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OCTOBER 1975 MATT-1154

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Available from
National Technical Information Service
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5285 Port Royal Road
Springfield, Virginia 22151
Price: Printed Copy $ _*__; Microfiche $1.45

*Pages	NTIS Selling Price
1-50	$ 4.00
51-150	5.45
151-325	7.60
326-500	10.60
501-1000	13.60

A Tensor Transformation Technique for The Transport Equation

by

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A step-wise tensor transformation technique is presented for the transformation of the single energy group transport equation to an arbitrary spatial coordinate system. Both gradient and divergence forms of the equation are given and the same method is applied to the derivation of the diffusion approximation. We demonstrate that using an orthogonal representation of the propagation vector will simplify the divergence form of the equation. The application of this technique is in the representation of the transport equation in coordinate systems other than the usual rectangular, cylindrical and spherical ones. Its use is demonstrated by transforming the transport equation to a toroidal coordinate system consisting of nested circular toroids.

I. INTRODUCTION

The transport equation for a single energy group,

$$\underline{\Omega} \cdot \nabla\Psi + \sigma\Psi = S \quad , \tag{1}$$

representing the conservation law of density in phase space, may be written in terms of the divergence of a 5-dimensional vector.

Drawbaugh,(1) using the metric,

$$g_{ij} = \left\| \begin{matrix} 1 & & & & \\ & 1 & & & \\ & & 1 & & \\ & & & (1-\delta^2) & \\ & & & & (1-\delta^2)^{-1} \end{matrix} \right\| ,$$

has demonstrated that this physical law is expressed by the tensor equation,

$$\text{div} \cdot M + \sigma\Psi = S \quad , \tag{2}$$

where,

$$\underline{M} = \underline{\Omega}\Psi \quad , \tag{3}$$

and

$$\text{div} \cdot \underline{M} = \frac{1}{\sqrt{g}} \frac{\partial}{\partial x^i} (g^{1/2} M^i) \tag{4}$$

In equation 4, $g = |g_{ij}|$, is the determinant of the metric and the summation of repeated indices is assumed.

A conservation law, such as equation 2, yields an integral form of the transport equation directly, which may be used for the derivation of conservative finite difference equations(2) in any system of coordinates. This has been illustrated by Drawbaugh in reference 1 by transforming to cylindrical and spherical coordinate systems. The most formidable stumbling block is that of inverting a transformation of the form,

$$x^i = x^i (\bar{\bar{x}}^1 \ldots \bar{\bar{x}}^5) \quad . \qquad i = 1 \ldots 5 \tag{5}$$

The notation used here is that the variables, x^i represent the coordinates of the original 5-dimensional Riemannian space, (following Drawbaugh we chose $x^1 = x$, $x^2 = y$, $x^3 = z$, (Cartesian spatial coordinates), $x^4 = \omega$ and $x^5 = \delta$ where δ is the component of $\underline{\Omega}$ along the Z direction and ω is the angle between the projection of $\underline{\Omega}$ on the xy plane and the positive x direction), while $\bar{\bar{x}}^i$ are the coordinates to which we chose to transform the equation. An alternative technique, used by Pomraning & Stevens(3) to transform the transport equation to a toroidal coordinate system consisting of nested concentric circular toroids, is to apply the chain rule of differentiation. Here, the transformation which must be inverted is a mapping of Euclidean 3-space onto itself which is a more tractable problem. However, the transformation process is complicated by the fact that in any non-Cartesian coordinate system the trajectory of a particle moving in a straight line is not in general along a geodesic curve of the coordinate surfaces. Consequently, the angle between the direction of motion and the coordinate directions will vary along the trajectory implying that Ψ will vary as a function of the angle variables as well as the spatial variables. The exception to this is for the case in which the coordinate system does yield straight geodesic curves for particular coordinate surfaces.

In this paper we will resolve the difficulty presented by either of the above cited methods by presenting a step-wise tensor formalism for the transformation of equation 1 to an arbitrary coordinate system (section II). We will then demonstrate the technique by applying it to the toroidal geometry treated by Pomraning and Stevens (section III), and also show that the diffusion approximation is readily obtainable. Finally we will prove in section IV that provided an orthogonal representation of the vector $\underline{\Omega}$ is used, the angle variable transformation is given by a group of motions in 3-space and consequently its Jacobian is equal to one. This is a desirable although not essential property.

