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ADJOINT METHOD FOR CONTROLLED CAVITATION INVERSE NOZZLE DESIGN

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ABSTRACT−A mathematical methodology is proposed for designing nozzle hole shapes producing controlled geometric cavitation. The proposed methodology uses an unstructured RANS flow solver, with the ability to compute sensitivity derivatives via an adjoint algorithm. The adjoint formulation for the N-S equations is presented while variation of the turbulence viscosity is not taken into account during the geometry modifications. The sensitivities are calculated in a mode independently of the shape parameterisation. The method is used to develop and evaluate conceptual shapes for nozzle hole cavitation reduction. The localized region at the hole inlet producing cavitation, is parameterised using its radius of curvature, while a cost function is formulated to eliminate the negative pressures present at this location. Sensitivity derivatives are used to assess the dependence of the localized region on the minimum pressure, and to drive the geometry to the targeted shape. The results show that the computer model can provide nozzle hole entry shapes that produce predefined flow characteristics, and thus can be used as an inverse design tool for nozzle hole cavitation control.

KEY WORDS : Adjoint method, Cavitation, Optimization, Sensitivity derivatives, Parameterisation

1. INTRODUCTION

Computational methods for designing geometries with desired flow characteristics are very appealing. Not until recently has computational fluid dynamics been proven a valid means of even predicting the formation of cavitation, and much less developing methods to control it. Brewer *et al.* (2003) developed a method for cavitation delay in hydrofoils. Controlling cavitation greatly depends on the nozzle design characteristics and operating conditions. In most diesel injectors operating at high pressure exceeding 1500bar, cavitation initiates to the entrance of the nozzle hole. Under most cases, the cavitating structures finally reach the nozzle hole exit. Although that the effect of cavitation on the spray formation still remains largely unknown, it is well recognised that uncontrolled cavitation induces spray-to-spray and cycle-to-cycle variations; that, in turn, increases engine exhaust pollutant emissions. The objective of the present study is to design nozzle hole shapes that reduce or even eliminate the local minimum/negative pressure region formed at the entry of hole-type nozzles, and in which geometric cavitation initiates.

The goal of any design optimization process is to systematically evolve from some initial design to an optimized design. Optimization problems can be addressed through the minimization of a 'cost function' with respect to some appropriately defined design variables. During the last decade numerous algorithms for gradient-based optimization have been developed. The adjoint method has been used in application from hydrodynamics and compressible flows (Soto and Löhner, 2001a; 2001b) or aerodynamics and compressible flows (Jameson, 1988; Jameson, 1994; Anderson and Venkatakrishnan, 1997; Petropoulou *et al.*, 2002).

The proposed method, like any other gradient-based method, requires gradient information, i.e. sensitivity derivatives. These are obtained by formulating and solving for the Adjoint equations. The latter are derived by enforcing the flow equations as constraints to the cost function via the concept of Lagrange multipliers.

In this work, an unstructured Reynolds-Average Navier-Stokes (RANS) flow solver capable of computing sensitivity derivatives is used. Unstructured grids can handle arbitrarily complex geometries, via a completely automated re-meshing approach. Sensitivity analysis allows computation of gradient-based information, which, in turn, gives information on how geometry modifications affect cavitation inception.

Furthermore, it is desirable that local geometry regions of importance to be defined by a minimum number of control points. This process of representing the actual

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geometry by control points is called parameterisation.

The optimization algorithm usually consists of a number of computational iteration cycles, during which the cost function is minimised. At each cycle, a solution of the flow equations (direct solution) and a solution of the adjoint equations (inverse solution) are performed. The shape to be optimised is modified using the derivatives of the cost function with respect to the design variables. The gradient of the cost function at each location of the design space are dependent on the flow field and the costate variables distribution along the wall boundary to be designed. So, the combined solution of the flow field and the adjoint equations may lead to the calculation of the exact values of the sensitivity derivatives.

