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On the 3-D inverse potential target pressure problem. Part 1. Theoretical aspects and method formulation

By P. CHAVIAROPOULOS,[1] V. DEDOUSSIS[1,2] AND K. D. PAPAILIOU[1]

[1] National Technical University of Athens, Laboratory of Thermal Turbomachines, PO Box 64069, 157 10 Athens, Greece

[2] Department of Industrial Management, University of Piraeus, 185 34 Piraeus, Greece

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An inverse potential methodology is introduced for the solution of the fully 3-D target pressure problem. The method is based on a potential function/stream function formulation, where the physical space is mapped onto a computational one via a body-fitted coordinate transformation. A potential function and two stream vectors are used as the independent natural coordinates, whilst the velocity magnitude, the aspect ratio and the skew angle of the elementary streamtube cross-section are assumed to be the dependent ones. A novel procedure based on differential geometry and generalized tensor analysis arguments is employed to formulate the method. The governing differential equations are derived by requiring the curvature tensor of the flat 3-D physical Eucledian space, expressed in terms of the curvilinear natural coordinates, to be zero. The resulting equations are discussed and investigated with particular emphasis on the existence and uniqueness of their solution. The general 3-D inverse potential problem, with 'target pressure' boundary conditions only, seems to be ill-posed accepting multiple solutions. This multiplicity is alleviated by considering elementary streamtubes with orthogonal cross-sections. The assumption of orthogonal stream surfaces reduces the number of dependent variables by one, simplifying the governing equations to an elliptic p.d.e. for the velocity magnitude and to a second-order o.d.e. for the streamtube aspect ratio. The solution of these two equations provides the flow field. Geometry is determined independently by integrating Frenet equations along the natural coordinate lines, after the flow field has been calculated. The numerical implementation as well as validation test cases for the proposed inverse methodology are presented in the companion paper (Paper 2).

1. Introduction

Optimal shape design in the context of applied aero-thermodynamics is one of the CFD challenges for the next decade. The development of reliable automated methods which will reduce the human expertise element in the design loop will increase the quality and duration of the products, while decreasing, on the other hand, their development cost. Although the concept is as old as the theory of aerodynamics itself, the maturation of analysis methods and the continuously increasing computing power have put it backstage. Comprehensive reviews on optimal shape design methods have been presented by Dulikravich (1990) and more recently by Labrujere & Sloof (1993).

First attempts in the field of optimal shape design are traced back to the mid-forties when inverse potential methods based on conformal mapping and potential theory were applied to the design of airfoils. In the fifties, Stanitz (1953) developed his inverse potential method for compressible flows. Applying a body-fitted coordinate transformation, Stanitz derived the inverse potential flow equations on a 'natural' computational plane employing the potential function and the stream function as independent variables. The two-dimensional (2-D) inverse problem can then be solved if 'target' velocity (or pressure) distributions are imposed over the complete boundaries of the domain. Stanitz's method, being more flexible than the conformal mapping ones, has been extended to axisymmetric flows (Nelson & Yang 1977) as well as to turbomachinery flows including the planar and the axisymmetric rotating or non-rotating cascades (Schmidt 1980; Hawthorne *et al.* 1984; Bonataki, Chaviaropoulos & Papailiou 1991). The 2-D potential target pressure problem has been recently reconsidered by Barron (1990), who provided an alternative formulation using the Von-Mises transformation, by Volpe (1990) who developed iterative profile closure conditions for compressible flows, and by Chaviaropoulos, Dedoussis & Papailiou (1993) who reformulated the airfoil design problem using differential geometry principles.

The computational cost of all the above-mentioned 'target pressure' (inverse) methods is equivalent to that of analysis (direct) methods. For reasons which will be explained below we will refer to these methods as 'single-pass' methods. The single-pass methods are very efficient in terms of the computational cost and provide a physical insight to the design problem. Conceptually, however, they are restricted to 2-D potential flows only. Some extensions to 2-D rotational flows using the Clebsch transformation are reported by Borges (1991) and Dedoussis, Chaviaropoulos & Papailiou (1993). Stanitz (1980, 1985) extended his original 2-D potential method to three dimensional (3-D) flows. A disadvantage of the single-pass methods is related to their inability to incorporate flow or geometrical side constraints. Thus, the designer's expertise remains crucial for determining the 'appropriate' target pressure distribution.

In the effort to circumvent the drawbacks of single-pass methods, optimization methods appeared in the design field as an alternative. These methods solve a general minimization problem, the cost function of which expresses desired flow properties along with flow or geometrical constraints. This cost function is computed using a standard direct solver and the designer may decide upon the complexity level of the state equations to be solved. The solution of the optimization problem (the 'target pressure' problem being one variant) is obtained as a sequence of direct problem solutions. Although the formulation of the design problem seems to be straightforward, these methods are still time consuming (some hundreds of direct problems are sometimes solved in the optimization process, plus the regridding overhead) while in complicated 3-D flows the grid deformation and adaption problem may become crucial for the convergence of the algorithm. Convergence may be accelerated using suitable parametrization techniques (Greff, Forbrich & Schwarten 1991) or hierarchical optimization techniques (Beux & Dervieux 1991). An alternative approach springs from the reformulation of the general optimization problem using optimal control theory (Cabuk, Sung & Modi 1991). Then the descend direction may be obtained from the solution of an 'adjoint' state equation which is usually similar to the state equation itself. This technique reduces the computational cost a lot, provided that the adjoint equation exists.

Although optimization methods appear to be a remedy for the design problem this is not completely true. There are difficulties in specifying the appropriate cost function for a precise problem. If, for example, the shock drag minimization problem is to be solved for a transonic airfoil, a hanging shock solution may be obtained if no curvature constraints are imposed on the profile. Optimization of lift versus drag at a specific incidence may cause, as a second example, severe off-design problems. It seems that the formulation of the optimization problem using global flow measures (such as lift and drag) in an automated procedure is a very risky policy. It is much better to control the flow behaviour at the local level and that explains why the target pressure conditions are widely used as optimality conditions by the optimization methods as well. Even in this case, however, the results may be misleading. If, for instance, the prescribed inviscid target pressure distribution is not consistent in terms of profile closure, the minimization algorithm will provide a solution which may be far from the desired one in physical terms (the transition point location may be altered or flow separation may be produced because of local deceleration of the flow). Additionally, optimization methods provide no information on the existence and the uniqueness of the solution of a flow (design) problem. They lack, therefore, the physical insight of single-pass methods.

