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Differential and BIE formulations of optimal heating solids

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ABSTRACT

Two types of sensitivity analysis methods are proposed for finding analytical sensitivity expressions of an integral objective functional in the case of optimal heating of solids. Basically, the adjoint variable method is utilized along with the differential heat equation and the corresponding BIE in the so-called differential and integral sensitivity formulations, respectively. The discretizations of the primary and adjoint problems are performed using the BEM. Numerical results are first compared with analytical (exact) results for a 1-dim. annular cylinder problem. Solutions are also provided for the optimal cooling of a 2-dim. turbine blade.

INTRODUCTION

Efficient and accurate calculations of gradients of functionals are very crucial for optimization problems, in general. If there exist many decision variables in the problem it might be time consuming to utilize the simple finite difference techniques. In addition, accuracies achieved by this method have been reported to be not agreeable in most cases. Other types of sensitivity analysis (SA) methods include implicit differentiation and adjoint variable methods (AVM) [1-4]. A choice is also possible in regard to the application of a particular SA technique before or after discretization of the physical system at hand. If a SA procedure is implemented before any discretization the sensitivity expressions are obtained in an analytical manner whose results are not affected by any post-SA approximation of the decision variables. This will be the basic approach to be adopted in the present paper.

Sensitivity analysis expressions are obtained using the AVM by utilizing two different SA procedures in the case of an optimization problem involving heat conducting materials. Material properties, heat sources and boundary heat fluxes constitute the decision variables. In the first SA formulation the differential heat equation is adopted as the system equation. As a result the associated adjoint variable function satisfies a similar differential equation with different boundary conditions. On the other hand, the boundary integral equation (BIE) corresponding to the heat equation constitutes the system equation in the integral SA formulation. As a consequence the associated adjoint function is also described directly by a boundary integral equation, however, of a different nature.

Discretizations are achieved by the BEM in all cases, i.e. for the primary and adjoint equations in both SA formulations. A simple transformation of variables is also utilized so that no domain integrations are required in the BEM implementations. Comparisions of the numerical solutions with analytical results are made in order to assess accuracies of the SA formulations. A more practical problem involving optimal cooling of turbine blades is also investigated by the proposed solution procedures.

OPTIMIZATION PROBLEM

A nondimensional form of equations describing the behavior of heat conducting solids may be given by using indicial notation as follows:

$$x_i \in \Omega : \quad k\,T_{,ii} + Q = 0 \tag{1}$$

$$x_i \in \Gamma_T : \quad T = 0 \tag{2}$$

$$x_i \in \Gamma_q : \quad q_n = -k\,T_{,i}\,n_i = q_0 \tag{3}$$

where x_i are the 3-dim. Cartesian coordinates; Ω is the solution domain with boundary $\Gamma = \Gamma_T \cup \Gamma_q$, as depicted in Fig.1; k denotes the thermal conductivity coefficient; T represents the temperature distribution; Q is the distributed heat source; q_0 indicates the boundary heat flux on Γ_q; n_i denotes the unit vector normal to Γ.

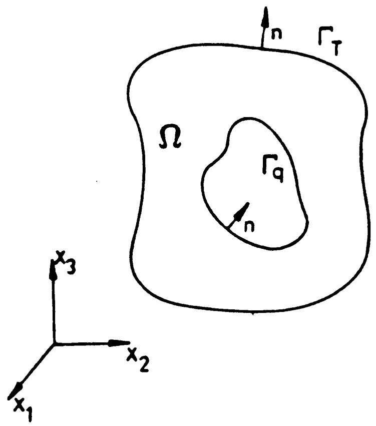

Fig. 1 Schematics of the general problem

Adopting a fixed geometry for the solid, the variables k, Q and q_0 may be taken as the decision variables in optimizing a desired physical objective [9-11]. This kind of problem may be termed as a material and load optimization problem, in general sense, in contrast to shape optimization problems [5-8]. In particular, it might be desirable to minimize an integral objective function given as follows:

$$I = \int_{\Gamma} g(T, q_n) \; d\Gamma \; + \; h(\varphi_i) \tag{4}$$

where I is the objective function (i.e., an integral performance criterion); g and h are continuous and differentiable functions of their arguments; and ϕ_i may represent finite number of some other decision parameters (i.e., constants). As can be noticed I has been defined over the boundary Γ only. The primary reason for taking a boundary integral functional stems from the fact that the BEM will be utilized later on for numerical calculations, and domain integrals are not particulary wanted in such procedures.