The adjoint method has a number of advantages relative to other gradient-based methods, for example finite differences. Apart from its fast convergence, it provides the gradients of the cost function in a way that the computational effort required for this calculation is independent of the number of the design variables. This is very important in nozzle re-design cases, were the parameters that effect cavitation may be numerous.

Following, the derivation of the Adjoint formulation and the overall algorithm for the inverse design calculation are described. Then, inverse design of an axisymmetric single-hole nozzle is performed. Experimental data for this nozzle are available in (König, 2002), which verify that the parameterisation parameters chosen indeed control and even eliminate cavitation inside the tested nozzle.

2. OPTIMIZATION PROCEDURE

In order to handle the problem of controlling cavitation as an inverse design problem, the cost function formed ensures increase of the pressure in the local areas where negative values appear. A desired target pressure distribution along the boundary of the nozzle is given, and then the following cost function is defined:

$$I_C=\frac{1}{2}\oint_{\partial V}(p-\bar{p}_t)^2 ds-\oint_{\partial V}\vec{n}(p-\bar{p}_t)\mu\frac{\partial\vec{u}}{\partial\vec{n}}ds\,, \qquad (1)$$

where p and $\bar{p}_t$ represent the current and target pressure respectively, $\vec{n}$ is the normal unit vector along the boundary and μ is the effective viscosity. W stands for wall and is the boundary of the geometry to be modified.

The last integral is zero for incompressible flows; nevertheless, it is added to the cost function for the well posedness of the problem.

The flow equations R(U), $U=(u, v, p)$ for incompressible flows, in tanist form reads:

$$\begin{aligned}&\frac{\partial\rho}{\partial t}+\nabla\cdot(\rho\vec{u})=0\,,\\&\frac{\partial}{\partial t}(\rho\vec{u})+\nabla\cdot(\rho\vec{u}\otimes\vec{u}-T)=\vec{f}_\sigma\end{aligned} \qquad (2)$$

where, $T=-pI+\mu(\nabla\otimes\vec{u}+(\nabla\otimes\vec{u})^T)$ and ${}^1f_\sigma$ is the source term in this case equal to ρg with g being the acceleration of gravity.

The GFS code, which is an unstructured RANS finite volume incompressible flow solver, has been used for the calculation of the single-phase internal nozzle flow distribution, using a pressure correction methodology.

Various differentiation schemes and solvers are used for the solution of the momentum equations while turbulence is modelled by the k-ε model. However, during the formulation of the Adjoint equations, the variation in the turbulence viscosity $\mu=\mu d+\mu t$ attributed to the geometry modifications has been considered negligible. There is the option of considering the variation $\delta\mu$ and formulate the adjoint of the turbulent equations. However, this approach requires a lot of computational time compared to the actual effect on the correctness of the adjoint solution and gradients.

The steady-state flow equations R(U) are integrated and introduced as constraints to the problem. Then, the state variables can be uniquely determined for a given set of control points in the domain of interest. The cost function I_C is augmented to the weak form of the constraints, through the Lagrange multiplier $\vec{\Psi}$ to give I_{aug}:

$$\begin{aligned}I_{aug}&=I_C+\int_V\vec{\Psi}\cdot R dV=\\&=I_C+\int_V\Psi_p\cdot\nabla\cdot(\rho\vec{u})dV+\int_V(\Psi_1,\Psi_2)\nabla\cdot(\rho\vec{u}\otimes\vec{u}-T)dV=\\&=I_C+\oint_{\partial V}\Psi_p\cdot(\rho\vec{u})\vec{n}ds+\oint_{\partial V}(\Psi_1,\Psi_2)\cdot(\rho\vec{u}\otimes\vec{u}-T)\vec{n}ds-\\&-\int_V\nabla\Psi_p\cdot(\rho\vec{u})dV+\int_V\nabla(\Psi_1,\Psi_2)\nabla\cdot(\rho\vec{u}\otimes\vec{u}-T)dV,\end{aligned} \qquad (3)$$

where, $\vec{\Psi}=(\Psi_1,\Psi_2,\Psi_p)^T$ is the vector of the costate variables, V is the computational domain bounded by its contour ∂V, and $\vec{n}=(n_x,n_y)$ is the outward normal vector along ∂V. The surface integrals are calculated from the application of the Green-Gauss theorem. The sensitivity derivatives of I_C with respect to the design variables are obtained by taking the variational form of I_{aug}.