Let us now address the question of existence and uniqueness of solution of the inverse target pressure problem using the simplest flow model, that is the incompressible potential flow. In 2-D this problem is equivalent to the solution of a Laplace equation for the velocity logarithm on the transformed plane with Dirichlet-type boundary conditions (Stanitz 1953). In this case the inverse target pressure problem is linear and accepts a unique admissible solution in simply connected regions. However, this is not true for multi-connected regions, the isolated airfoil case for example, where additional constraints should be satisfied by the target pressure distribution in order to ensure the closure of the profile. A set of integral constraints has been developed by Lighthill (1945) for incompressible potential flows, but no explicit set of such constraints is available for compressible flows. It is well known, on the other hand, that even if these constraints are satisfied the closed profile may be non-admissible (re-entering airfoils for example). In 3-D the question has not been answered even for the simplest case of incompressible potential flows in simply connected geometries. Stanitz's (1980, 1985) work indicates that in contrast to the 2-D case the 3-D problem is nonlinear. He also reported convergence difficulties in several test cases he tried. In the authors' opinion this is due to the non-uniqueness of the solution.

The purpose of this work is to present a single-pass inverse potential method for the solution of the general 3-D target pressure problem. Similar to the approach proposed by Stanitz (1980), a potential function ϕ and two stream functions ψ and η are introduced as the 'natural' coordinates. A body-fitted coordinate transformation is employed to map the physical (x, y, z)-space on which the boundaries of the flow field are unknown onto the natural (ϕ, ψ, η)-space. Computational boundaries on the latter space are fixed simply because, in inviscid flows, lateral boundaries are stream surfaces, i.e. $\psi = \text{const.}$ or $\eta = \text{const.}$ surfaces, and inflow and outflow boundaries can be considered to be potential ones. Thus, assuming that the velocity distribution (or prescribed pressure) is given on the lateral as well as on the inflow and outflow boundaries of the flow field, one is faced with solving a boundary value problem on the (ϕ,ψ, η)-space.

The novelty of the present method is that the inverse target pressure problem is treated as a geometrical problem rather than a fluid dynamics one. A mathematically formal way, employing differential geometry and generalized tensor analysis arguments has been adopted in order to formulate the problem and derive a novel set of governing equations. Actually the metrics of the (ϕ, ψ, η) natural space, which are expressed in terms of flow quantities, should satisfy the zero curvature condition of the 3-D Euclidean (flat) space. A closed set of three partial differential equations (p.d.e.s) is, thus, derived in terms of the velocity magnitude V, and the aspect ratio t and the skew angle θ of the elementary streamtube cross-section. Both the formulation of the method and the resulting equations are quite different from those proposed by Stanitz (1980), although the same set of dependent and independent variables has been used.

It is seen that the 3-D inverse problem with velocity (or pressure)-only boundary conditions is an ill-posed problem accepting multiple solutions. This is due to the insufficient number of available boundary conditions. The extra boundary conditions required to remove this multiplicity may be introduced in several ways, e.g. appropriate, desirable, θ-values may be prescribed along the lateral boundaries (stream surfaces). In this work we removed this multiplicity by decreasing the degrees of freedom of the problem. We seek a particular solution in the resulting reduced space of geometries. We avoid, in this way, introducing any extra information which is not always available. In this context, it has been shown that the problem accepts as a particular solution elementary streamtubes with orthogonal cross-sections. Thus, the number of dependent variables is reduced by one and the governing equations simplify to an elliptic-type p.d.e. for the velocity magnitude and to a second-order o.d.e. for the streamtube aspect ratio. The solution of these two equations provides the flow field in a single-pass manner without requiring any feedback from the geometry. In a subsequent step, geometry is determined independently by integrating Frenet equations along the natural coordinate lines. The decoupling of flow and geometry equations is obviously attractive from the computational point of view. However, the present method being a single-pass one, cannot inherently incorporate sophisticated flow or geometrical constraints. Some control on the geometry is effected *a priori* via the flow-field boundary conditions, e.g. Dirichlet velocity conditions on the boundary of the natural coordinate space are related to the arclength of the boundary streamlines, while Neumann velocity conditions are related to local streamline curvature. It is worth noting that the present method is, in itself, a simple flow solver which employs a very specific body-fitted coordinate transformation. In that respect it can be incorporated as the state equation in any optimization loop. The replacement of analysis flow solvers with the inverse one alleviates the regridding penalty due to the moving of the boundaries within the iterative process. This is because the inverse solver handles the governing equations in a simple rectangular natural body-fitted coordinate space. The present authors have applied this approach to 2-D duct optimization (Workshop on Selected Inverse and Optimum Design Problems, organized by Brite Euram Project 1082 partners, June 1992).

Part 1 of the study, this paper, focuses on the theoretical aspects and the formulation of the method. The numerical implementation and some validation tests cases of the proposed methodology in 3-D internal configurations are presented in Part 2 (Dedoussis, Chaviaropoulos & Papailiou 1995).

2. Problem statement and basic equations

The inverse target pressure problem can be stated as: 'Given a prescribed target velocity (pressure) distribution on the entire (lateral, inflow and outflow) boundary of a 3-D flow field determine the corresponding boundary shape'. In the present work it has been assumed that the flow is three-dimensional steady, compressible inviscid and irrotational. It has been also assumed that the fluid is a perfect gas.

Under the above assumptions the flow equations simplify to
continuity equation

$$\nabla \cdot (\rho V) = 0; \tag{1}$$

irrotationality condition

$$\nabla \times V = 0; \tag{2}$$

density equation (energy conservation for isentropic changes)

$$\rho = \left[1 + \frac{\gamma - 1}{2} M_\infty^2 (1 - V^2)\right]^{1/(\gamma-1)}. \tag{3}$$

In the above equations the velocity V is normalized with a reference value V_∞ and the density ρ with the corresponding ρ_∞ value. M_∞ is the Mach number at the reference point and γ is the ratio of specific heats c_p/c_v.