In the present investigation k and Q are simply taken as constants, representing uniform distributions of thermal conductivity and heat source in the solid. Hence, the decision variables in the present optimization problem consist of k, Q and ϕ_i parameters and the boundary heat flux function q_0 defined over Γ_q. The SA procedures to be proposed in the next sections are, in general, by no means constrained by the choice of uniform decision parameters.

With constant k and Q decision parameters a simple transformation can be introduced in the following manner:

$$u = \frac{k}{Q} T + \frac{x_k x_k}{2d} \tag{5}$$

where $d = \delta_{ii}$ and δ_{ij} is the Kronecker delta. Equations (1)-(3) are then transformed into the following:

$$x_i \in \Omega : \quad u_{,ii} = 0 \tag{6}$$
$$x_i \in \Gamma_T : \quad u = \frac{x_k\, x_k}{2\, d} \tag{7}$$
$$x_i \in \Gamma_q : \quad u_{,n} = -\frac{q_0}{Q} + \frac{x_i\, n_i}{d} \tag{8}$$

where $u_{,n}$ denotes the normal derivative of u over Γ. The present optimization problem is now defined as follows: Minimize the objective function I, Equation (4), subject to the subsidiary system equations (6)-(8) with respect to decision parameters k, Q and ϕ_i and the decision function q_0 over Γ_q. It may be noted that I depends on the variable u implicitly through Equation (5). In the next two sections two SA formulations will be presented in order to find analytically the sensitivities of I with respect to k, Q, ϕ_i and q_0.

DIFFERENTIAL SENSITIVITY ANALYSIS (DSA)

In this formulation, which will be indicated by DSA in short, the primary problem describing the systems behavior is given by Equations (6)-(8). These equations are incorporated into the objective function I in terms of an adjoint function as follows:

$$\tilde{I} = \int_\Omega \bar{u}\, u_{,ii}\, d\Omega + \int_\Gamma g\,(T, q_n)\, d\Gamma + h(\phi_i) \tag{9}$$

where $\tilde{I}$ represents the augmented functional. A simple procedure is now followed which may be summarized as follows:

i) Take the first variation of $\tilde{I}$

ii) Use the Green's second identity

iii) Introduce the variations of δT and δq_n through the use of Equation (5)

iv) Introduce the variations of δu, $\delta u_{,n}$ over boundary segments Γ_T and Γ_q

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v) Define an adjoint (differential equation) problem given by

$$x_i \in \Omega : \quad \bar{u}_{,ii} = 0 \tag{10}$$

$$x_i \in \Gamma_T : \quad \bar{u} = \frac{\partial g}{\partial q_n} Q \tag{11}$$

$$x_i \in \Gamma_q : \quad \bar{u}_{,n} = \frac{\partial g}{\partial T} \frac{Q}{k} \tag{12}$$

It may be seen that the adjoint problem for $\bar{u}$ has the same type of equations as for u but with different boundary conditions.

If the primary problem, Equations (6)-(8), is solved for a set of decision variables the expressions on the right hand sides of Equations (11) and (12) may be found directly. Solution of the adjoint problem is then implemented by using the same type of solution procedure as for u. The first variation of I is then given as follows:

$$\delta I = \left[-\frac{1}{k} \int_\Gamma T \frac{\partial g}{\partial T} \, d\Gamma \right] \delta k$$

$$+ \left\{ \int_\Gamma \left[\frac{T}{Q} \frac{\partial g}{\partial T} + \left(\frac{x_i n_i}{d} - u_{,n} \right) \frac{\partial g}{\partial q_n} \right] d\Gamma - \frac{1}{Q^2} \int_{\Gamma_q} q_0 \left(Q \frac{\partial g}{\partial q_n} - \bar{u} \right) d\Gamma \right\} \delta Q$$

$$+ \int_{\Gamma_q} \left(\frac{\partial g}{\partial q_n} - \frac{\bar{u}}{Q} \right) \delta q_0 \, d\Gamma + \frac{\partial h}{\partial \phi_i} \delta \phi_i \tag{13}$$

which indicates the sensitivity of I with respect to the decision variables. It may be noticed that since k and Q are constants their variations are positioned out of the integrals in Equation (13). On the other hand, the variation δq_0 remains inside of integral since it is a function of position over the boundary segment Γ_q. It may be emphasized that the sensitivity expression given by Equation (13) corresponds to the primary problem defined by differential equations (1)-(3). It thus constitutes the sensitivity expression of I using the DSA formulation.