In the next paragraph, the formulation of the Adjoint equations is discussed in detail.

2.1. Formulation of the Adjoint Equations

The derivation of the Adjoint equations and the sensitivity derivatives of the cost function with respect to the design variables closely follow classical techniques from the calculus of variation and the theory of Lagrange multipliers. Any modification of the design variables $\delta\vec{D}$ results to a corresponding variation to the body shape. This, in return, produces a variation to the computational domain and the flow solution $\vec{U}$. The variation of the flow variables values consist of a convective part (due to the displacement of the domain boundary) and the local variation $\delta\vec{U}$. Thus, the new values of the flow variables read:

$$\vec{U}^{new}=\vec{U}^{old}+\nabla\vec{U}\cdot(\delta x,\delta y)+\delta\vec{U} \quad (4)$$

Applying the formula of Eq. (4) along with the variations of the geometrical quantities to I_{aug}, its variational form is obtained. Terms are grouped into field and surface integrals that multiply variations $\delta\vec{U}$, $\delta\vec{\Psi}$ and $\delta\vec{D}$. In order to obtain δI_{aug} independently from the variation of $\delta\vec{U}$ and the costate $\delta\vec{\Psi}$ variables, the corresponding integrals must be vanished. Eliminating the field and surface integrals that multiply $\delta\vec{\Psi}$, the flow equations and their boundary conditions are obtained, whilst the corresponding elimination of terms multiplying $\delta\vec{U}$ provide the costate equations along with their boundary conditions. Due to the presence of the derivatives of the velocity components u and v appearing in the diffusion part of the flow equations the grouping of terms multiplying the variation of velocities δu and δv is not straightforward. It is accomplished by a second application of the Green-Gauss theorem. This gives rise to second derivatives of the co-state variables multiplying the variations $\delta\vec{U}$ and the surface integral containing first derivatives of the vector of the costate variables $\vec{\Psi}$. The later integrals, multiplying variations $\delta\vec{U}$ along boundaries, contribute to the boundary conditions for the Adjoint equations. After the addition of the time variation of the costate variables, the Adjoint equations take the form:

$$\frac{\partial\rho}{\partial t}-\nabla\cdot\left(\rho\vec{\Psi}\right)=0$$
$$\frac{\partial}{\partial t}\left(\rho\vec{\Psi}\right)-\rho\vec{u}(\nabla\otimes\vec{u}+(\nabla\otimes\vec{u})^T)-\nabla\cdot T=\vec{f_\sigma}\,, \quad (5)$$
$$\text{where } T_{adj}=-\rho\Psi_p I+\mu\left(\nabla\otimes\vec{\Psi}+\left(\nabla\otimes\vec{\Psi}\right)^T\right).$$

Appling the no slip flow condition in equation (5) and combining the remaining terms with the boundary terms, the cost function $\vec{\Psi}=-\vec{n}(p-\bar{p}_t)$ is obtained as boundary condition for the shape to be modified. The resulting system of equations is a convection-diffusion system, where information transfer takes place in the opposite direction of the information propagation of the costate variables in relation to the flow variables.