The irrotationality condition of the velocity field expressed by (2) is satisfied identically, by requiring the velocity vector to be the gradient of a scalar function, i.e. potential function. The potential function ϕ is defined by the relation

$$V = \nabla \phi. \tag{4}$$

The continuity equation (1) can be identically satisfied by introducing two stream functions ψ, η (Yih 1957) defined by the relation

$$\rho V = \nabla \psi \times \nabla \eta. \tag{5}$$

Equation (5) indicates that the velocity vector is tangent to both $\psi = \text{const.}$ and $\eta = \text{const.}$ surfaces, which are appropriately termed as stream surfaces. Obviously intersections of stream surfaces, which belong to a different family, are streamlines. Schematically, potential and stream surfaces are shown in figure 1(*a*).

The potential function ϕ and the two stream functions ψ, η are considered to be the independent variables. The physical (x, y, z)-space, on which the boundaries of the flow field sought are unknown, is mapped onto the natural (ϕ, ψ, η)-space via a body-fitted coordinate transformation.

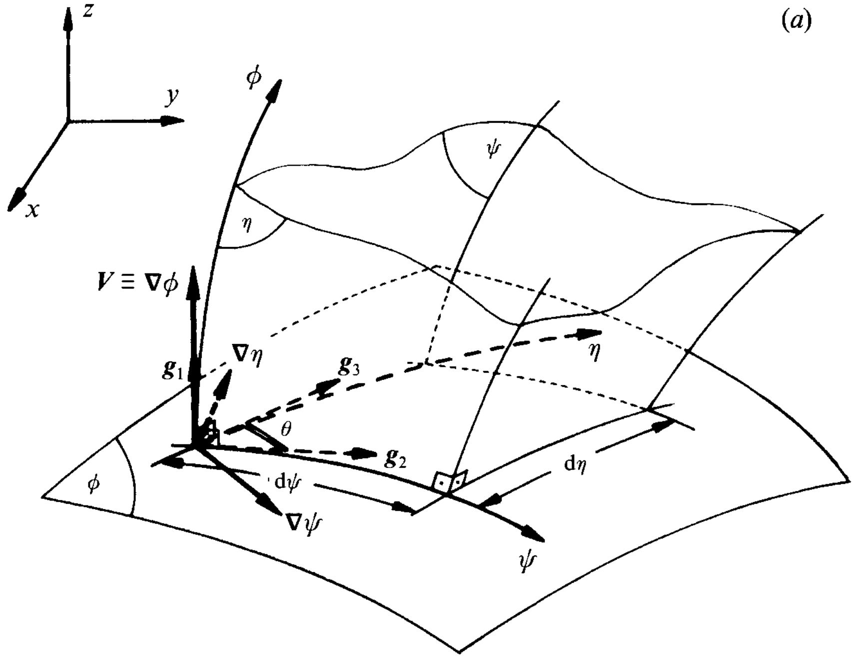
3. The concept

Differential geometry and generalized tensor analysis arguments are employed in order to derive the governing equations. For completeness an overview of differential geometry principles has been included in the Appendix. The line of thought is as follows.

Consider a representation of the 3-D (x, y, z) Euclidean space in terms of the natural curvilinear coordinates (ϕ, ψ, η). Euclidean space, being flat, has zero curvature. Referring to the Ricci curvature tensor the zero-curvature condition reads

$$R_{rm} = 0 \quad \text{with} \quad r, m = 1, 2, 3. \tag{6}$$

From the definition of the Ricci tensor and the Christoffel symbols Γ_{ij}^k, see (A 8)–(A 10), it is observed that the zero-curvature condition is expressed in terms of the elements of the metrics tensor and their first- and second-order partial derivatives. In that sense, the flat-space condition provides six metric compatibility conditions which have to be satisfied for any parametrization of the physical space, including the (ϕ, ψ, η) one. In the present formulation the (ϕ, ψ, η) natural coordinates have been adopted,



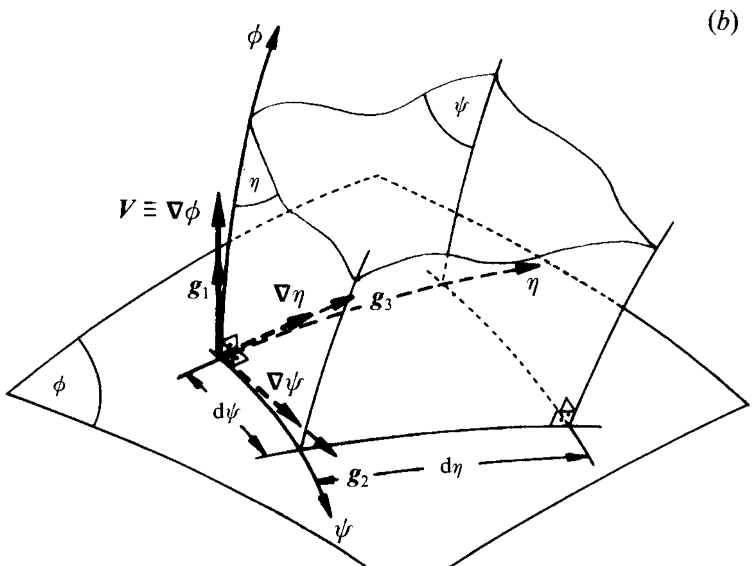


FIGURE 1. Natural (ϕ, ψ, η) coordinate system and elementary streamtubes. (*a*) General 3-D case. (*b*) 3-D case with orthogonal ψ- and η-family stream surfaces.

having the advantage that the corresponding metrics tensor is expressed in terms of flow quantities only. The governing equations of the inverse flow problem in the (ϕ, ψ, η)-space, therefore, are provided via the satisfaction of the zero curvature conditions.

