

Geometrical inverse problems in three-dimensional non-linear steady heat conduction

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This paper presents results of research involving the inverse thermal design of coolant flow passage shapes in arbitrary, three-dimensional, internally cooled configurations. A computer program has been developed to demonstrate this methodology in which a thermal systems designer can simultaneously enforce the desired temperature and heat flux distribution on the hot outer surface of the object while enforcing either the desired temperature, desired heat flux or desired convective heat transfer boundary conditions on the cooled interior surfaces of the coolant flow passages. The program's objective is to meet the overspecified thermal boundary conditions of the outer surface by iteratively altering the geometries of the coolant passages. This is achieved with an automatic, constrained optimization algorithm that minimizes the difference between the user-specified and the intermittently computed hot outer surface heat flux distribution. A quasi-Newtonian gradient search algorithm was used for the optimization. A simple method for escaping stationary points was employed and involved the switching of the objective function when the optimization process stalled at a local minimum. The analysis of the steady-state, non-linear heat conduction within the solid was done using the boundary element method.

Key words: Boundary element method, non-linear optimization, inverse shape design, quasi-Newtonian algorithm.

1 INTRODUCTION

The design of turbines within turbojet and turbofan engines introduces a unique set of requirements for high performance, endurance, light weight and compact size. To meet these requirements, turbines must operate at elevated temperature and pressure levels and must use air as a coolant to be capable of withstanding large numbers of thermal cycles, high heat fluxes and thermal stress levels. An engineer who might wish to reduce the high thermal plastic strains that cause cracks to form in the coolant passage walls of a turbine blade must simultaneously try to maximize the heat transfer out of the blade to avoid melting. This thermal design problem could be accomplished by allowing the engineer to develop a coolant system geometry that satisfies a specific desired temperature field within the configuration.

The design of internal coolant flow passages within turbine blades is usually accomplished using approximate empirical methods, repetitive numerical analysis of intuitively modified coolant flow passage shapes and expensive experimentation. The development of high speed computers and adequate numerical techniques

has made it possible to approach the design problem differently and to solve it more efficiently and with greater accuracy. During the past several years, we have developed a fully automatic inverse thermal design method¹⁻⁹ based on the boundary element method (BEM),¹⁰ which allows a thermal cooling systems designer to determine the proper sizes, shapes and locations of arbitrary coolant fluid passages within internally cooled configurations. The methodology has been successfully demonstrated on simple two-dimensional geometries,¹¹⁻¹³ on realistic coated and non-coated turbine blade airfoils¹⁻⁹ and on scramjet combustor struts.¹⁴ Elementary examples of three-dimensional design applications involved a coolant passage in a rocket nozzle periodic wall section⁹ and a three-dimensional gas turbine blade.¹⁵

2 THEORY

The mathematical model for steady-state heat conduction within an internally cooled solid object can be represented by a boundary value problem over a multiply connected domain. The desired temperature field

within a fixed configuration is intrinsically related to a single set of well-posed thermal boundary conditions specified on the entire object's surface. If additional boundary conditions are enforced on parts or all of the object's surface, the over-specified boundary value problem might not have a solution. The methodology presented in this paper demonstrates that this problem may be solved by iteratively altering the geometry of the configuration until the over-specified thermal boundary conditions are appropriately satisfied. This steady state shape design inverse problem is fundamentally different from the classical inverse heat conduction transient problem where the small changes in the initial data may result in erroneous solutions.

Steady-state heat conduction in a nonhomogeneous, isotropic medium with a variable coefficient of thermal conductivity is governed by the following partial differential equation in the region, Ω , of a conducting solid

$$\nabla \cdot (\lambda(T) \nabla T) = 0 \quad (1)$$

Here T is the temperature and $\lambda(T)$ is the temperature-dependent coefficient of thermal conductivity. This equation represents a boundary value problem having essential boundary conditions, T_0 , and natural boundary conditions, Q_0 , specified on the surfaces Γ_u and Γ_q , respectively. Equation (1) can be linearized by the application of the classical Kirchoff's transformation,¹⁶ which defines the heat function, Θ , as

$$\Theta = \int_0^T \frac{\lambda(T)}{\lambda_0} dT \quad (2)$$

Here, λ_0 is the reference conductivity. Utilizing this transformation, eqn (1) can be transformed into Laplace's equation and solved for the heat function, Θ , instead of the temperature, T :

$$\nabla^2 \Theta = 0 \quad (3)$$

Results obtained for the heat function must be transformed back into temperatures using the inverse of the transformation given in eqn (2).