The remaining terms correlate the variation of I_{aug} with the variation of the design variables, for the derivation of the sensitivities. Having the Adjoint equations being solved, the sensitivity derivatives can be easily computed. They consist of the boundary distribution of the costate variables and their derivatives combined with terms arising from δ_{IC} plus the remaining terms resulting from the diffusive part of the Adjoint system calculation that multiplies the variation of the velocities δu and δv. Terms involving $\nabla\vec{U}\cdot(\delta x,\delta y)$ are eliminated from the boundary conditions. So the variation of I_{aug} reads:

$$\delta I_{aug}=\frac{1}{2}\oint_W (p-\bar{p}_t)^2\,\delta(ds)+\oint_W p\vec{\Psi}\,\delta(\vec{n}ds)$$
$$+\oint_W \vec{n}\left(\mu\left(\nabla\otimes\vec{\Psi}+\left(\nabla\otimes\vec{\Psi}\right)^T\right)\right)\delta\vec{u}\,. \quad (6)$$

Expressing the velocities on the new surface in a Taylor series and noting that the velocities on the old and new surface are both zero, the variation of the velocity components can be written in the following manner that contribute to the sensitivity derivatives:

$$\delta\vec{u}=-\frac{\partial\vec{u}}{\partial x}\delta x-\frac{\partial\vec{u}}{\partial y}\delta y \quad (7)$$

The above variational expressions can be also significantly simplified by the substitution of the normal vector's definition:

$$\delta(\vec{n}ds)=\delta((n_x,n_y)ds)=$$
$$=\delta\left(\left(\frac{dy}{ds},\frac{dx}{ds}\right)ds\right)=(\delta(dy),-\delta(dx)) \quad (8)$$

Considering the design points to be Di where $i = 1, n$, the variations of the geometrical quantities in δI_{aug} read:

$$\delta(ds)=\sum_{i=1}^{n}\frac{\partial(ds)}{\partial D_i}\delta D_i,$$
$$\delta(dy)=\sum_{i=1}^{n}\frac{\partial(dy)}{\partial D_i}\delta D_i, \quad (9)$$
$$\delta(dx)=\sum_{i=1}^{n}\frac{\partial(dx)}{\partial D_i}\delta D_i.$$

After replacing the variations $\delta(dx)$, $\delta(dy)$ and $\delta(ds)$ of δI_{aug}, an expression for the sensitivity derivatives is obtained. So the final form of the sensitivity derivatives with respect to the design variables will be concluded after the definition of the shape parameterisation and the consequence derivation of the variations of the above geometrical entities.

The update of the control points location is carried out through a steepest descend scheme, reading:

$$D_i^{new}=D_i-\eta\frac{\partial I_{aug}}{\partial D_i}, \quad (10)$$

for positive η values. By using the gradient of the cost function, the search on the design space is limited to a specific direction, rather than randomly searching the entire n-dimensional space. The proper choice of the scalar parameter η provides the minimum for the current search direction.

2.2. Solution Procedure

The optimization procedure is constituted by individual cycles for the progressive improvement of the nozzle shape as the cost function tends to zero. Each cycle consists of the flow field calculation and the Adjoint equations calculation, as well as the computation of the objective function derivatives with respect to the design variables. Finally a correction scheme for updating the values taken on by the design variables (using the steepest descent scheme) is used. The numerical solution of the flow and the Adjoint equations bear almost exclusively the burden of computational cost. Having in mind that the computational cost for the solution of the Adjoint equations is almost equal to the computational time for the direct problem, each design cycle is almost equivalent to two direct solutions.

The same numerical scheme used for the flow solution is used for the solution of the Adjoint system of equations. Nevertheless the variation of the turbulent viscosity is considered to be negligible and does not play significant part in the gradient calculation. This is a convenient assumption from the numerical point of view and quite realistic for slight changes of the geometry from cycle to cycle.

For the parameterisation of the modified geometry the radius of curvature at the hole inlet is used as the only parameter. In this way, only the localized region affecting cavitation inception is parameterised and reproduced in every optimization cycle. The hole diameter, the hole length as well as the upstream nozzle geometry remain unaffected. Work is in progress to include more parameters in the parameterisation like the hole inlet diameter and the needle seat angle as well as extension of the method for 3D nozzles.