It is emphasized, however, that the six metrics compatibility conditions (6) are not independent, since in Riemannian geometry the Ricci tensor elements satisfy the following Bianchi identities (Synge & Schild 1978):

$$g^{rm}R_{rm,k}-g^{rm}R_{rk,m}-g^{ij}R_{ik,j}=0 \quad \text{with} \quad i,j,k,r,m=1,2,3. \tag{7}$$

Bianchi identities provide three ($k=1,2,3$) equations interrelating the covariant derivatives ($R_{ij,k}$) of the curvature tensor elements, thus reducing the overall number of independent metrics compatibility conditions to three only. According to the discussion in Malvern (1969), satisfaction of either the diagonal zero-curvature conditions, equations (6), or the off-diagonal ones only, is not sufficient for the flatness of the physical 3-D space. For a simply connected region, this is established if any one of the set of the three conditions is satisfied in the interior of the field and the other one on the boundaries. Evidently, this combination results in a *boundary value* problem.

4. Method formulation

The contravariant base of the natural curvilinear (ϕ,ψ,η) coordinate system is

$$\boldsymbol{g}^1=\boldsymbol{\nabla}\phi, \quad \boldsymbol{g}^2=\boldsymbol{\nabla}\psi, \quad \boldsymbol{g}^3=\boldsymbol{\nabla}\eta, \tag{8}$$

where indices 1, 2, 3 are associated with the ϕ,ψ,η coordinates respectively.

The metrics and the conjugate (contravariant) metrics of the $(\phi,\ \psi,\ \eta)$ system are evaluated, using (4) and (5) and standard tensor relations. In terms of flow quantities the metrics and conjugate metrics of the (ϕ,ψ,η) coordinate system are

$$\left.\begin{aligned} g_{11}&=\frac{1}{V^2}, & g^{11}&=V^2;\\ g_{22}&=1/(\rho Vt\sin\theta), & g^{22}&=\rho Vt/\sin\theta;\\ g_{23}=g_{32}&=1/(\rho V\tan\theta), & g^{23}&=g^{32}=-\rho V/\tan\theta;\\ g_{33}&=t/(\rho V\sin\theta), & g^{33}&=\rho V/(t\sin\theta);\\ g_{12}=g_{21}=g_{13}=g_{31}&=0, & g^{12}&=g^{21}=g^{13}=g^{31}=0,\end{aligned}\right\} \tag{9}$$

where θ is the angle between $\boldsymbol{g}_2$ and $\boldsymbol{g}_3$ (or the angle at which a $\psi=$ const. surface intersects a $\eta=$ const. stream surface on a potential, $\phi=$ const., surface, see figure 1*a*) and t is a variable defined as

$$t^2=g_{33}/g_{22}. \tag{10}$$

Variable t represents the aspect ratio of the cross-section ($\phi=$ const. section) of the elementary streamtube defined by the stream surfaces ψ, $\psi+\mathrm{d}\psi=$ const. and η, $\eta+\mathrm{d}\eta=$ const., with $\mathrm{d}\psi=\mathrm{d}\eta$.

The off-diagonal elements of the metrics and conjugate metrics tensor, g_{ij} and g^{ij} (with $i=1$ and $j=2,3$) respectively, are zero since via the defining relations (4) and (5) both $\boldsymbol{\nabla}\psi$ and $\boldsymbol{\nabla}\eta$ are normal to $\boldsymbol{\nabla}\phi$, i.e. $\boldsymbol{\nabla}\phi\cdot\boldsymbol{\nabla}\psi=\boldsymbol{\nabla}\phi\cdot\boldsymbol{\nabla}\eta=0$ (note that in general $\boldsymbol{\nabla}\psi\cdot\boldsymbol{\nabla}\eta=g^{23}\neq0$).

The elementary distance $\mathrm{d}s$ expressed in terms of the natural coordinates is

$$\mathrm{d}s^2=g_{11}\,\mathrm{d}\phi^2+g_{22}\,\mathrm{d}\psi^2+g_{33}\,\mathrm{d}\eta^2+2g_{23}\,\mathrm{d}\psi\,\mathrm{d}\eta. \tag{11}$$

Introducing (9) in the defining relations of the Christoffel symbols (see (A 8) and

(A 9)), expressions of the latter in terms of the dependent variables V, ρ, t, θ are derived. For example

$$\left.\begin{aligned} \Gamma^1_{11} &= -(\ln V)_\phi, \\ \Gamma^2_{11} &= (\rho/Vt\sin\theta)(\ln V)_\psi - (\rho/V\tan\theta)(\ln V)_\eta, \\ \Gamma^3_{11} &= (-\rho/V\tan\theta)(\ln V)_\psi + (\rho t/V\sin\theta)(\ln V)_\eta, \end{aligned}\right\} \tag{12}$$

where indices ϕ, ψ and η denote partial derivatives.

The governing p.d.e.s for V, t and θ are derived by the following combinations of the zero conditions for the elements of the Ricci tensor;

$$-R_{11}/g_{11} = 0, \tag{13}$$

$$-R_{22}/g_{22} + R_{33}/g_{33} = 0, \tag{14}$$

$$R_{22}/g_{22} + R_{33}/g_{33} - 2R_{23}/g_{23} - R_{11}/g_{11} = 0. \tag{15}$$

Equations (13)–(15) supplemented by (3) constitute a closed set of p.d.e.s for the quantities V, ρ, t, θ. Satisfying only three compatibility conditions is in accordance with the number of independent variables considered (V, t, θ) as well as with the overall number of independent conditions. Strictly, (13)–(15) constitute necessary but not sufficient conditions for the flatness of the 3-D space considered. However, the 'sufficient' character of the conditions is indicated by the satisfactory reproduction calculations presented in Part 2.

As will be demonstrated in the following sections, this particular linear combination of the individual Ricci tensor elements leads to a tractable set of governing equations, which can be solved for the flow quantities in a self-contained, single-pass, manner requiring no geometry feedback. The geometry is determined in a subsequent step by transforming the flow solution on the natural space, to the physical, Cartesian, one.