The Laplace equation can be accurately and most efficiently solved using the BEM.¹⁰ By introducing an approximation, u , to the exact solution, Θ , an error function or residual is produced in the domain and on the boundary. The residual in the domain is given by $R = \nabla^2 u$. The residuals in the essential and natural boundary conditions are

$$R_u = u - \Theta_0 \quad \text{and} \quad R_q = \partial u / \partial n - Q_0 \quad (4)$$

respectively. These error functions have non-zero values unless u is the exact solution. The weighted average of the residual over the domain and on the boundary may be set to zero by the weighted residual statement:

$$\int_{\Omega} u^* \nabla^2 u \, d\Omega - \int_{\Gamma_q} (q - Q_0) u^* \, d\Gamma + \int_{\Gamma_u} (u - \Theta_0) q^* \, d\Gamma = 0 \quad (5)$$

where u^* represents the weight function, which is usually called the fundamental solution,¹⁰ while $q = \partial u / \partial n$ and $q^* = \partial u^* / \partial n$ where n is the direction of the outward normal to the surface Γ . After integrating by parts twice, the boundary integral equation for Laplace's equation is obtained:

$$\int_{\Omega} u \nabla^2 u^* \, d\Omega + \int_{\Gamma} u^* q \, d\Gamma = \int_{\Gamma} q^* u \, d\Gamma \quad (6)$$

The weight function is a Green's function solution for a point-source subject to the homogeneous boundary conditions. For the three-dimensional Laplace equation it is

$$u^* = \frac{1}{4\pi r} \quad (7)$$

where $r = |\mathbf{x}_i - \mathbf{x}_j|$, \mathbf{x}_i is the position vector of the arbitrarily located observation point at which u and q are to be evaluated, and \mathbf{x}_j is the position vector of the point-source location. The bounding surface Γ is discretized into N_{SP} surface elements bounded by N end-nodes. After discretizing the surface and utilizing the properties of the Dirac's delta function, the boundary integral equation (6) can be written as

$$c_i u_i + \sum_{j=1}^{N_{sp}} \int_{\Gamma_j} u q^* \, d\Gamma_j = \sum_{j=1}^{N_{sp}} \int_{\Gamma_j} q u^* \, d\Gamma_j \quad (8)$$

for each i th node. The term c_i indicates the scaled internal angle¹⁰ formed by the neighboring panels meeting at the i th surface node. It is produced when the first surface integral of eqn (6) is integrated in the sense of Cauchy's principal value. The functions u and q are assumed to vary bilinearly along each quadrilateral surface element and, therefore, they can be defined in terms of their nodal values and interpolation functions. The whole set of equations for the N nodal values of u and q can be expressed in matrix form as

$$[\mathbf{H}]\{\mathbf{U}\} = [\mathbf{G}]\{\mathbf{Q}\} \quad (9)$$

where $\{\mathbf{U}\} = (U_1, U_2, \dots, U_N)$ and $\{\mathbf{Q}\} = (Q_1, Q_2, \dots, Q_{N_{sp}})$ are vectors containing the nodal potentials and surface panel fluxes, respectively, while the terms in the $[\mathbf{H}]$ and $[\mathbf{G}]$ matrices are assembled by properly adding the contributions from each surface integral. After the $[\mathbf{H}]$ and $[\mathbf{G}]$ matrices are formed, all boundary conditions are applied and a set of linear algebraic equations, $[\mathbf{A}]\{\mathbf{X}\} = \{\mathbf{F}\}$, is constructed. Known or specified surface potentials, U_j , and fluxes, Q_j , are multiplied by their respective $[\mathbf{H}]$ or $[\mathbf{G}]$ matrix row and assembled on the right-hand side of the equation set, thus forming the vector of knowns $\{\mathbf{F}\}$. All unknown potentials or fluxes are assembled on the left-hand side of the equation set and are represented by a coefficient matrix $[\mathbf{A}]$ multiplying a vector of unknown quantities $\{\mathbf{X}\}$.

The integration for each surface panel in eqn (8) was performed with three-point Gaussian quadrature.

Whenever the surface panel integral included a singularity at one of the quadrilateral's vertices, a localized transformation¹⁷ was performed to eliminate the singularity, and the order of the Gaussian quadrature was automatically increased to a five-point integration.

3 THE OPTIMIZATION TECHNIQUE

The complexity of the analysis of the temperature field in an irregular, three-dimensional, multiply connected domain calls for the use of a relatively simple, but robust and fast, optimization technique for constrained, non-linear optimization. The Davidon-Fletcher-Powell (DFP) quasi-Newtonian algorithm¹⁸ was implemented because it requires a relatively low number of objective function evaluations and because of its ability to converge quickly near minima. This optimization procedure is iterative in nature and involves repetitive solutions of the thermal field within the solid configuration. A first-order numerical approximation was used to compute the gradients of the objective function, and the univariant line search was handled using quadratic polynomial fitting.