The mesh generation is fully automated, taking place at the beginning of each optimisation cycle after the parameterisation. The required computational unstructured grid is generated using an inhouse software based on a typical advancing front method. The grid generation software is very fast, so it is repetitively used within each cycle to create the computational grid for every new nozzle shape.

3. TEST CASE–RESULTS

A single-hole axisymmetric nozzle hole has been selected to test the capability of the developed computer code. The actual nozzle designs are shown in Figure 1. For this injector detailed experimental and computational results have been presented recently (König and Blessing, 2002; Giannadakis *et al.*, 2004). Three transparent nozzles, corresponding to 0%, 9.5% and 18% hydrogrinding have been made (König, 2002) and operated under a variety of injection and back pressures. The diameters of the

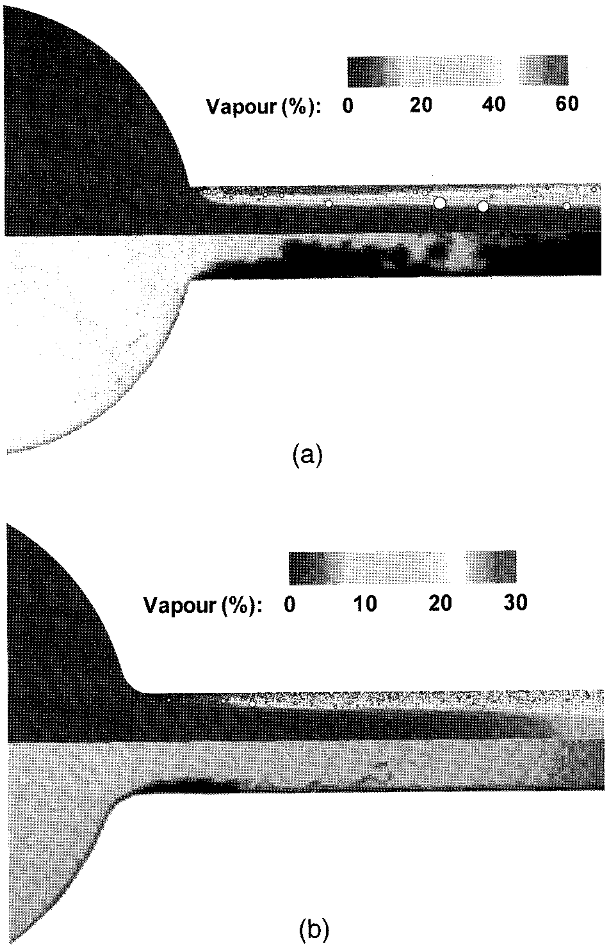

Figure 1. Single-hole nozzles for (a) 0% and (b) 9.5% hydrogrinding. The calculated void fraction distribution is shown for comparison with the CCD images, taken from (Giannadakis *et al.*, 2004).

nozzles were $D_{0\%HE}$=205 μm. The needle lift for both cases was h=250 μm. In all cases pressure boundary conditions were applied for both the inlet and the outlet of the nozzle. The simulations were steady-state and constant injection pressure of p_{Inj}=1000 bar and constant outlet pressure of p_{Exit}=20 bar were used. The sharp-inlet nozzle, shown in Figure 1a, was found to be highly cavitating, the 9.5% nozzle, shown in Figure 1b, was less cavitating while the last one, the 18% nozzle, was cavitation-free for all cases tested. As clear, changing the hole inlet radius of curvature, the cavitation intensity can be modified. That also affects the nozzle discharge coefficient which varies considerably between the non-cavitating and the fully cavitating cases.

