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Inverse problems and design in heat conduction

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ABSTRACT: Our work during the past ten years on developing solution methods for shape inverse problems and for boundary condition inverse problems has been demonstrated in the case of two -and three-dimensional steady linear and non-linear heat conduction, and documented in a large number of our publications. The method for shape design of coolant flow passages utilizes standard optimization algorithms to minimize the difference between the specified and computed thermal boundary conditions thus arriving at a *de facto* shape inverse problem solution. Our new method for finding unknown steady thermal boundary conditions on parts of the boundaries where such quantities are unknown is quite unique since it does not utilize any standard unsteady inverse heat conduction problem formulation. Instead, our approach to inverse boundary value problems is based on a non-iterative boundary element formulation, and consequently, it is very fast and robust.

1 INVERSE SHAPE DESIGN

During the past ten years we have developed an inverse design method (Kennon and Dulikravich 1985, 1986a, 1986b; Chiang and Dulikravich 1986; Dulikravich, Chiang and Hayes 1986; Dulikravich 1988, 1992; Dulikravich and Kosovic 1992; Dulikravich and Martin 1992a, 1992b) that allows a thermal system designer to determine the minimum proper number, and correct sizes, shapes, and locations of coolant flow passages in arbitrarily shaped internally cooled configurations. The design methodology has been successfully demonstrated on two-dimensional coated and non-coated turbine blade airfoils and scram jet combustor struts. Our most recent success is the extension of this inverse shape design algorithm to fully three-dimensional configurations (Martin and Dulikravich 1993b; Dulikravich and Martin 1994).

Using this method the designer is free to guess the number, sizes, shapes, and locations of the coolant flow passages. The designer is also free to specify desired temperature distributions on the outer surface of the heat conducting object and on the surfaces of the guessed internal coolant flow passages. In addition, the designer must specify the desired heat flux distribution on the outer surface or on the walls of the coolant flow passages. The heat fluxes can be obtained either experimentally or computationally. That is, the coolant fluid flow or hot fluid flow analysis code which accepts wall temperature boundary conditions will automatically compute the corresponding wall heat flux distributions. In addition, the designer is free to specify the minimum allowable distances between any cooling passage and the outer surface of the object and between any two neighboring cooling passages. Since we deal with steady heat conduction, the designer has to specify only coefficients of heat conductivity for the main material of the solid object and for the solid's coating material if such coating exists. Each coefficient of heat conductivity is allowed to be temperature-dependent according to a fourth order polynomial

$$\lambda(T) = \lambda_o \left(A\,T^{-1} + B + C\,T + D\,T^2 + E\,T^3 \right) \quad (1)$$

where T is the temperature. λ_o is the reference thermal conductivity coefficient and the coefficients A, B, C, D and E must be specified by the user.

Afterwards, the design process does not require any intervention on the part of the designer since it uses an automatic constrained optimization algorithm (Vanderplaats 1984) to minimize the least-square differences between the specified and the computed surface heat fluxes by automatically relocating, resizing, reshaping and reorienting the initially guessed cooling passages. All unnecessary initially guessed passages are automatically reduced to negligible size and eliminated (Dulikravich and Kosovic 1992; Dulikravich and Martin 1992a, 1992b), while honoring the specified minimal manufacturing distances between the neighboring passages and between any passage and the object's coating if such coating exists. The computer code is highly reliable and geometrically flexible since it utilizes the boundary element method (Brebbia and Dominguez 1989) for thermal field analysis.

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

$$\nabla \bullet \left(\lambda(T)\, \nabla T \right) = 0 \qquad (2)$$

This can be converted into linear Laplace's equation

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

by the application of the classical Kirchoff's transformation which defines the heat function, Θ, as

$$\Theta = \int_0^T \frac{\lambda(T)}{\lambda_o}\, dT \qquad (4)$$

Laplace's equation can be easily solved for the heat function, Θ, instead of the temperature, T. Afterwards, results must be transformed back into T using the inverse of the transformation given in equation (4).