The primary goal of the optimization procedure is the minimization of the objective function $f(\mathbf{x})$, where \mathbf{x} contains the N_{VAR} design variables which make up the geometry of the internal coolant passages. During the optimization process, local minima can occur and halt the process before achieving an optimal solution. In order to overcome such a situation, a simple technique has been devised.¹⁴ In this approach, whenever the optimization stalls, the formulation of the objective function is automatically switched to some other valid formulation. The new objective function provides a departure from the local minima and further convergence towards the global minima.

Specifically, the objective of the optimization procedure is to minimize the difference between the specific heat fluxes, Q^{spec} , and the calculated values, Q^{calc} , at the outer boundary. Thus, the objective function can be mathematically formulated in the sense of the normalized least squares of the global error:

$$f(\mathbf{x}) = \frac{\sum_{j=1}^N (Q_j^{\text{spec}} - Q_j^{\text{calc}})^2}{\sum_{j=1}^N (Q_j^{\text{spec}})^2 + \epsilon} \quad (10)$$

or as a local normalized error at each panel on the outer boundary:

$$f(\mathbf{x}) = \sum_{j=1}^N \frac{(Q_j^{\text{spec}} - Q_j^{\text{calc}})^2}{(Q_j^{\text{spec}})^2 + \epsilon} \quad (11)$$

Here, ϵ is a very small user-specified parameter to avoid division by zero.

In summary, the optimization procedure consists of the following steps:

- (1) The geometry of the outer surface of the turbine blade is assumed fixed.
- (2) The desired temperature and heat flux profile are specified on the hot outer surface of the turbine blade. The temperature is used as a Dirichlet-type boundary condition on the outer surface, while the outer surface heat fluxes are used in the objective function formulation of the optimization procedure described previously. In addition, boundary conditions such as temperature, heat flux must be specified on the three-dimensional coolant passage surfaces. Their configurations are, as yet, unknown.
- (3) The user may specify almost any type of equality or inequality constraints to the program as a subroutine. Such constraints could be allowable minimum or maximum wall thickness, minimum distance between multiple coolant passage walls, minimum or maximum cross-sectional areas of the coolant channels, material properties, etc.
- (4) The user supplies an initial guess for the design variables that define the geometry of the three-dimensional coolant flow passages.
- (5) The BEM is used to solve for the temperature field within the current configuration. Since the temperature boundary conditions are specified on the outer surface, the BEM algorithm automatically computes the heat flux distribution on that surface. The computed heat flux distribution is, in general, not the same as the user-specified desired heat flux distribution.
- (6) An objective function is formulated using the computed and user-specified outer surface heat fluxes. Note that the use of heat fluxes in the objective function is not a requirement nor a limitation. The user is free to develop any objective function or set of weighted objective functions that may utilize not only boundary values such as temperature and heat flux, but also convective heat transfer coefficients and ambient temperatures, temperatures at points within the solid, thermal stresses and strains and many other functions of the temperature field.
- (7) The optimization procedure automatically perturbs the design variables in order to minimize the objective function while satisfying the constraints. In order to minimize this function properly and efficiently, a feasible and descent line search direction is found by computing the gradient of the function. This requires one thermal field analysis using the BEM per design variable. Once the line search direction is obtained from the DFP update formula, a

univariant suboptimization procedure minimizes the objective function along that direction.

- (8) The optimization continues to the next cycle, beginning with step 5.

4 VERIFICATION OF THE NON-LINEAR BOUNDARY ELEMENT FORMULATION

The accuracy of the BEM analysis program for the non-linear heat conduction in a 1.0 m long by 0.1 m high by 0.1 m wide parallelepiped was verified. The rectangular box was discretized with 42 square surface panels each measuring 0.1 m by 0.1 m. Four sides of the object were kept adiabatic ($Q_0 = 0$) and the remaining two opposite sides were subject to different temperatures ($T_{\text{hot}} = 100 \text{ K}$ and $T_{\text{cold}} = 0 \text{ K}$). The temperature-dependent thermal conductivity was given as a polynomial function:

$$\lambda(T) = \lambda_0(AT^{-1} + B + CT + DT^2 + ET^3) \quad (12)$$

In our test $\lambda_0 = 1.0 \text{ W/mK}$, $B = 1.0$, and $A = D = E = 0$. Temperature data were collected for various degrees of non-linearity given by the parameter C . The results shown in Fig. 1 were compared with the one-dimensional analytic solution:¹⁶

$$\begin{aligned} \frac{C}{2}T^2 + T &= \left(T_{\text{hot}} + \frac{C}{2}T_{\text{hot}}^2\right) \\ &- \left(1 + \frac{C}{2}(T_{\text{hot}} + T_{\text{cold}})\right) \frac{(z - z_{\text{hot}})}{(z_{\text{cold}} - z_{\text{hot}})} \\ &\times (T_{\text{hot}} - T_{\text{cold}}) \end{aligned} \quad (13)$$