Figure 2 shows the predicted blockage (dimensionless cross sectional area at the nozzle hole exit occupied by cavitation bubbles), as calculated by a recently developed cavitation model (Giannadakis *et al.*, 2004). This is a

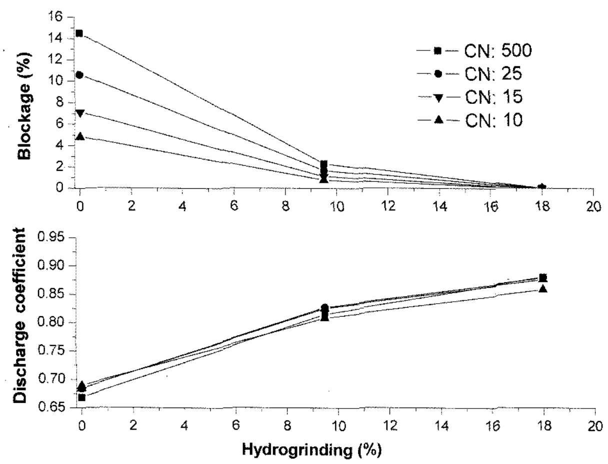

Figure 2. Predicted nozzle hole exit blockage and discharge coefficient as function of inlet radius of curvature and cavitation number.

function of the hole inlet radius of curvature and the cavitation number. Here, the cavitation number is defined as $CN=(P_{INJ}-P_{BACK})/(P_{BACK}-P_{VAPOUR})$. As it has been shown in a number of studies, for example (Soteriou *et al.*, 1995), the cavitation number is the major dimensionless number used to characterise the onset of cavitation, the flow regimes formed inside the injection hole and the reduction of the discharge coefficient with increasing cavitation levels. Based on those flow characteristics, the cost function was formulated in such a way that a targeted pressure distribution along the wall surface, for fixed inlet and back pressure conditions, is specified. Two target pressure distributions are shown in Figure 3.

The target pressure distribution in all the cases is calculated using the flow solver for a target geometry. Experimental data for this geometry indicate that it is cavitation free.

On the same graph, the pressure distribution corresponding to the initial nozzle design is also plotted. The model was then employed to re-construct the geometry of the targeted pressures. The corresponding results are also presented on the same Figure 3.

As it is clear, after a few iterative solutions for the flow field and the Adjoint equations, the code converges to the desired pressure and nozzle shape. Parametric runs (not shown here) starting from different initial nozzle designs

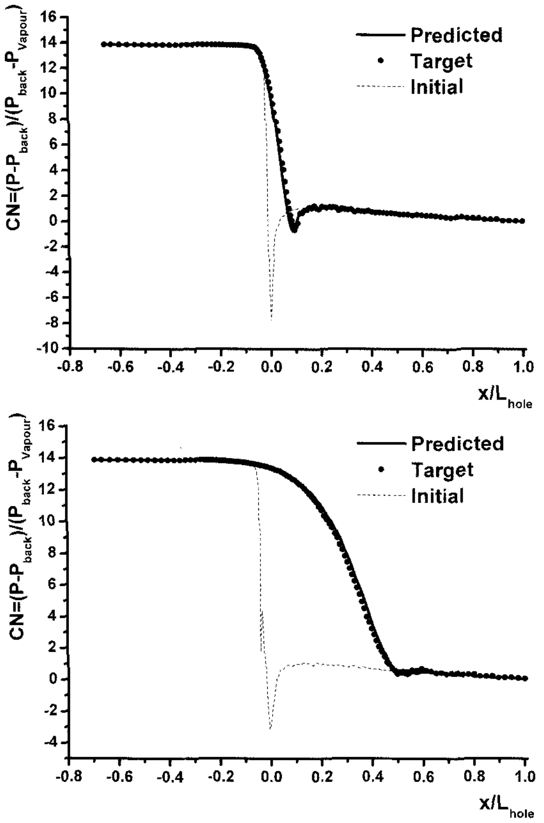

Figure 3. Target dimensionless (CN) pressures for two nozzle designs, pressure corresponding to an initial geometry and model predictions after convergence.