1.1 Boundary Element Method Formulation

The Laplace's equation can be accurately and efficiently solved using a variety of numerical techniques. Nevertheless, the most versatile, robust and economical numerical method for this class of potential field problems is the boundary element method (BEM). By introducing an approximation, u, to the exact solution, Θ, an error or residual $R = \nabla^2 u$ is produced in the domain and on the boundary. The weighted average of the error over the domain and on the boundary may be set to zero by the weighted residual statement. After integrating by parts twice, the boundary integral equivalent of the Laplace's equation is obtained

$$\int_\Omega u\, \nabla^2 u^*\, d\Omega + \int_\Gamma u^*\, q\, d\Gamma = \int_\Gamma q^*\, u\, d\Gamma \qquad (5)$$

where u^* represents the weight function which is usually called the fundamental solution, while $q = \partial u/\partial n$ and $q^* = \partial u^*/\partial n$ and **n** is the direction of the outward normal to the object's surface, Γ. The weight function is a Green's function solution for a point-source subject to the homogeneous boundary conditions. After discretizing the surface Γ into N_{sp} surface elements or panels and utilizing the properties of the Dirac's delta function, the boundary integral equation (5) can be written as

$$c_i\, u_i + \sum_{j=1}^{Nsp} \int_{\Gamma_j} u\, q^*\, d\Gamma_j = \sum_{j=1}^{Nsp} \int_{\Gamma_j} q\, u^*\, d\Gamma_j \qquad (6)$$

for each "i-th" surface node. The term c_i indicates the scaled internal angle formed by the neighboring panels meeting at the i-th surface node. The functions u and q are assumed to vary bi-linearly 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

$$[\mathbf{H}]\,\{\mathbf{U}\} = [\mathbf{G}]\,\{\mathbf{Q}\} \qquad (7)$$

with $\{\mathbf{U}\}$ and $\{\mathbf{Q}\}$ as vectors containing the nodal potentials and surface panel fluxes, respectively, while the terms in the $[\mathbf{H}]$ and $[\mathbf{G}]$ geometric influence 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 assembled on the right-hand-side of the equation set and are multiplied by their respective $[\mathbf{H}]$ or $[\mathbf{G}]$ matrix row 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 equation (7) was performed with Gaussian quadrature. Whenever the surface panel integral included a singularity at one of the quadrilateral's vertices, a localized cubic transformation (Telles 1987) was performed to eliminate the singularity and subsequently numerically integrated with Gaussian quadrature.

1.2 *Optimization Formulation*

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, nonlinear optimization. The Davidon-Fletcher-Powell (DFP) quasi-Newton algorithm (Vanderplaats 1984) 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 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 (Dulikravich 1988; Dulikravich and Kosovic 1992). In this approach, whenever the optimization stalls, the formulation of the objective function is automatically switched to some other valid objective function. This provides a departure from the local minima and further convergence towards the global minimum.

The objective of the optimization procedure is to minimize the difference between the specified 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 global normalized least squares error

$$f(\mathbf{x}) = \frac{\sum_{j=1}^{N} (Q_j^{spec} - Q_j^{calc})^2}{\sum_{j=1}^{N} (Q_j^{spec})^2 + \varepsilon} \tag{8}$$

or as a local normalized least squares error at each panel on the outer boundary.

$$f(\mathbf{x}) = \sum_{j=1}^{N} \frac{(Q^{spec} - Q^{calc})^2_j}{(Q^{spec})^2_j + \varepsilon} \tag{9}$$

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

1.3 *Example results for inverse shape design*

We have developed both two-dimensional and fully three-dimensional BEM computer codes capable of accurate analysis and inverse shape design in steady heat conduction. The accuracy of the codes was tested against simple geometries where the analytical solutions were known. Similarly, accuracy of the codes to compute problems with temperature-dependent thermal conductivity was verified against simple geometries where the analytical solutions were known. Our codes proved to be highly accurate averaging less than 0.5% error (Dulikravich and Kosovic 1992; Dulikravich and Martin 1993) despite the fact that we used only flat panels and linear distribution of u and q on the boundaries.