Figure 1 shows that the non-linear BEM results compared very well with the analytic solution, averaging an error of less than 0.5%.

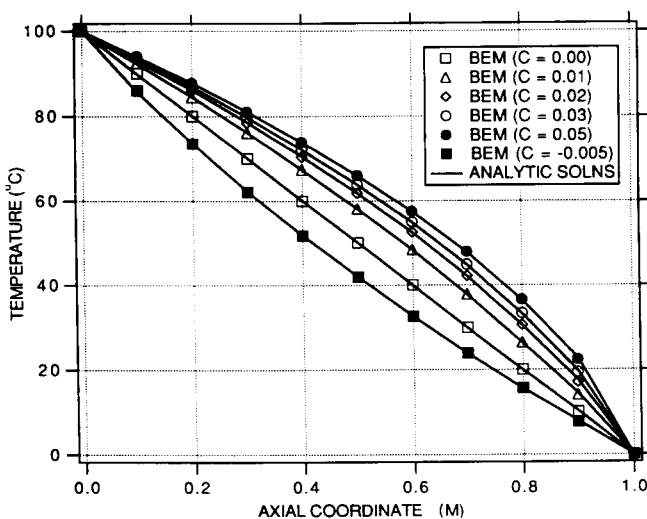


Fig. 1. Comparison of temperature distribution in a parallelepiped with different degrees of thermal dependency of heat conductivity coefficient.

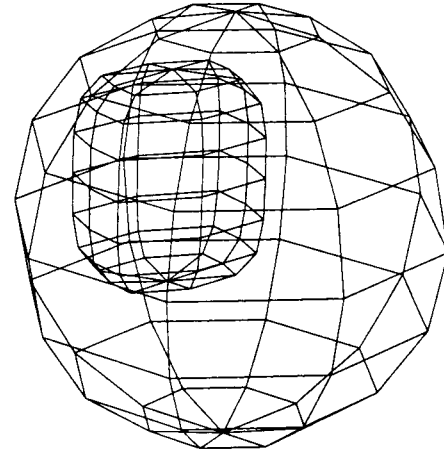


Fig. 2. Initial configuration for a three-dimensional inverse shape design: a super-elliptic off-center cavity in a sphere.

5 INVERSE DESIGN OF A SUPER-ELLIPTIC CAVITY WITHIN A SPHERE

This test case was used to demonstrate the fully three-dimensional inverse design capability⁶ of the optimization algorithm with the BEM thermal field analysis scheme. The geometry consisted of a unit sphere with an off-centered cavity of a three-dimensional super-elliptic shape given by

$$\left(\frac{x - x_0}{a}\right)^n + \left(\frac{y - y_0}{b}\right)^n + \left(\frac{z - z_0}{c}\right)^n = 1 \quad (14)$$

Seven design variables are derived from this equation: the center of the super-elliptic cavity (x_0, y_0, z_0), its semi-major axes (a, b, c) and the super-elliptic exponent, n . The outer spherical surface and the internal super-elliptic cavity (Fig. 2) were discretized with 64 isoparametric quadrilateral panels, respectively. A temperature of 100 K was specified on the outer surface and 50 K on the inner super-elliptic surface. The normal

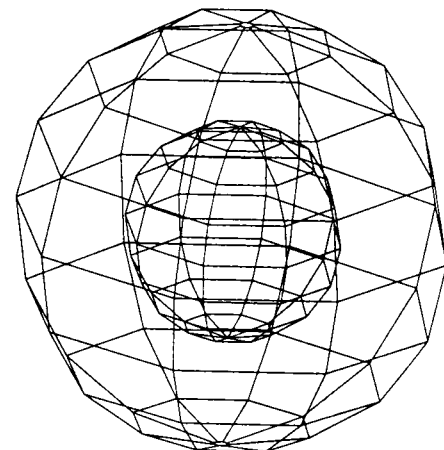


Fig. 3. Final converged configuration for a three-dimensional inverse shape design: a centered spherical cavity in a sphere.