INTEGRAL SENSITIVITY ANALYSIS (ISA)

In this formulation, which will be denoted by ISA, the differential equation for u, given by Equation (6), is first transformed into a BIE given as follows [12-13] :

$$\xi \in \Gamma \ : \ c(\xi)\, u(\xi) + \int_{\Gamma(x)} u^*_{,n}(x,\xi)\, u(x)\, d\Gamma(x) - \int_{\Gamma(x)} u^*(x,\xi)\, u_{,n}(x)\, d\Gamma(x) = 0 \tag{14}$$

where $u^*(x,\xi)$ and $u^*_{,n}(x,\xi)$ are the fundamental solutions; $c(\xi)$ is the solid angle of Γ ; x and ξ represent the field and source points, respectively. The forms of the fundamental solutions are, for example, in a 2-dim. domain, given as follows [13]:

$$u^*(x,\xi) = \frac{1}{2\pi} \ln(\frac{1}{r}) \tag{15}$$

$$u^*_{,n}(x,\xi) = \frac{\partial u^*(x,\xi)}{\partial n(x)} = -\frac{r_i n_i(x)}{2\pi r^2} \tag{16}$$

where

$$r_i = x_i - \xi_i \qquad\qquad r^2 = r_i r_i \tag{17}$$

The BIE given by Equation (14) is adopted as the system equation, instead of Equation (6). Thus, the primary problem is given by an integral equation on which the present SA formulation will be based, hence the name ISA. The neccesary boundary conditions are again given by Equations (7) and (8).

Following the general procedure of AVM, an augmented functional $\tilde{I}$ is constructed by incorporating Equation (14) into the same objective function as has been used in the DSA formulation, i.e., Equation (4), as follows:

$$\tilde{I} = \int_{\Gamma(\xi)} \left\{ g + \hat{u}(\xi) \left[c(\xi)u(\xi) + \int_{\Gamma(x)} u^*_{,n}(x,\xi)u(x)d\Gamma(x) - \int_{\Gamma(x)} u^*(x,\xi)u_{,n}(x)d\Gamma(x) \right] \right\} d\Gamma(\xi) + h(\phi_i) \tag{18}$$

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where $\hat{u}$ is the associated adjoint function. It is noted that $\tilde{I}$ involves doubly-nested boundary integrals defined over Γ.

A simple procedure, slightly different from the previous one, is implemented as follows:

i) Take the first variation of $\tilde{I}$

ii) Substitute the variation δT and δq_n as before

iii) Interchange the order of nested integrations

iv) Rename the dummy variables of integrations

v) Insert the variational forms of the boundary conditions

vi) Define an adjoint problem for $\hat{u}$ by the following:

$$\xi \in \Gamma_T \quad : \quad \int_{\Gamma(x)} u^*(\xi, x)\hat{u}(x)d\Gamma(x) = -\frac{\partial g}{\partial q_n} Q \tag{19}$$

$$\xi \in \Gamma_q \quad : \quad c(\xi)\hat{u}(\xi) + \int_{\Gamma(x)} u^*_{,n}(\xi, x)\hat{u}(x)d\Gamma(x) = -\frac{\partial g}{\partial T}\frac{Q}{k} \tag{20}$$

Some interesting features of the above equations may be noted. The primary BIE, Equation (18), is a mixed type of integral equation defined in the same form for all points on Γ. On the other hand, Equations (19) and (20) define a BIE of Neuman type given in different forms depending on the location of ξ, i.e., whether on Γ_T or Γ_q. The kernels in these equations are given by

$$u^*(\xi, x) = \frac{1}{2\pi} \ln(\frac{1}{r}) \tag{21}$$

$$u^*_{,n}(\xi, x) = \frac{\partial u^*}{\partial n(\xi)} = \frac{r_i n_i(\xi)}{2\pi r^2} \tag{22}$$

The kernels have been introduced during the interchanging of nested integration's variables. It is seen that although $u^*(\xi, x)$ symmetric in x and ξ, $u^*_{,n}(\xi, x)$ is given differently than $u^*_{,n}(x, \xi)$ (cf. Equations (16) and (22)). The right hand sides of Equations (19) and (20) are free terms which are calculated after the solution of the primary problem u. Hence, they do not require any volume integrations as in the case of nonuniform distributed sources in the domain [13]. In fact, they may be considered as corresponding to singular types of boundary conditions on Γ given in terms of Dirac delta functions. Another intresting feature of the free-terms in Equations (19) and (20) is that they are exactly the boundary conditions (with a negative sign) for the $\bar{u}$ problem, as given by Equations (11) and (12).