With these BEM analysis codes and our version of the Davidon-Fletcher-Powel optimization code we have developed a powerful and practical shape design tool. For example (Dulikravich and Martin 1992b), a ceramically coated gas turbine blade airfoil needed to be cooled with three coolant flow passages. Airfoil outer surface temperature and heat flux distributions were specified, as were the temperatures on the walls of the three guessed cooling passages. The three passages were initially guessed to be of identical circular shape and size standing side-by-side (Figure 1). The BEM code, using the temperatures specified on the airfoil outside (hot) surface and the walls of the cooling passages, predicted the heat flux distribution on the outer (hot) surface that was quite different from the specified (desired) hot surface heat flux distribution. A series of small perturbations of the locations, sizes and shapes of each of the three holes was then performed to find sensitivity derivatives and the search gradient of the optimization code. The geometry of each hole was analytically described with parameters of a two-dimensional Lame (super-elliptic) function (Dulikravich and Martin 1992a, 1992b) that involves six variables per hole: x and y coordinates of its center, semi-minor and semi-major axis of the hole, Lame exponent, and angle of inclination of the hole. The optimization code perturbed the Lame curve parameters for each of the holes to evaluate uni-directional search gradients and to consequently update all six Lame parameters per each hole. The minimum allowable distance between any two holes and between any hole and the metal/ceramic interface was specified and incorporated (Dulikravich and Kosovic 1992) in the objective functions (equations 8 and 9) via a barrier function (Vanderplaats 1984). Each time when a local minimum was detected, the design code automatically switched between the two forms of the objective functions (equations 8 and 9). The geometric evolution of the iterative optimization process is captured in Figure 1. Similar results for strictly circular holes were obtained earlier (Chiang and Dulikravich 1988; Dulikravich and Kosovic 1992; Matsumoto, Tanaka and Hirata 1993

We have also obtained examples with the design of three-dimensional cooling passages in the walls of regeneratively cooled rocket engine nozzles (Martin and Dulikravich 1993b) by allowing for the "growth" of an optimized cooling fin on one wall of the passage. The same concept was applied to a three-dimensional internally cooled turbine blade (Dulikravich and Martin 1994) depicted in Figure 2.

1.4 *Future research on inverse shape design*

Presently we are developing a version of the inverse design code that will allow for the design of arbitrary cross section shapes of the three-dimensional coolant flow passages instead of the present shapes that must belong to a Lame curve (super-elliptic function) family of curves. We are also completing a version of the inverse design code that will allow for multiple three-dimensional coolant flow passages with arbitrary number of cooling fins in each of the passages. The design code will also allow for regions of distinctly different materials having different temperature-dependent thermal properties.

2 INVERSE DETERMINATION OF TEMPERATURES AND HEAT FLUXES ON INACCESSIBLE SURFACES

We have recently developed a new method (Martin and Dulikravich 1993a; 1994a; 1994b) that has the capability to determine thermal boundary conditions (temperatures and heat fluxes) on surfaces of conducting arbitrarily shaped solids where such thermal quantities are unknown. The method is extremely fast since it uses a non-iterative direct approach based on the BEM in solving what is usually called the steady inverse heat conduction problem. It should be pointed out that our method differs conceptually from the standard approaches to inverse boundary value problems. Specifically, in the field of heat conduction, the classical approach is based on an unsteady heat conduction model (Stolz 1960) and is known as the inverse heat conduction problem (Beck, Blackwell and St. Clair 1985). The solution of the unsteady model is time consuming and involves complex mollification (regularization) algorithms (Busby and Trujillo 1985; Hills and Hensel 1986; Hsu, Sun, Chen and Gong 1992; Murio 1993) in order to control numerical errors and keep the iterative solution process stable (Dorri 1990). Our method is non-iterative and does not have any need for regularization.

This means that given any over-specified thermal boundary conditions (such as temperatures and heat fluxes specified simultaneously on surfaces where such data are readily available), the algorithm computes the temperature field within the object and any unknown thermal boundary conditions on surfaces where the thermal boundary values are unavailable.