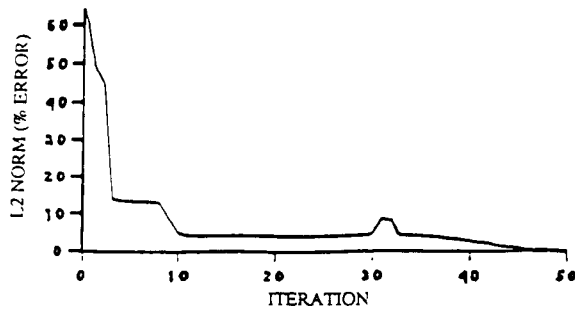


Fig. 4. Convergence history of the objective function for the cavity-in-the-sphere design.

temperature derivative specified on the outer surface was taken from the analytic solution ($\partial T/\partial n = 59.3 \text{ K/m}$) corresponding to the desired (target) configuration consisting of a centered spherical cavity with radius of 0.5 m. The material properties were assumed such that the thermal conductivity $\lambda_0 = 1.0 \text{ W/m K}$, $A = D = E = 0$, $B = 1.0$, and $C = 0.01 \text{ K}^{-1}$.

The initial guess for the design variables was: $x_0 = 0.2 \text{ m}$, $y_0 = 0.2 \text{ m}$, $z_0 = 0.2 \text{ m}$, $a = 0.3 \text{ m}$, $b = 0.4 \text{ m}$, $z = 0.5 \text{ m}$, and $n = 4.0$. The DFP optimization algorithm nearly reached the fully converged sphere-within-a-sphere configuration (Fig. 3) in 50 optimization cycles with the remaining objective function value of 0.32%. The convergence history (Fig. 4) of the composite objective function shows a spike at the 30th iteration, indicating an automatic cost function switch from global to local (eqn (10) to eqn (11)). The entire optimization required 647 calls to the BEM analysis routine and consumed approximately 2235 s of CPU time on an IBM 3090 computer.

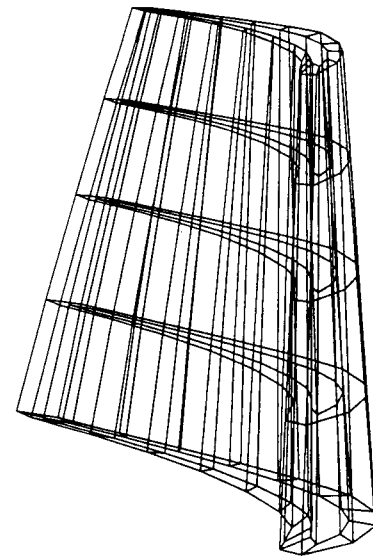


Fig. 5. Initial configuration for a three-dimensional turbine blade with surface discretization.

6 INVERSE DESIGN OF A COOLANT PASSAGE WITHIN A TURBINE BLADE

This example involved the application of the inverse design technique to a three-dimensional turbine blade of realistic shape.¹⁵ The turbine blade was given a single internal coolant flow passage. The blade inner surface was generated at each radial cross-section by first determining the mean thickness curve from the local blade airfoil geometry. At each blade cross-section this mean thickness curve was then reduced by a fraction