5. Governing equations of the flow field

The developed form of the governing equations (13)–(15) is:

velocity (V) equation

$$\begin{aligned} &(\ln\rho)_{\phi\phi} + (\ln V)_{\phi\phi} - (\ln\rho)_\phi[(\ln\rho)_\phi + (\ln V)_\phi] \\ &\quad + \tfrac{1}{2}(1+\cot^2\theta)\{[(\ln\rho)_\phi + (\ln V)_\phi + (\ln\sin\theta)_\phi]^2 - (\ln t)^2_\phi\} \\ &\quad - \tfrac{1}{2}\cot^2\theta[(\ln\rho)_\phi + (\ln V)_\phi + (\ln\tan\theta)_\phi]^2 \\ &\quad + (\rho t/V\sin\theta)\{(\ln V)_{\psi\psi} - (\ln V)_\psi[(\ln\rho)_\psi + (\ln V)_\psi + (\ln\sin\theta)_\psi - (\ln t)_\psi]\} \\ &\quad + (\rho/tV\sin\theta)\{(\ln V)_{\eta\eta} - (\ln V)_\eta[(\ln\rho)_\eta + (\ln V)_\eta + (\ln\sin\theta)_\eta + (\ln t)_\eta]\} \\ &\quad + (\rho\cot\theta/V)\{-(\ln V)_{\psi\eta} + (\ln V)_\psi[(\ln\rho)_\eta + (\ln V)_\eta + (\ln\tan\theta)_\eta] \\ &\qquad\qquad + (\ln V)_\eta[(\ln\rho)_\psi + (\ln V)_\psi + (\ln\tan\theta)_\psi]\} = 0; \end{aligned} \tag{16}$$

aspect ratio (t) equation

$$\begin{aligned} &(\ln t)_{\phi\phi} - (\ln t)_\phi[(\ln\rho)_\phi + 2(\ln\sin\theta)_\phi] \\ &\quad + (\rho\sin\theta/V)\left\{t(\ln V)_{\psi\psi} - \frac{1}{t}(\ln V)_{\eta\eta} + t(\ln V)_\psi(\ln\rho)_\psi - \frac{1}{t}(\ln V)_\eta(\ln\rho)_\eta \right. \\ &\qquad \left. + (1/\cos\theta)[(\ln V)_\eta(\ln\sin\theta)_\psi - (\ln V)_\psi(\ln\sin\theta)_\eta]\right\} = 0; \end{aligned} \tag{17}$$

skew angle (θ) equation

$$
\begin{aligned}
&(\ln\sin\theta)_{\phi\phi} - (\ln\rho)_\phi (\ln\sin\theta)_\phi \\
&\quad + \cot^2\theta\left\{(\ln t)_\phi^2 + (\ln\cos\theta)_\phi^2 - (\rho\sin\theta/V)\left[t(\ln V)_{\psi\psi} + \frac{1}{t}(\ln V)_{\eta\eta}\right]\right\} \\
&\quad + (\rho\cot\theta/V)\,[2(\ln V)_{\psi\eta} + (\ln V)_\psi(\ln t)_\eta - (\ln V)_\eta(\ln t)_\psi] \\
&\quad + (\rho\cos\theta/V)\left[t(\ln V)_\psi(\ln\rho)_\psi + \frac{1}{t}(\ln V)_\eta(\ln\rho)_\eta\right] = 0,
\end{aligned} \tag{18}
$$

where $\cot\theta = (\tan\theta)^{-1}$.

Noting that ρ is expressed in terms of V via (3), equations (16)–(18) form a closed system of p.d.e.s for the dependent variables V, t and θ. The above equations, therefore, represent the *governing equations for the general* 3-*D inverse potential problem*. This system of equations forms a boundary value problem for the main three dependent variables. According to the definition of the target pressure inverse problem, complete boundary conditions are only available for the velocity magnitude, while there are no boundary conditions for t and θ along the lateral boundaries.

Following the discussion presented in the previous section it was investigated whether the two compatibility conditions which have not been taken into account could provide this extra information for t and θ. The development of these conditions revealed that it is not possible to obtain a set of equations which contains information intrinsic to the lateral boundary only. This is mainly due to the presence of second-order mixed derivatives, e.g. $(\ln V)_{\phi\psi}$ in the $R_{12} = 0$ condition, along with first-order ones with respect to all three coordinate directions. These cannot by eliminated using the available information. It could be argued therefore that the 3-D inverse potential target pressure problem, as addressed above, is *ill-posed*, accepting multiple solutions.

The multiplicity of the solution could be removed by providing extra information for either t or θ along the lateral boundaries (stream surfaces). An alternative way of removing the multiplicity of the solution without introducing extra *a priori* unknown information is by reducing the degrees of freedom of the problem. In this work the latter strategy has been adopted. Actually the dependency of the solution on θ may be removed by observing that the θ-equation (18) is satisfied identically for constant $\theta = 90°$. This implies that a flow with elementary streamtubes with orthogonal cross-section (see figure 1*b*) represents a *particular* solution of the inverse potential target pressure problem. Assuming that $\theta = \text{const.} = 90°$, the θ-equation becomes redundant, while the V- and t-equations, (16) and (17) respectively, are simplified considerably and a unique solution may be obtained with the available velocity boundary conditions.

Hereafter, therefore, we deal with the following *well-posed* version of the general 3-D inverse target pressure problem: 'Given a prescribed target velocity (pressure) on the entire boundary of a 3-D flow field *made up of orthogonal elementary streamtubes*, determine the corresponding boundary shape.'

With the assumption of orthogonal streamtubes the resulting governing equations are:

velocity (V) equation

$$
\begin{aligned}
&(\ln V)_{\phi\phi} + (\ln\rho)_{\phi\phi} + (\rho t/V)(\ln V)_{\psi\psi} + (\rho/tV)(\ln V)_{\eta\eta} + \tfrac{1}{2}[(\ln V)_\phi^2 - (\ln t)_\phi^2 - (\ln\rho)_\phi^2] \\
&\quad - (\rho t/V)(\ln V)_\psi[(\ln V)_\psi - (\ln t)_\psi] - (\rho/tV)(\ln V)_\eta[(\ln V)_\eta + (\ln t)_\eta] = 0;
\end{aligned} \tag{19}
$$

aspect ratio (t) equation

$$(\ln t)_{\phi\phi}-(\ln\rho)_{\phi}(\ln t)_{\phi}+(\rho t/V)[(\ln V)_{\psi\psi}+(\ln V)_{\psi}(\ln\rho)_{\psi}] -(\rho/tV)[(\ln V)_{\eta\eta}+(\ln V)_{\eta}(\ln\rho)_{\eta}]=0. \quad (20)$$

6. Discussion of the flow equations

Appropriate boundary conditions for the solution of the flow equations are discussed in this section. The analysis is restricted to the compressible form of the governing equations which have been derived with the assumption of orthogonal streamtubes cross-section.