The basic concept works as follows. In case of a well-posed boundary value problem, either $u = U$ (Dirichlet boundary condition) or $q = Q$ (von Neumann boundary condition), will be known at each boundary node. Hence, the resulting equation set (equation 7) will have N unknowns and N equations that can be solved by any standard matrix solver.

But, if at some boundary nodes both $u = U$ and $q = Q$ are specified, while at the other nodes neither is known, the BEM equation set can have three cases. If the total number of known boundary values of U and Q equals the total number of unknown boundary values of u and q, the system is fully determined and will have a solution. If the number of equations is greater than the number of unknowns, the system is over-determined and will have a highly accurate numerical solution. If the number of equations is less than the number of unknowns, the system is under-determined and will have a solution which might not be unique (Okuma and Kukil 1993). All of the unknowns are collected on the left-hand side, while all of the knowns are assembled on the right. Since the vector on the right-hand side is known, it may be multiplied by its coefficient matrix to form a vector of knowns, {**F**}, that is,

$$[\mathbf{A}]\{\mathbf{X}\} = \{\mathbf{F}\} \tag{10}$$

This equation set is highly singular and most standard matrix solvers will not work well enough to produce a correct solution. Such numerical results could erroneously be interpreted as multiple-valued solutions. Instead, there exist techniques for dealing with sets of equations that are either singular or very close to singular. These techniques, known as Singular Value Decomposition (SVD) methods, are widely used in solving most linear least squares problems. In this work we used a SVD algorithm (Press, Teukolsky, Vetterling and Flannery 1992) to solve the equation set (10). If additional data are available in the form of temperature or heat flux measurements at locations within the solid domain, they can be readily added to the equation set in order to enhance the accuracy of the inversely determined steady thermal boundary conditions. Once the matrix [**A**] is solved, the entire thermal field within the solid can be determined from the BEM integral formulation.

2.2 *Example results for inverse boundary conditions*

A two-dimensional steady-state BEM program has been developed to perform automatic non-iterative determination of both temperatures and heat fluxes on parts of the interior and exterior boundaries. Recently, we added a feature where additional measured temperatures and/or heat fluxes at isolated points on different surfaces and/or within the interior of the material of the body could be incorporated in the input data. The accuracy of our computer code in solving a highly singular matrix problem arising in this inverse algorithm was tested on several simple geometries where the analytic solutions for steady heat conduction were known (Martin and Dulikravich 1993a; 1994a; 1994b). Numerical results obtained were in excellent agreement with the analytic values (Chapman 1960).

Here, we will demonstrate the usefulness and the reliability of our inverse boundary value code on an example representing a cross-section of one of the cooling passages that are imbedded in the wall of the rocket engine nozzle. There are typically 70-120 such identical small cross-section passages that are equidistantly located along the circumference of the nozzle. Because of their very small size (only a few millimeters across) and the extreme environment (liquid hydrogen is pumped along the passages), it is practically impossible to experimentally measure the temperatures and the heat fluxes on the walls of the cooling passages. We used (Quentmyer 1992) the hot gas wall heat flux $Q = - 5.72 \times 10^7$ (W m^{-2}) and the outer nozzle boundary temperature $T = 305$ (K). As an over-specified boundary, the outer nozzle surface heat flux was assumed to be zero. A circumferentially periodic section containing one entire cooling passage cross section and half of the surrounding conducting metal was generated. The meridional or symmetry planes between the passages (upper and lower walls in Figure 3) were assumed to be adiabatic.

The isotherms generated by our inverse boundary condition code for four different configurations of the cooling channel cross section are given in Figures 3a-d. It is clear that the nozzle hot surface section (left vertical wall) and the entire cooling channel wall surface will be the progressively cooler as the left vertical wall of the channel (channel "hot" surface) deviates more radically from its original flat (Figure 3a) shape. A double triangular fin configuration (Figure 3d) will generate a thermal field with the minimum thermal stresses and the coolest hot surfaces of the nozzle and the cooling channel. In other words, this simple sequence of candidate configurations for the cooling passage configuration clearly demonstrates the power and the reliability of our inverse method. From the inversely obtained values of temperatures and heat fluxes on the four walls of the cooling passage it is easy to find the temperature field at any point using the standard integral formulation. The resulting isotherms are smooth, although only one boundary was over-specified.