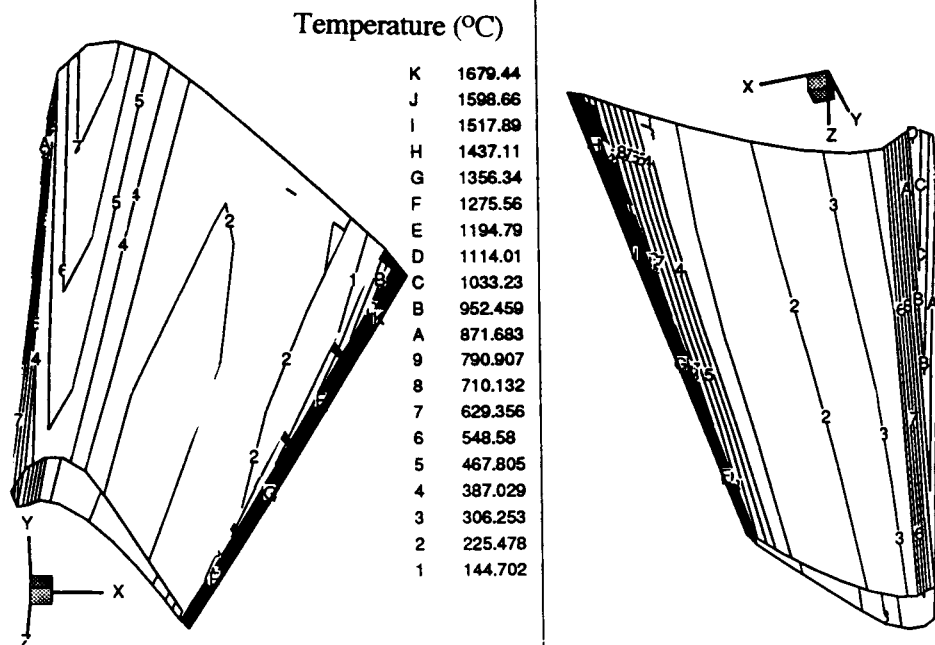


Fig. 6. Specified distribution of temperature on the outer surface of the three-dimensional blade.

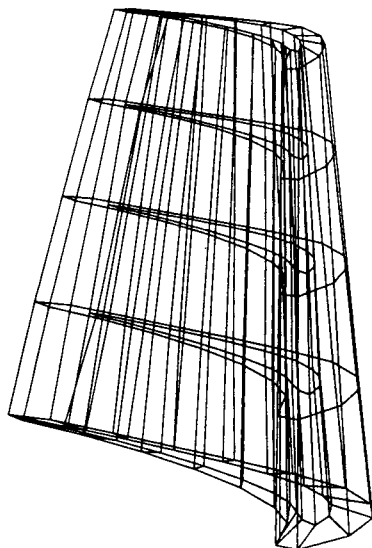


Fig. 7. Specified (desired or target) configuration of the coolant passage inside the three-dimensional turbine blade.

of its total length from the leading and trailing edges, p_{le} and p_{te} , respectively. At each blade cross-section, the local blade airfoil inner contour was then constructed by defining a wall thickness function versus the blade airfoil outer contour-following coordinate, s . The local wall thickness was defined to be a fraction of the straight line distance from a point on the blade airfoil outer contour to the corresponding point on the reduced mean thickness curve. The wall thickness, $t(s)$, was approximated by a Chebyshev polynomial¹⁹ of

degree n , given as

$$t(s) \approx \sum_{j=1}^n c_j P_{j-1}(s) - \frac{c_1}{2} \tag{15}$$

where the Chebyshev coefficients are

$$c_j = \frac{2}{n} \sum_{k=1}^n t \left[\cos \left(\frac{\pi(k-1/2)}{n} \right) \right] \times \cos \left(\frac{\pi(j-1)(k-1/2)}{n} \right) \tag{16}$$

and

$$P_j(s) = \cos(j \arccos s) \tag{17}$$

The polynomial of eqn (15) can be truncated to a lower degree $m \ll n$ due to the nature of the Chebyshev approximation. Thus, the design variables that made up the coolant passage geometry consisted of m Chebyshev coefficients for each cross-section of the blade in addition to the two quantities, p_{le} and p_{te} , that determine by what fraction the mean thickness curve is reduced from the trailing and leading edges of each local blade airfoil.

The outer surface and the initial guess to the inner surface geometry of the three-dimensional turbine blade are shown in Fig. 5. The outer surface of the blade was generated by creating airfoil sections of the blade at each of the five locations measured radially from the turbine axis. Each turbine blade section between two consecutive radial cuts was discretized with 20 clustered quadrilateral flat surface panels around its outer surface in addition to the same number of quadrilateral flat surface panels on its inner surface. There were also

