indicate the presence of a fuel core stream that locally propagates in a region around the centerline, as well as the effects of the fuel injection that takes place near the downstream end of the recirculation region. The floor streamlines are indicative of fairly localized influence of fuel injection bounded in the vicinity of the symmetry plane. The fuel mass fraction distributions in Fig. 14(b) also suggests rather localized fuel propagation predominantly in the recirculation zone closer to the symmetry plane. Consequently little fuel is contained in the outflow at the exit, where rather weak streamwise vorticity is observed.



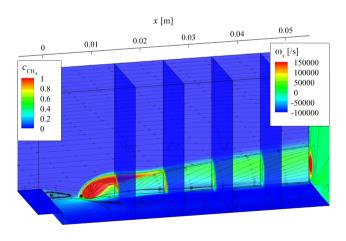
(b) fuel mass fraction

Fig. 15 Flowfields of S₁ configuration

The S₁ configuration is characterized with a higher injection angle, downstream injector position, and a half step height, as compared to the baseline geometry. The injector is located downstream of the nominal end of the recirculation zone in contrast to the baseline case, as seen in the floor streamlines in Fig. 15(a). In spite of these differences in the geometric arrangements, however, the major characteristics of the flowfield appear to be similar to those observed with the baseline injector as a whole, in terms of the extent of the jet-crossflow interactions. The fuel mass fraction distributions plotted in Fig. 15 (b), on the other hand, reveal a different behavior of the injected fuel in the recirculation zone, where its propagation appears to be rather inactive, in comparison with the baseline case according to the fuel distributions on the symmetry and floor planes. This difference, however, has resulted in a rather small decrease in the fuel massflow deficit (Fig. 13), suggesting a large portion of the fuel remains in recirculation, off the symmetry plane and floor wall. A considerably higher total pressure recovery is achieved at the exit with this configuration, which may be attributed primarily to a moderate shock loss due to a lower backward step height and secondarily to a slightly increased fuel massflow, which possesses higher total pressure than the airflow (as seen in Table 1).



(a) Mach number



(b) fuel mass fraction

Fig. 16 Flowfields of S₂ configuration

The S_2 configuration is also characterized with a high injection angle and low step height, similarly to the S_1 configuration, but features a relative injector position that is similar to the baseline geometry, in that the fuel injector is submerged in the recirculation region. The resultant

flowfield in Fig. 16(a), however, reveals a distinctly different flow structure characterized by various features typically observed in transverse fuel injection into supersonic crossflow such as the presence of a supersonic region within the under-expanded jet bounded by a barrel shock and Mach disk[31]. This characteristic flowfield, similar to that observed experimentally by Kuratani *et al*.[15], can be attributed to the relatively strong injection at a near-normal angle, which penetrates the recirculation zone and reaches out to the main airstream, where the corner expansion around the backward-facing step is not too immense for the resultant bow shock to suppress the growth of the fuel jet at the interface, in contrast with the baseline case in Fig. 14(a). As a consequence a large portion of the fuel is injected into the outer crossflow and mixed with the air owing to strong counter-rotating streamwise vortices, as seen in Fig. 16(b). A small fraction of the injected fuel is fed into the recirculating flow in this case, resulting in virtually no fuel massflow deficit measured at the exit (Fig. 13).

3.4 Summary

Key insights obtained in this study are summarized in Table 3 with respect to the effects of the major design parameters, *i.e.*, injection angle and step height, on the performance parameters:

Table 3 Effects of major design parameters

	Δp_0	h_f	$\Delta \dot{m}_f$	Γ
$\alpha_j \uparrow$		\uparrow	\	\uparrow
$h_s \uparrow$	\uparrow	_	\downarrow	\uparrow

4 Conclusions

A multi-objective design optimization has been performed for methane injected into crossflow downstream of a backward-facing step located in supersonic freestream at Mach 2, assuming fuel injection and mixing for supersonic combustion in scramjet engines. Hybrid optimization approaches combining evolutionary algorithms and local-search methods assisted by surrogate modeling have been applied to the fuel injector design, coupled with high-fidelity computational

fluid dynamics. Four design parameters are employed as the decision variables, namely, the injector angle, streamwise position, and hole radius, as well as the height of the backward step. The total pressure loss and fuel penetration height are used as the objective functions to be minimized and maximized, respectively. Sensitivity analysis has been applied to these parameters along with other two design criteria, that is, the fuel massflow deficit and streamwise circulation. Injection flowfields have been scrutinized for selected configurations. Two classes of flow structures have been identified, characterized by pronouncedly different shock structures resulting from jet crossflow interactions. The injection angle and backward step height have been found to be the dominant design factors, while the other two play a subordinate role in fuel mixing for the configurations and variable ranges considered in this study. High injection angle and low step height are favored for higher total pressure saving and fuel penetration as well as enhanced fuel/air mixing at the downstream exit. However, lower injection angle and low step height may be preferred if priority is given to fuel mixing and flame holding in the recirculation region behind the backward step. Shock-tunnel experiments are planned by the authors in order to examine the insights gained through the present investigation.

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