It should be pointed out that our inverse boundary value code works as a direct non-iterative method only because it uses an integral BEM formulation.

2.3 *Future research on inverse boundary value problems*

We are presently improving the accuracy of this algorithm for two-dimensional objects with multiple voids (Martin and Dulikravich 1994b) and are extending its capability to arbitrarily shaped three-dimensional objects that can have regions of different temperature-dependent thermal properties. Notice that this algorithm can also determine correct variation of unknown convective heat transfer coefficient on the surfaces where it cannot be measured or predicted accurately otherwise.

In addition, we are presently applying this approach to elasticity and other linear field problems. The ultimate goal is to perform a truly conjugate heat transfer computation of realistic three-dimensional internally cooled configurations.

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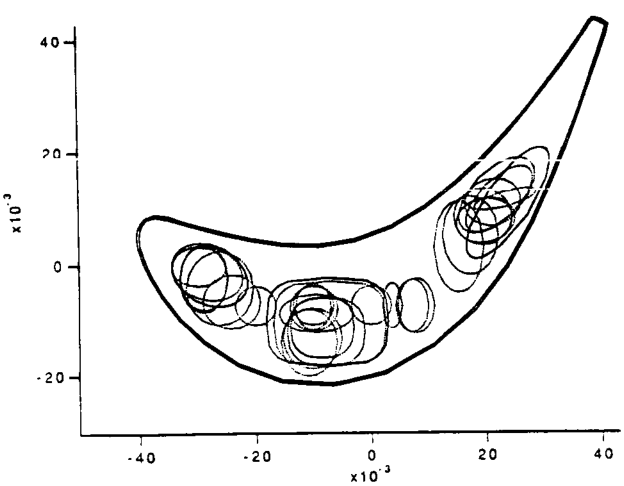


Figure 1. Geometric convergence history for an internally cooled turbine blade airfoil using Lame curve shapes for the three holes: intermediate configurations (dotted lines) and final configuration (solid lines).

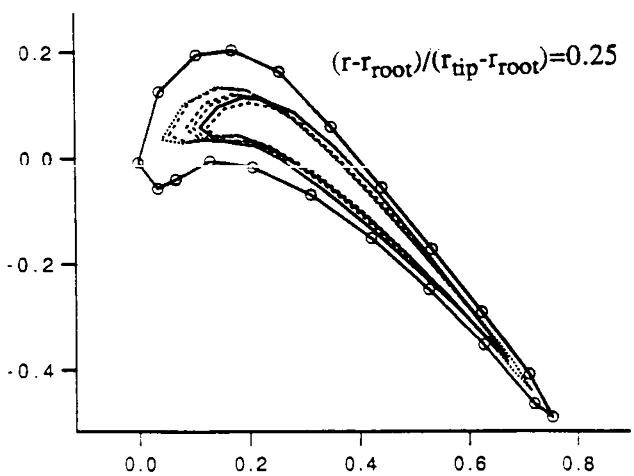
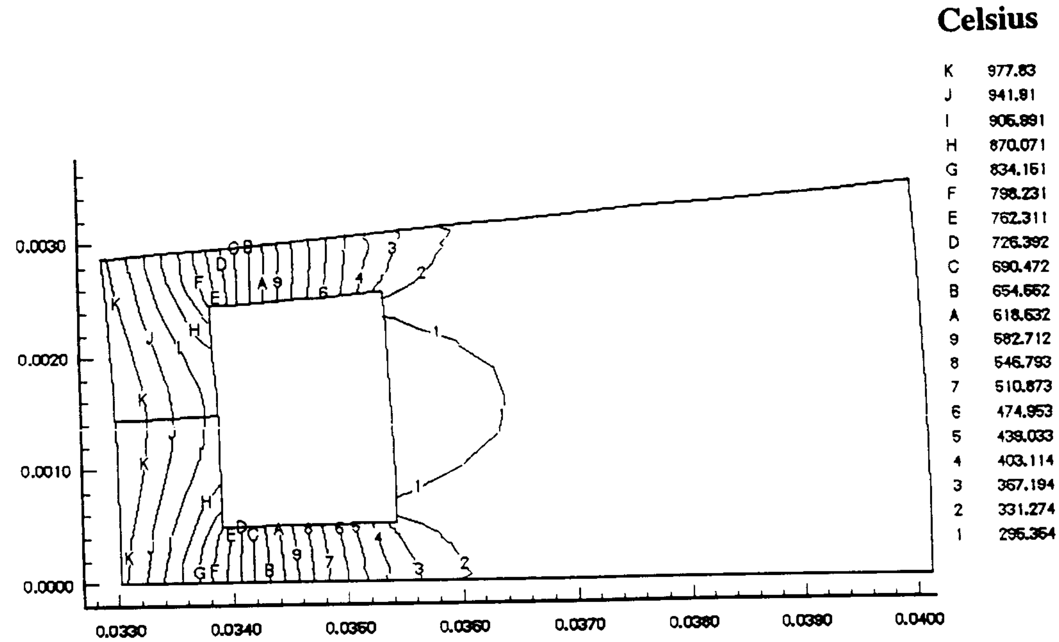