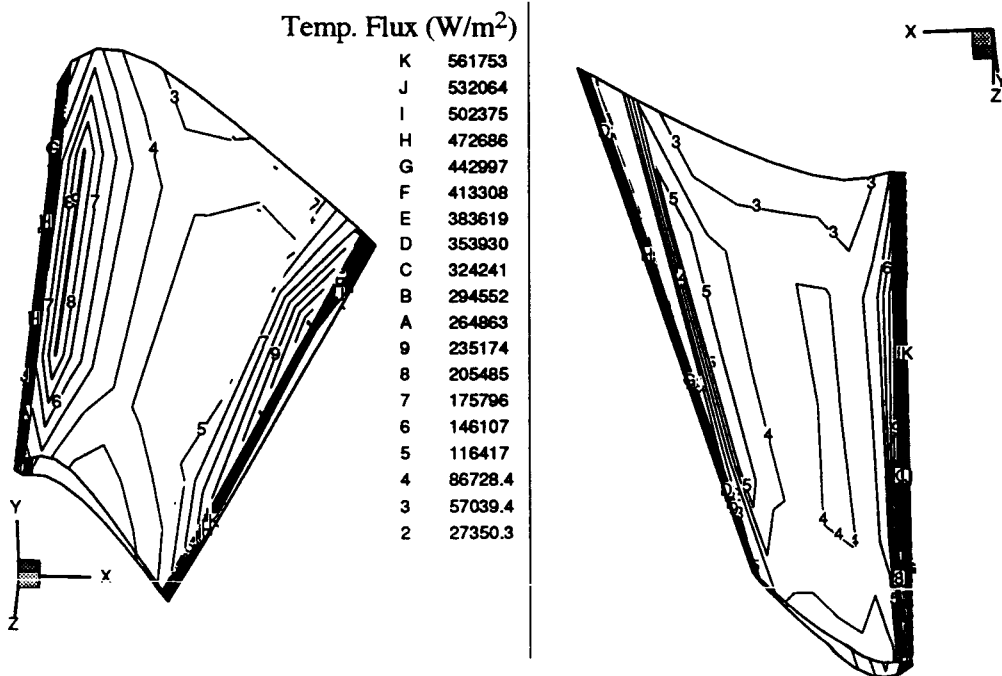


Fig. 8. Specified (desired or target) distribution of heat fluxes on the outer surface of the three-dimensional blade.

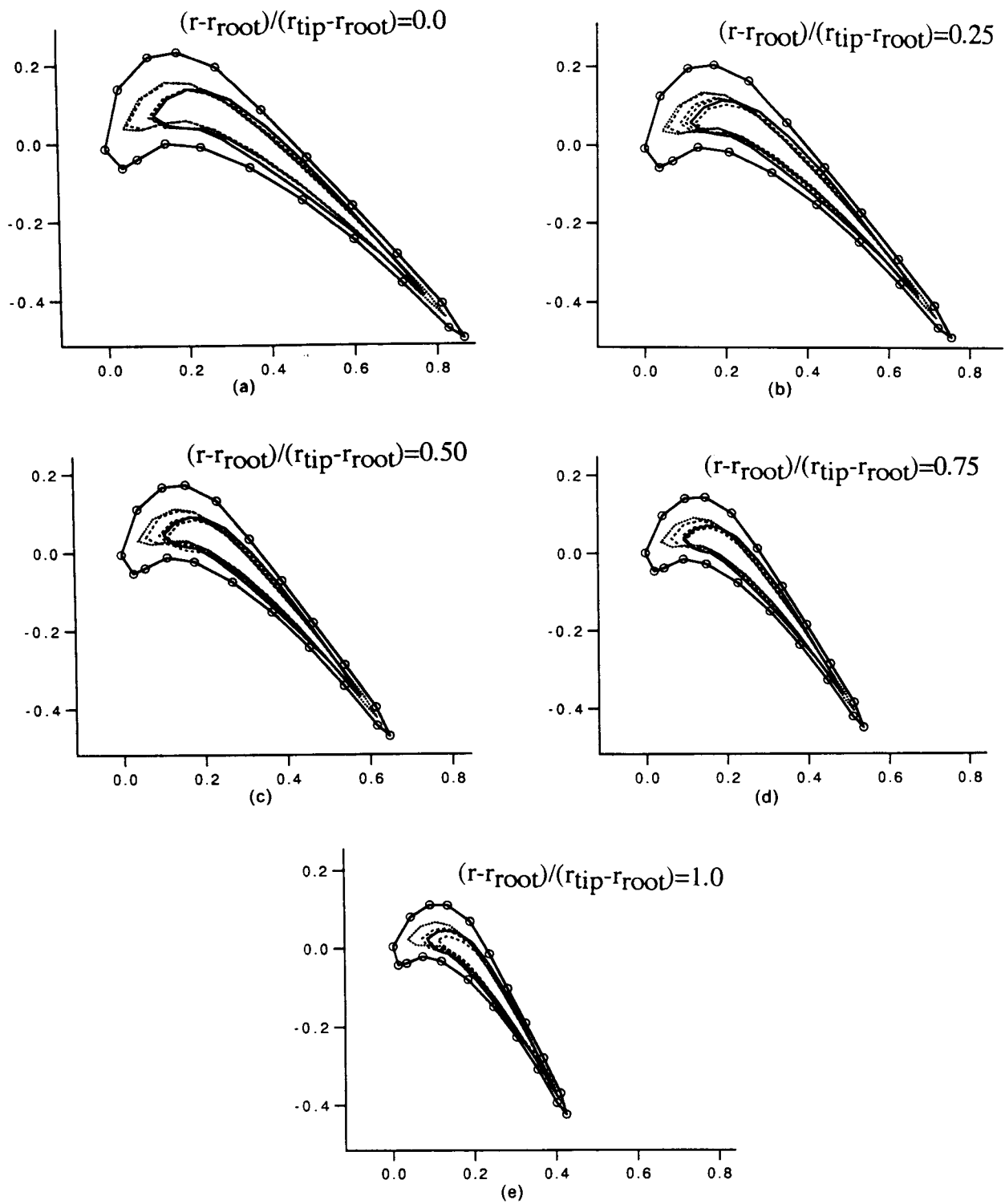


Fig. 9. Geometric evolution of thickness distributions on individual cross-sections of the three-dimensional blade.