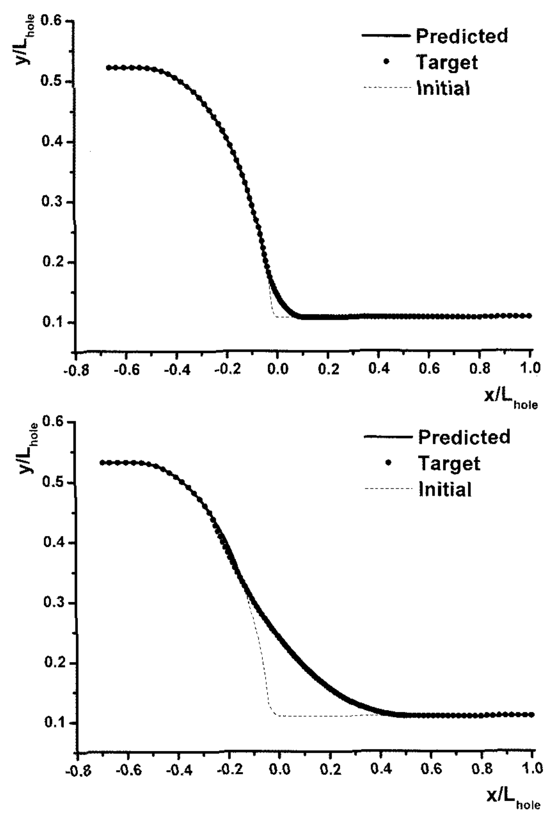

Figure 4. Initial and targeted nozzle designs and model predictions for the two test cases investigated.

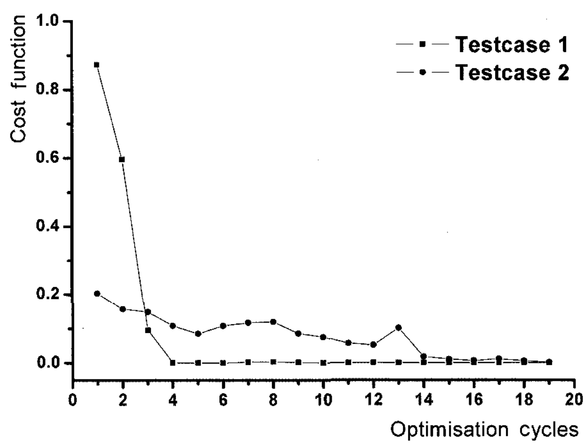

Figure 5. Convergence history of the cost function for the two test cases investigated.

have resulted to the same final geometry. Figure 4 shows the initial geometry, the targeted geometry and the geometry predicted by the computer model after convergence for the two test cases investigated. The model predicts the specified pressure distribution and nozzle geometry. Finally, Figure 5 shows the convergence history for the two test cases. As can be seen, for the test case selected, the model converges after a few iterations and stabilises to almost zero cost function value.

4. CONCLUSION

A mathematical methodology has been described for inverse design of diesel nozzle hole geometries. The method was used to develop and evaluate conceptual shapes for nozzle hole cavitation reduction. The target pressure distribution along the nozzle hole wall can be selected in such a way that the nozzle can be either cavitation-free or to have a specified cavitation intensity, which corresponds to a required nozzle discharge coefficient. The proposed methodology uses an unstructured RANS flow solver, with the ability to compute sensitivity derivatives via an Adjoint equations algorithm. The localized region affecting cavitation inception is parameterised and represented by its radius of curvature. An objective function was formulated in such a way that the negative pressures present at the hole inlet for sharp inlet corners are reduced or even eliminated. Sensitivity derivatives were used to assess the dependence of the localized region on the minimum pressure region, and to drive the localized modification to the targeted shape.

The results have demonstrated that the developed methodology converges to the targeted nozzle shapes only after a few iterations. Work is in progress for applying the developed methodology to multi-hole nozzles, where more complicated parameterisation is required for describing the nozzle design.

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