If the primary and adjoint problems, i.e., Equations (14), (19) and (20), are satisfied by a set of decision variables during an iterative solution process of optimization the sensitivity of I is given by the following expression:

$$
\begin{aligned}
\delta I = & \left[-\frac{1}{k} \int_{\Gamma(\xi)} T \, \frac{\partial g}{\partial T} \, d\Gamma(\xi) \right] \delta k \\
& + \left\{ \int_{\Gamma(\xi)} \left[\frac{T}{Q} \frac{\partial g}{\partial T} + \left[\frac{x_i n_i}{d} - u_{,n} \right] \frac{\partial g}{\partial q_n} \right] d\Gamma(\xi) \right. \\
& \left. - \frac{1}{Q^2} \int_{\Gamma_q(\xi)} q_0 \left[Q \frac{\partial g}{\partial q_n} + \int_{\Gamma(x)} u^*(\xi, x) \, \hat{u}(x) d\Gamma(x) \right] d\Gamma(\xi) \right\} \delta Q \\
& + \int_{\Gamma_q(\xi)} \left[\frac{\partial g}{\partial q_n} + \frac{1}{Q} \int_{\Gamma(x)} u^*(\xi, x) \, \hat{u}(x) \, d\Gamma(x) \right] \delta q_0 \, d\Gamma(\xi) \\
& + \frac{\partial h}{\partial \phi_i} \delta \phi_i
\end{aligned}
\tag{23}
$$

The above equation represents the sensitivity expression of I with respect to the decision variables k, Q, ϕ_i and q_0 . It may be noticed that doubly-nested integrals are involved in the sensitivity coefficients of δQ and δq_0 in Equation (23).

If the sensitivity expressions obtained by the DSA and ISA formulations , i.e., Equations (13) and (23), are compared the sensitivity coefficient for δk is seen to be the same in both formulations, i.e.,

$$\frac{\delta I}{\delta k} = \Pi_k = -\frac{1}{k} \int_{\Gamma(\xi)} T \ \frac{\partial g}{\partial T} \ d\Gamma(\xi) \tag{24}$$

where Π_k denotes the associated sensitivity coefficient. The sensitivity coefficients for Π_Q and Π_{q_0} in Equations (13) and (23) are, on the other hand, equal to each other if and only if the following expression is satisfied:

$$\xi \in \Gamma_q \quad : \qquad \bar{u} \ = \ - \int_{\Gamma(x)} \ u^*(\xi, x) \, \hat{u}(x) \, d\Gamma(x) \tag{25}$$

The above expression gives a relationship between the adjoint functions $\bar{u}$ and $\hat{u}$ introduced in the DSA and ISA formulations, respectively, over the boundary segment Γ_q. The functions are, however, defined over all of the boundary Γ.

BOUNDARY ELEMENT DISCRETIZATIONS

The boundary element method (BEM) is utilized in order to discretize all equations given in the last sections. It is noted that the primary and adjoint problems in the DSA formulation are given by differential equations, i.e., Equations (6) and (10). The differential equation for u has already been transformed into a BIE, Equation (14). The same type of BIE may be used for the solution of the $\bar{u}-$ problem.

Constant boundary elements are used in all discretizations in the present paper. For the solution of the $u-$ and $\bar{u}-$ problem the following element matrices may be defined [13]:

$$G_{ij}^e = \int_{\Gamma^e(x)} \ u^*(x, \xi) \ d\Gamma(x) \tag{26}$$

$$H_{ij}^e = \int_{\Gamma^e(x)} \ u_{,n}^*(x, \xi) \ d\Gamma(x) \tag{27}$$

where $u^*(x, \xi)$ and $u_{,n}^*(x, \xi)$ are given by Equations (15) and (16). When the element matrices are assembled the whole set of equations can be expressed in matrix form by using Equation (14) as

$$\mathbf{HU} = \mathbf{GQ} \tag{28}$$

where **H** and **G** are (n x n) matrices; n is the total number of boundary nodes on Γ; **U** and **Q** denote (n x 1) vectors representing the nodal values of u and $u_{,n}$, respectively.