20 quadrilateral flat panels covering the blade root cross-section and 20 quadrilateral flat panels covering the blade tip cross-section. This means that the blade wall thickness at the root and at the tip sections was discretized by single rows of flat quadrilateral panels. Consequently, we used a total of 200 flat quadrilateral surface panels connected between 200 nodes at the panels' vertices.

The desired temperature was prescribed along the outer surface of the turbine blade according to a simple formula:

$$T(s) = T_{\min} + (T_{\max} - T_{\min}) \left[\cos \left(\frac{2\pi s}{s_{\max}} \right) \right]^2 \quad (18)$$

with $T_{\min} = 500$ K and $T_{\max} = 1000$ K at the blade root section. Each of them was increased by 50 K at each of

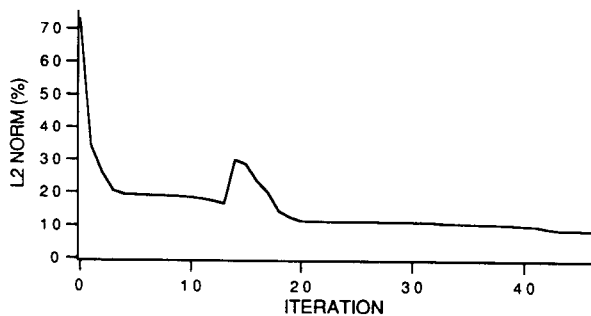


Fig. 10. Convergence history of the objective function for the three-dimensional turbine blade wall thickness optimization.

the four remaining consecutive sections so that their values at the blade tip section were $T_{\min} = 700$ K and $T_{\max} = 1200$ K. The three-dimensional blade surface isotherms are illustrated in Fig. 6. In addition, a desired constant temperature was specified on the inner surface, $T_{\text{inner}} = 300$ K. The reference coefficient of thermal conductivity was $\lambda_0 = 23.0$ W/m K and the parameters of eqn (12) were $A = D = E = 0$, $B = 1.0$, and $C = 0.01$ K $^{-1}$.

Next, a desired (target) configuration for the three-dimensional coolant passage geometry was generated (Fig. 7). The BEM was run once for this configuration with the desired temperature boundary conditions described above. The computed outer surface heat fluxes (Fig. 8) were then used as the desired (target) over-specified boundary conditions for the optimization process's objective function.

Figures 9(a)–(e) illustrate the evolution of the coolant passage geometry throughout the optimization process. Each figure represents a consecutive cross-section of the turbine blade showing nodes on the outer surface of the airfoil shape, the initial guess geometry (finely dotted line), several intermittent contours depicting the coolant passage cross-section geometry after every 10 iterations (dashed lines) and the target configuration (solid line). The final configurations are almost geometrically equivalent to the target configurations. The optimization process was completed after 46 iterations with the objective function reducing from an initial value of 74% to its final value of 8.64% (Fig. 10). A single objective function automatic switch occurred at the 14th iteration. The objective function declined very rapidly initially and then levelled off to a rather slow rate of decrease. This is typical of most optimization procedures. Although the program was terminated at the 46th optimization cycle, the process could be resubmitted in order to refine further the coolant passage geometry. The entire optimization process required 2996 calls to the BEM analysis routine and consumed approximately 2550 s of CPU time on a Cray C-90 computer with a single processor.

7 SUMMARY

The concept of inverse design of three-dimensional configurations subject to overspecified thermal boundary conditions has been found to be feasible. Future research possibilities in the field of three-dimensional shape inverse design using the presented methodology could be directed toward complex design tools involving thermal convection, radiation and conduction as well as thermal stress-deformation field analysis and electromagnetic field problems. The same optimization procedure with boundary integral analysis described herein can be used for problems governed by Poisson's equation. This work is presently being extended into unsteady, fully three-dimensional, non-linear heat conduction involving latent heat, multiple coolant passages and multiple domains with different properties.

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