Figure 2. Geometric convergence history for a section of a fully three-dimensional internally cooled blade having specified outside temperatures and heat fluxes and interior temperatures: intermediate configurations (dotted lines) and final configuration (solid line) of the inner surface.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B 654.552
A 618.632
9 582.712
8 546.793
7 510.873
6 474.953
5 439.033
4 403.114
3 367.194
2 331.274
1 295.354
0.0030
0.0020
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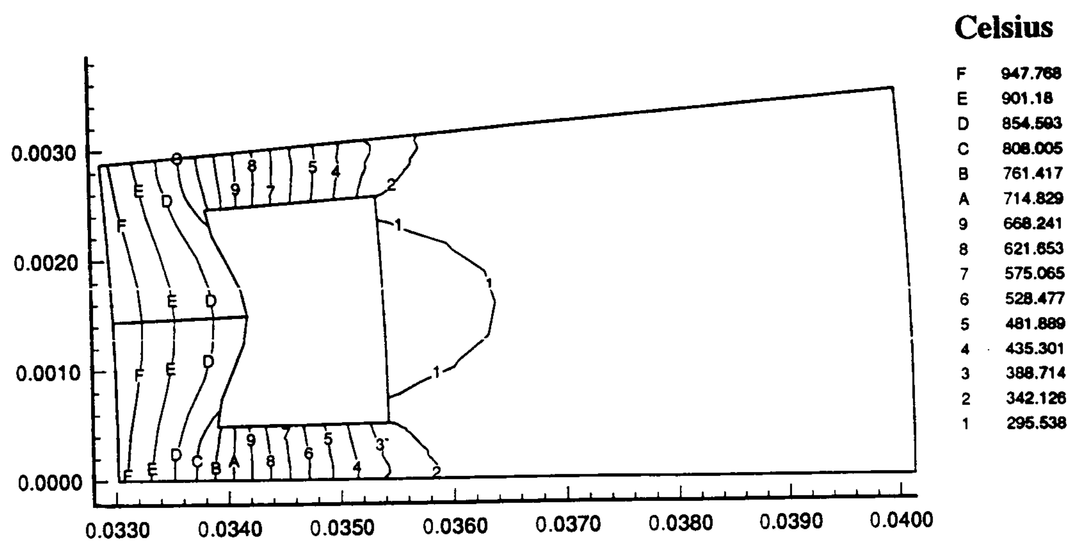
3a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6 528.477
5 481.889
4 435.301
3 388.714
2 342.126
1 295.538
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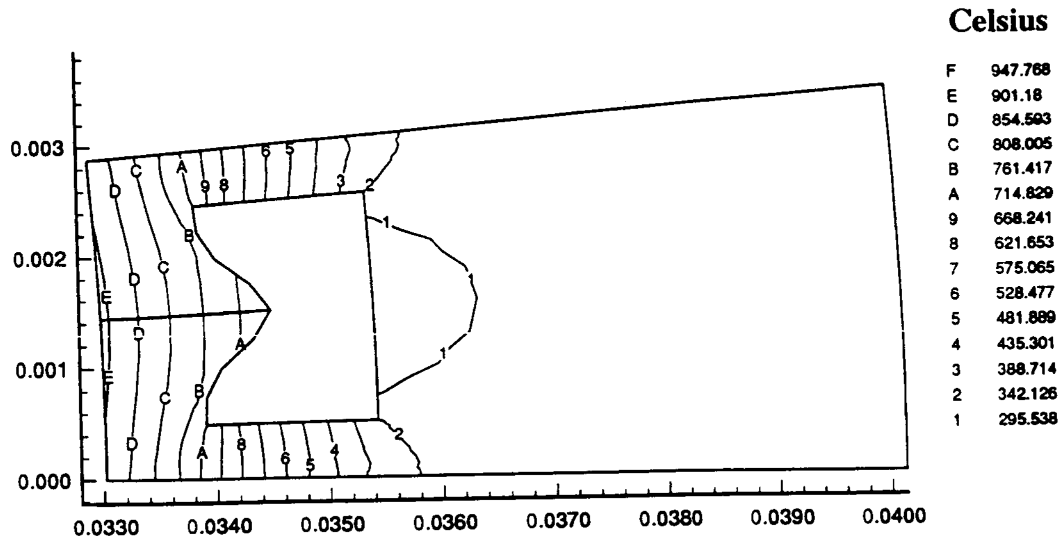
3b