Assuming a given t-field, then (19) represents an elliptic-type quasi-linear p.d.e. for ($\ln V$). In accordance with the standard 'full-potential' equations the mathematical, elliptic or hyperbolic, character of the velocity equation (19), in the streamwise sense, is controlled by the size of the local Mach number, i.e. subsonic or supersonic flow conditions respectively. Considering (3), it can be shown that

$$(\ln\rho)_{\phi}=-M^2(\ln V)_{\phi}, \quad (21)$$

where M is the local Mach number. Introducing (21) into (19) and rearranging the second-order partial derivative terms, it is straightforward to show that the resulting equation is elliptic in the streamwise (ϕ) direction when $M<1$, and hyperbolic when $M>1$. Evidently, for subsonic flows, velocity boundary conditions should be specified all round the integration domain.

The aspect ratio equation (20) may be considered as a second-order o.d.e. along the streamlines, i.e. in the ϕ-direction. In that respect, (20) forms a boundary value problem requiring boundary conditions for t on the inflow and outflow boundaries only, which are considered to be potential surfaces. It is emphasized that the closed set of equations (19) and (20), which govern the flow field without requiring any geometry feedback, form a strongly nonlinear problem for V and t, even for the simplest, the potential incompressible, 3-D case.

When the pure target pressure problem is treated, Dirichlet-type boundary conditions are imposed on the velocity. An interesting alternative is the 'mixed' problem, where part of the boundary geometry is specified, while a target pressure distribution is prescribed on the remaining part. Considering that the fixed part of the boundary geometry belongs to a $\eta=$ const. surface, then the Gaussian curvature K_{η} of this surface reads

$$K_{\eta}=\frac{1}{4g_{33}}(\ln g_{11})_{\eta}(\ln g_{22})_{\eta}. \quad (22)$$

This relation is derived via a suitable combination of (A 7) with the assumption of orthogonal natural coordinates. Substituting the metrics expressions (9) in (22) it yields for $\theta=90°$

$$K_{\eta}=\frac{\rho V}{2t}(\ln V)_{\eta}[(\ln V)_{\eta}+(\ln\rho)_{\eta}+(\ln t)_{\eta}]. \quad (23)$$

Thus, for a given K_{η}-distribution, (23) forms a nonlinear Neumann-type boundary condition on V and t variables. In general, the implementation of condition (23) to the solution of the inverse problem, is rather inconvenient. However, there is a class of surfaces, including the planar, the cylindrical and the conical surface (very common in engineering applications) which have identically zero Gaussian curvature. In such a case the two derivative factors of condition (23) are decoupled, yielding linear Neumann-type boundary conditions.

It should be noted that the Gaussian curvature K_η of an η = const. surface can be expressed in terms of quantities intrinsic to the surface as (Synge & Schild 1978)

$$K_\eta = -\frac{1}{(g_{11}g_{22})^{1/2}}\left\{\left[\frac{(g_{22}^{1/2})_\phi}{g_{11}^{1/2}}\right]_\phi + \left[\frac{(g_{11}^{1/2})_\psi}{g_{22}^{1/2}}\right]_\psi\right\}. \tag{24}$$

Equating the right-hand sides of (22) and (24) a metrics compatibility condition is derived which is not independent of the flatness conditions (6). Linear combination of the Gaussian curvatures compatibility conditions for K_η, K_ψ and K_ϕ provide the governing equations (19) and (20) in an alternative way.

7. Reduced forms of the flow equations

In order to check the validity of the new governing equations proposed for the 3-D inverse problem, some simple cases have been examined.

7.1. 1-*D incompressible case* (*point source flow field*)

The flow field generated by a point source exhibits spherical symmetry about the source itself. Consider an orthogonal streamtube originating from the source. Since the velocity vector is directed radially away from the source, the radial coordinate R is associated with ϕ while the ψ- and η-coordinates, being normal to ϕ, measure surfaces of concentric spheres. For this case both ψ- and η-derivatives vanish and the proposed flow equations (19) and (20) become

$$(\ln V)_{\phi\phi} + \tfrac{1}{2}(\ln V)_\phi^2 = 0, \qquad (\ln t)_{\phi\phi} = 0. \tag{25}$$

This system of equations is satisfied by the solution $V \sim \phi^2(\sim 1/R^2)$ and t = const. which is indeed the known solution of the point source flow problem.

The above solution is valid even when the considered streamtube, defined by ψ = const. and η = const. surface, is non-orthogonal. It is also noted that for this 1-D case, an arbitrary but constant streamtube skew-angle θ satisfies (18) identically. This is in accordance with the conclusion that multiple geometrical solutions may be obtained if only velocity boundary conditions are imposed.

7.2. 2-*D compressible case*

The 2-D form of the compressible flow equations is derived by considering that the flow derivatives vanish along one of the ψ- or η-directions and that the corresponding metric is constant, say equal to one. Obviously, the assumption of orthogonal streamtubes is valid also for the 2-D case. Assuming that $g_{33} = 1$ and $\theta = 90°$, then t is implicitly defined via the metrics expressions (9) as

$$t = \rho V. \tag{26}$$

With t given by (26) and taking into account that η-derivatives vanish, (19) and (20), governing the V- and t-fields respectively, become identical with one another, reducing to

$$(\ln V)_{\phi\phi} + (\ln\rho)_{\phi\phi} + \rho^2(\ln V)_{\psi\psi} - (\ln\rho)_\phi(\ln V)_\phi - (\ln\rho)_\phi^2 + \rho^2(\ln\rho)_\psi(\ln V)_\psi = 0. \tag{27}$$

Equation (27) is the well-known equation of Stanitz (1953) for 2-D potential compressible flows. This equation has been used by the present authors for the design of 2-D ducts (Dedoussis *et al.* 1993) and airfoils (Chaviaropoulos *et al.* 1993).