If there exist n_t and n_q number of nodes on Γ_T and Γ_q, respectively, with $n_t + n_q = n$, n_t values of u and n_q values of q are known on Γ. Equation (28) may be reordered with all the unknowns on the left hand side and a vector on the right hand side obtained by multiplying matrix elements by the known values of potential and flux. This gives

$$\mathbf{A}\,\mathbf{Y} = \mathbf{F} \tag{29}$$

where **Y** is the vector of unknowns $u_{,n}$'s on Γ_T and u's on Γ_q, written as

$$\mathbf{Y} = \left\{ \begin{array}{c} \mathbf{Q_T} \\ \mathbf{U_q} \end{array} \right\} \tag{30}$$

where $\mathbf{Q_T}$ and $\mathbf{U_q}$ are vectors of dimension (n_tx1) and (n_qx1), respectively.

In the case of the ISA formulation, the adjoint function $\hat{u}$ is given in terms of a different type of integral equation, namely, Equations (19) and (20). Using constant boundary elements again the following element matrices may be defined:

$$\hat{G}^e_{ij} = G^e_{ij} = \int_{\Gamma^e(x)} u^*(\xi, x)\, d\Gamma(x) \tag{31}$$

$$\hat{H}^e_{ij} = \int_{\Gamma^e(x)} u^*_{,n}(\xi, x)\, d\Gamma(x) \tag{32}$$

where $u^*(\xi, x)$ and $u^*_{,n}(\xi, x)$ are given by Equations (21) and (22). After the element assembly the whole set of equations may be expressed in matrix form using Equations (19) and (20) as follows:

$$\left[\begin{array}{c} \hat{\mathbf{G}} \\ --- \\ \hat{\mathbf{H}} \end{array} \right] \left\{ \hat{\mathbf{U}} \right\} = \left[\begin{array}{c} \mathbf{B_T} \\ --- \\ \mathbf{B_q} \end{array} \right] \tag{33}$$

where $\hat{\mathbf{G}}$ and $\hat{\mathbf{H}}$ matrices are of dimensions (n_t x n) and (n_q x n), respectively; $\hat{\mathbf{U}}$ represents the unknown nodal values of u with a dimension (n_t x 1); $\mathbf{B_T}$ and

$\mathbf{B_q}$ denote the free term vectors whose elements are calculated directly by the right hand side of Equations (19) and (20).

The above equation is already in a form in which the unknown values are on the left hand side in contrast to Equation (28). It may be noticed that only nodal values of $\hat{u}$ are calculated and that no direct information is acquired regarding the nodal values of $\hat{u}_{,n}$. This aspect along with the presence of free-terms (with no integrals) represent interesting features of the BIE associated with the $\bar{u}-$ problem.

NUMERICAL EXAMPLES

Two example problems with different geometries are solved by using the presented SA formulations. In order to check the accuracy of the sensitivity expressions a 1-dim. annular cylinder problem is analyzed first (see Fig.2), where the inner and outer radii are taken as $r_1 = 1$ and $r_2 = 2$, respectively. An unconstrained optimization problem is considered with the following objective functional:

$$I = \frac{1}{2}\int_{\Gamma_q} (T - T_r)^2 \ d\Gamma \tag{34}$$

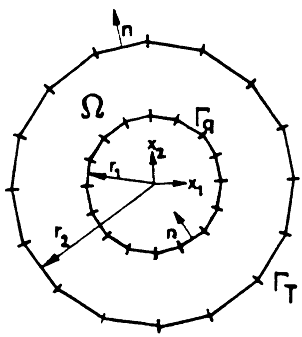

Fig. 2 Annular cylinder geometry and boundary elements

where T_r is the reference temperature with a value of 1. It may be seen from Fig.2 that Γ_q corresponds to the inner boundary surface, while Γ_T is the outer surface. The sensitivity coefficient of I with respect to constant values of k, Q and q_0 are calculated by the DSA and ISA formulations as well as by analytical means. The numbers of constant boundary elements is 16 for both Γ_T and Γ_q,

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with a total of 32. The percentage errors in the numerical results as compared to the exact ones, indicated by $e(\Pi_k)$, $e(\Pi_Q)$ and $e(\Pi_{q_0})$, are tabulated in Tables I, II and III by varying one decison parameter while holding the other two fixed.

The sensitivity coefficient Π_k results are the same for the two formulations, as they are given by the same expression, Equation (24). Better results are obtained by the ISA formulation for Π_Q and Π_{q_0}. It is emphasized that better accuracies have been obtained even though doubly-nested integral exist in the integral formulation. An explanation can be offered for this as follows: The adjoint function $\bar{u}$ and also its normal derivative $\bar{u}_{,n}$ introduced in the DSA formulation belong to L_2 ,the square-integrable functions space, as dictated by the BIE of the form (14). On the other hand, Equations (19) and (20), require that only the adjoint function $\hat{u}$, introduced in the ISA formulation, belong to L_2, leaving its normal derivative free. This freedom obviously leads to higher accuricies for the sensitivity coefficients Π_Q and Π_{q_0}, which involve inner integrals with $\hat{u}$.