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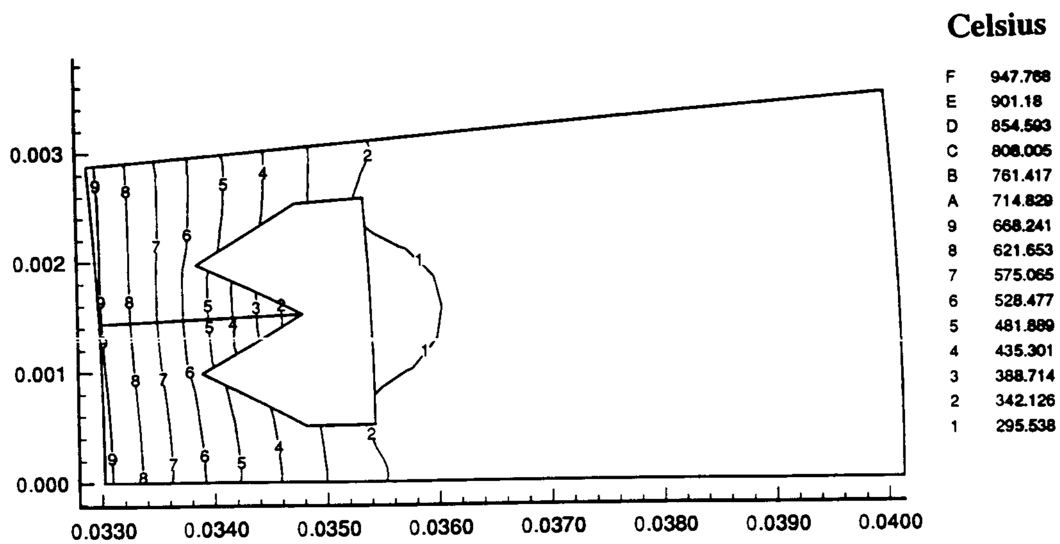

3d

Figure 3. Isotherms obtained from the inverse boundary value code for a periodic internally cooled section of a rocket engine nozzle: geometry is given, but temperatures and heat fluxes were initially unknown on the inner four walls. Only the right hand side wall has over-specified thermal boundary conditions.