7.3. *Axisymmetric compressible case*

Another case where the assumption of orthogonal streamtubes is self-evident is the axisymmetric flow with zero azimuthal velocity component. Associating $\eta = \text{const.}$ surfaces with meridional planes and, thus, neglecting the η-derivatives, (19) and (20) are reduced to

$$(\ln V)_{\phi\phi} + (\ln \rho)_{\phi\phi} + (\rho t/V)(\ln V)_{\psi\psi} + \tfrac{1}{2}[(\ln V)^2_\phi - (\ln t)^2_\phi - (\ln \rho)^2_\phi] \\ - (\rho t/V)(\ln V)_\psi [(\ln V)_\psi - (\ln t)_\psi] = 0, \quad (28)$$

$$(\ln t)_{\phi\phi} - (\ln \rho)_\phi (\ln t)_\phi + (\rho t/V)[(\ln V)_{\psi\psi} + (\ln V)_\psi (\ln \rho)_\psi] = 0. \quad (29)$$

The above set of equations has been applied successfully to reproduction test cases of non-annular axisymmetric ducts (Dedoussis, Chaviaropoulos & Papailiou 1992). Treating the axisymmetric case as a particular 3-D one, one gets the advantage of solving the V- and t-equations simultaneously. In this way, the need to iterate between the flow-field and geometry solutions, required by other axisymmetric approaches which are extensions of standard 2-D inverse methods and have the local radial distance R as a principal variable (e.g. Nelson & Yang 1977), is alleviated. The flow-field and geometry calculation procedures, therefore, remain entirely independent. Effectively, the t-equation plays the role of an R-equation. It can be shown that t is proportional to R^2.

8. Implications and limitations of the orthogonal streamtubes assumption

The assumption of orthogonal elementary streamtubes is not directly associated with any particular topology of the flow boundaries. There are several ways to group the individual streamlines into streamtube filaments. Considering, for example, the internal flow case presented in figure 2, one could use two different ways – and H- and an O-type – of partitioning the flow field with orthogonal elementary streamtubes. Obviously these two partitionings correspond to different t-field inflow boundary conditions.

With the H-type partitioning the implementation of the governing equations and their boundary conditions is straightforward. The consequence of this partitioning is that the lateral flow boundaries must have four right-angled edges, implying non-smooth cross-sectional boundary contours. Although this may be quite adequate for many design applications (see, for example, the test cases presented in Part 2) it certainly limits the generality of the proposed inverse method.

An O-type orthogonal streamtubes partitioning, on the other hand, does not imply edged-type boundaries and is therefore more appropriate for designing smooth contoured shapes. It is seen that in this case the assumption of orthogonal streamtubes is not all that restrictive as far as the boundary of the designed geometry is concerned. However, O-type partitioning exhibits a singular streamline along which the streamtube aspect ratio cannot be defined (point O of figure 2). In this case the governing V- and t-equations, (19) and (20) respectively, can be solved only if V is specified along the singular streamline. Evidently, different velocity distributions on this streamline lead to different flow-field shapes. It is observed again that the attempt to increase the degrees of freedom of the geometry sought leads to multiple solutions.

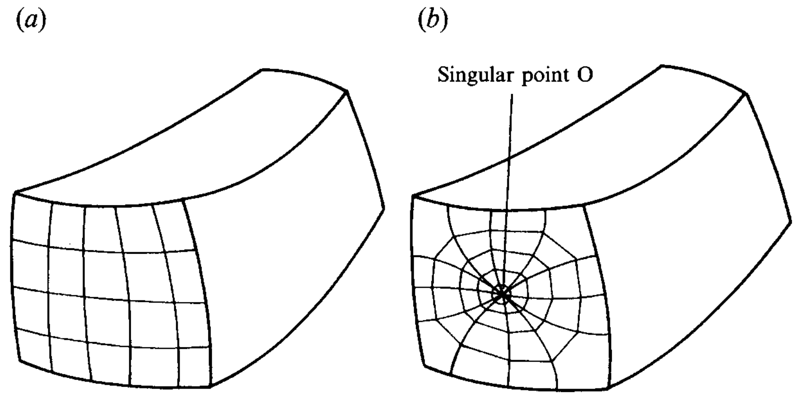


FIGURE 2. Alternative partitionings of an internal flow field with orthogonal elementary streamtubes. (*a*) H-type. (*b*) O-type.

9. Geometry calculation

Ultimately, the objective of an inverse method is to calculate the geometry which complies with the prescribed flow qualities (properties). In the previous sections it has been shown that the flow equations (19) and (20) governing the 3-D inverse potential target pressure problem form a closed set of p.d.e.s on the natural coordinates space, requiring no information – feedback – from the physical geometry itself. The purpose of this section is to demonstrate how the target geometry is obtained, once the flow field has been determined.

According to the analysis presented in the Appendix the Cartesian coordinates of the geometry position vector $\boldsymbol{r}$ can be evaluated in two steps by integrating (A 7) and (A 1) along any one of the natural coordinates lines. If, for example, a $\psi = \text{const.}$, $\eta = \text{const.}$ streamline is considered, (A 7) provides the following system of o.d.e.s:

$$\frac{\mathrm{d}}{\mathrm{d}\phi}\begin{bmatrix} g_1 \\ g_2 \\ g_3 \end{bmatrix} = \boldsymbol{A}_\phi \begin{bmatrix} g_1 \\ g_2 \\ g_3 \end{bmatrix}; \quad \boldsymbol{A}_\phi = \begin{bmatrix} \Gamma^1_{11} & \Gamma^2_{11} & \Gamma^3_{11} \\ \Gamma^1_{21} & \Gamma^2_{21} & \Gamma^3_{21} \\ \Gamma^1_{31} & \Gamma^2_{31} & \Gamma^3_{31} \end{bmatrix}. \tag{30}$$

where the matrix $\boldsymbol{A}_\phi$ elements, being a sub-set of the 27 Christoffel symbols, are analytical expressions of the (known) flow quantities and their partial derivatives on the natural space.