Table I Percentage errors in sensitivity coefficients by DSA and ISA for different k ($Q = 25$, $q_0 = 1$)

	$e(\pi_k)$		$e(\pi_Q)$		$e(\pi_{q_o})$	
k	DSA	ISA	DSA	ISA	DSA	ISA
0.25	2.7	2.7	2.5	2.3	1.6	0.1
0.50	2.9	2.9	2.7	2.5	1.8	0.1
0.75	3.1	3.1	3.0	2.8	2.0	0.4

Table II Percentage errors in sensitivity coefficients by DSA and ISA for different Q ($k = 1$, $q_0 = 1$)

	$e(\pi_k)$		$e(\pi_Q)$		$e(\pi_{q_o})$	
Q	DSA	ISA	DSA	ISA	DSA	ISA
25.00	3.5	3.5	3.4	3.1	2.4	0.8
30.10	3.1	3.1	3.0	3.0	2.1	0.5
35.00	2.9	2.9	2.8	2.7	1.9	0.3

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Table III Percentage errors in sensitivity coefficients by DSA and ISA for different q_0 ($k = 1$, $Q = 25$)

q_0	$e(\pi_k)$		$e(\pi_Q)$		$e(\pi_{q_0})$	
	DSA	ISA	DSA	ISA	DSA	ISA
0.25	3.0	3.0	3.0	2.9	2.0	0.4
0.50	3.2	3.2	3.1	3.0	2.2	0.5
0.75	3.3	3.3	3.2	3.1	2.4	0.8

A 2-dim. problem involving optimal cooling of turbine blades is also analyzed (see, Fig.3). In this unconstrained optimization problem the same objective function (cf.Equation (4)) is used, as before. Simultaneous optimization of k, Q and q_0 parameters lead to the following optimal values : By the DSA formulation; $k = 0.041367$, $Q = 9.0873$ and $q_0 = 0.001$. By the ISA formulation; $k = 0.041367$, $Q = 0.90871$ and $q_0 = 0.001$. In the iterative solution of optimization 49 and 50 iterative steps have been needed in the DSA and ISA formulations, respectively. The CPU time required in the ISA formulation, however, was 22of $k = 0.455$ has been obtained by the two methods when Q and q_0 parameters were fixed with values of 10 and 0.001, respectively. The ISA formulation needed 43 iterative steps for convergence, in contrast to 52 steps in the DSA procedure.

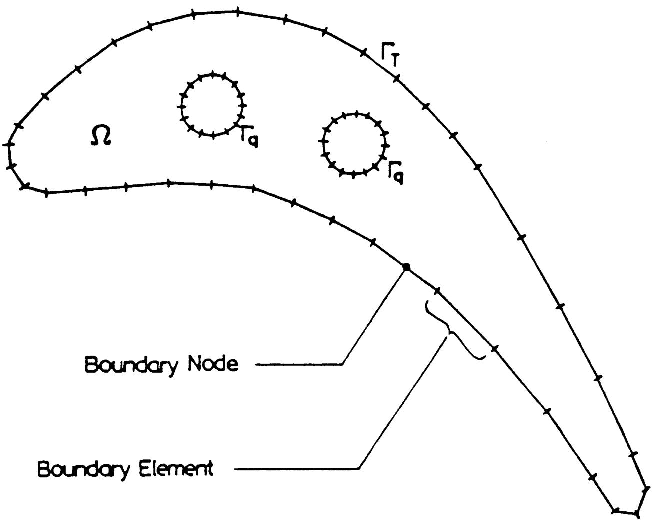

Fig. 3 Turbine blade geometry and boundary elements

CONCLUSION

Two different SA formulations have been presented for the optimal heating of solids. In the differential formulation the physics of the problem has been described by the heat differential equation, while in the integral formulation the asssociated boundary integral equation is adopted as the system equation. As aunique feature of the so-called SA formulation the relevant adjoint problem is described by an integral equation of Neumann type. Another interesting feature is that doubly-nested integrals appear in the sensitivity expressions of an integral functional. Better sensitivity results are obtained through the ISA formulation as no continuity requirements exist for the associated adjoint function in the integral formulation. Further studies are in progress in regard to the effectiveness of the two methods for nonhomogenous distributed heat sources and objective functions defined over the domain, as well.

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