Equations (30), which represent a generalized form of the Frenet equations, may be integrated to provide the covariant vector base if appropriate initial conditions are prescribed for (g_1, g_2, g_3). The Cartesian coordinates of the geometry can be evaluated then, by integrating the covariant base, i.e. (A1), along any one of the natural coordinates. Starting, therefore, from a known position $\boldsymbol{r}_0$ and integrating along a streamline, for instance, we get

$$\boldsymbol{r} = \boldsymbol{r}_0 + \int_{\phi_0}^{\phi} g_1 \,\mathrm{d}\phi. \tag{31}$$

It should be noted that the evaluation of the $\boldsymbol{A}_\phi$ matrix elements involves inner flow information even when the integration of (30) is performed along the flow-field boundaries. This is the reason why the solution of the flow-field equations precedes the geometry calculation.

10. Conclusions

An inverse potential methodology is introduced for the solution of the 3-D target pressure problem. The method is based on a body-fitted coordinate transformation which maps the physical space onto a natural one. A potential function and two stream functions are used as the natural coordinates (independent variables), whilst the velocity magnitude as well as the aspect ratio and the skew angle of the elementary streamtube cross-section are considered to be the dependent ones.

A novel set of governing equations for the inverse 3-D problem is proposed which is derived using differential geometry and generalized tensor analysis arguments. The general 3-D inverse problem is treated as a geometrical one which has to satisfy the zero-curvature metrics compatibility conditions of the 3-D Euclidean, flat, space. It seems that in the general case the 3-D inverse target pressure problem is ill-posed, accepting multiple solutions.

A particular solution of the 3-D inverse problem is shown to be the one with elementary streamtubes with orthogonal cross-section, i.e. orthogonal stream surfaces are assumed. The governing equations and their boundary conditions are presented and discussed for this case. Reduced forms of these equations for point source, 2-D and axisymmetric flows are also examined. It is shown that the resulting system of governing equations can be solved with velocity-only boundary conditions because of the special form of the streamtube aspect ratio equation. On the natural coordinates space the flow field is determined in a self-contained manner without requiring any feedback from the actual geometry. The geometry is determined after the flow solution has been calculated, by integrating the generalized Frenet equations along the natural coordinates lines. A brief discussion on the implications and limitations of the assumption of orthogonal stream surfaces on the geometry is also included.

The numerical implementation as well as two validation duct design test cases of the proposed inverse method are presented in Part 2.

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Appendix. Differential geometry overview

In this Appendix key elements of differential geometry are presented. More details may be found in any differential geometry or tensor calculus book, e.g. Synge & Schild (1978).

Let x^i $(i = 1,2,3)$ be the Cartesian coordinates and u^j $(j = 1,2,3)$ a body-fitted parametrization of the flow field considered. Let $\boldsymbol{g}_i$ and $\boldsymbol{g}^j$ represent the covariant and contravariant orthonormal vector bases defined as:

$$\boldsymbol{g}_i = \frac{\partial \boldsymbol{r}}{\partial u^i}, \quad \boldsymbol{g}^j = \nabla u^j; \quad \boldsymbol{g}_i \cdot \boldsymbol{g}^j = \delta_i^j, \tag{A 1}$$

where

$$\boldsymbol{r} = (x^1, x^2, x^3); \quad \nabla = \left(\frac{\partial}{\partial x^1}, \frac{\partial}{\partial x^2}, \frac{\partial}{\partial x^3}\right) \tag{A 2}$$

are the position vector and the gradient operator respectively. δ_i^j is the Kronecker delta.

The covariant and contravariant metrics tensors are defined respectively as

$$g_{ij} = \boldsymbol{g}_i \cdot \boldsymbol{g}_j, \quad g^{ij} = \boldsymbol{g}^i \cdot \boldsymbol{g}^j. \tag{A 3}$$

The contravariant metrics (or conjugate metrics) g^{ij} represent the cofactors of the covariant metrics satisfying the following identity:

$$g^{ij}g_{jk} = \delta^i_k, \tag{A 4}$$

where repeated indices denote summation (Einstein convention).

The Jacobian J of the coordinate transformation may be expressed in terms of the covariant (or contravariant) metrics as

$$J^2 = \det(g_{ij}) = \det^{-1}(g^{ij}), \tag{A 5}$$

and the metric (infinitesimal distance) is expressed on the transformed domain as

$$\mathrm{d}s^2 = g_{ij}\,\mathrm{d}u^i\,\mathrm{d}u^j. \tag{A 6}$$

The partial derivatives of the covariant (and contravariant) bases with respect to the curvilinear coordinates are expressed in terms of the Christoffel symbols of the second kind Γ^k_{ij} as

$$\frac{\partial \boldsymbol{g}_i}{\partial u^j} = \Gamma^k_{ij}\boldsymbol{g}_k. \tag{A 7}$$

The Christoffel symbols of the first and second kind, $[ij, k]$ and Γ^k_{ij} respectively, are defined in terms of partial derivatives of the metrics tensor as

$$[ij,k] = \frac{1}{2}\left(\frac{\partial g_{ik}}{\partial u^j} + \frac{\partial g_{jk}}{\partial u^i} - \frac{\partial g_{ij}}{\partial u^k}\right), \tag{A 8}$$

$$\Gamma^k_{ij} = g^{km}[ij,m]. \tag{A 9}$$

The space curvature tensor is expressed in terms of the Christoffel symbols and their derivatives. It has six independent entries that form the symmetric Ricci curvature tensor R_{rm}, defined as

$$R_{rm} = \frac{\partial \Gamma^n_{rn}}{\partial u^m} - \frac{\partial \Gamma^n_{rm}}{\partial u^n} + \Gamma^p_{rn}\Gamma^n_{pm} - \Gamma^p_{rm}\Gamma^n_{pn}. \tag{A 10}$$

The Euclidean space, being flat, has zero curvature. Referring to the Ricci curvature tensor the zero-curvature condition reads

$$R_{rm} = 0 \quad \text{with} \quad r,m = 1,2,3. \tag{A 11}$$

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