II. Tensor Transformation Technique

Consider the transport equation,

$$\frac{1}{\sqrt{g}} \frac{\partial}{\partial x^i} (g^{1/2} M^i) + \sigma\Psi = S \quad , \tag{6}$$

where Ψ, σ and S are the angular flux, cross section and source function, and M^i is defined in terms of the propagation vector $\underline{\Omega}$ by equation 3 in the 5-dimensional Riemannian space having coordinates $x^1 = x$, $x^2 = y$, $x^3 = z$, $x^4 = \omega$ and $x^5 = \delta$ for which the choice of metric tensor, g_{ij}, introduced by Drawbaugh (see section I) is made. The physical components of $\underline{\Omega}$ in this space are,

$$\begin{aligned} \alpha &= \left\{ 1- \{\delta\}^2 \right\}^{\frac{1}{2}} \cos \omega \\ \beta &= \left\{ 1- \{\delta\}^2 \right\}^{\frac{1}{2}} \sin \omega \\ \delta &= \delta \quad , \end{aligned} \tag{7}$$

while the five-dimensional vector M^i has components,

$$M^i = \left\{\alpha, \beta, \delta, o, o\right\} \quad \Psi(x^i) \tag{8}$$

We will use the notation Ω^i to denote the vector portion of M^i and note that,

$$\frac{\partial}{\partial x^i} \left(\sqrt{g}\, \Omega^i\right) = 0 \qquad (9)$$

The representation of the equation in any other 5-dimensional Riemannian space having coordinates $\bar{\bar{x}}^i$ may be found by the following procedure:

i) Introduce a transformation, T_1, of the spatial coordinates x^1, x^2, x^3 but preserve the choice of angle variable x^4, x^5. Thus,

$$T_1: \quad \begin{aligned} x^1 &= x^1\,(\bar{x}^1 \ldots \bar{x}^3) \\ x^2 &= x^2\,(\bar{x}^2 \ldots \bar{x}^3) \\ x^3 &= x^3\,(\bar{x}^1 \ldots \bar{x}^3) \\ x^4 &= \bar{x}^4 \\ x^5 &= \bar{x}^5 \end{aligned}$$

ii) Transform the metric tensor.

Since g_{ij} is a rank two covariant tensor it transforms under T_1 according to

$$\bar{g}_{ij} = g_{ek} \frac{\partial x^e}{\partial \bar{x}^i} \frac{\partial x^k}{\partial \bar{x}^j} \qquad (10)$$

(We are using the bar notation to denote a representation in the $\bar{x}^i$ coordinate system.)

iii) Transform the covariant components of $\underline{\Omega}$.

Since the x^i spatial coordinates are Cartesian, the covariant and contravariant components of $\underline{\Omega}$ are identical. We form $\overline{\Omega}_i$ by

$$\overline{\Omega}_i = \Omega_j \frac{\partial x^j}{\partial \overline{x}^i} \quad . \tag{11}$$

iv) Form the associated contravariant tensor $\overline{g}^{ij}$.

This requires the solution of the equations

$$\overline{g}^{ij} \quad \overline{g}_{jk} = \delta^i_k \quad , \tag{12}$$

where δ^i_k is a Kronecker delta. The transformation T_1 will affect the spatial variables only. Consequently even for a choice of non-orthogonal coordinates the metric tensor will be partitioned as follows:

$$\overline{g}_{ij} = \left\| \begin{array}{ccc|cc} X & X & X & 0 & 0 \\ X & X & X & & \\ X & X & X & 0 & 0 \\ \hline 0 & 0 & 0 & (1-\delta^2) & 0 \\ 0 & 0 & 0 & 0 & (1-\delta^2)^{-1} \end{array} \right\| ,$$

and the inverse will be of the form:

$$\bar{g}^{ij} = \left\| \begin{array}{ccc|cc} & A^{-1} & & 0 & 0 \\ & & & 0 & 0 \\ \hline 0 & 0 & 0 & (1-\delta^2)^{-1} & 0 \\ 0 & 0 & 0 & 0 & (1-\delta^2) \end{array} \right\| ,$$

where A^{-1} is the inverse of the 3 x 3 matrix occupying the upper left partition of $\bar{g}_{ij}$.

v) Form the contravariant components of $\underline{\Omega}$ in $\bar{x}^i$.

The relationship between the contravariant and covariant components is given by,

$$\bar{\Omega}^i = \bar{g}^{ij} \bar{\Omega}_j \quad . \tag{13}$$

vi) Form the physical components of $\underline{\Omega}$ along the coordinate curves.(4)

These components will be given by,

$$\bar{\lambda}_i = \frac{\bar{\Omega}_i}{\sqrt{g_{i|i}}} \quad . \tag{14}$$

(The notation $i|i$ indicates no sum on i). The $\bar{\lambda}_i$ will be used in constructing the transformation of the angle variables necessary to represent $\underline{\Omega}$ in the $\bar{x}^i$ spatial coordinates. If they do not form an orthogonal triad, it may, in some cases, be convenient to chose directions which do not lie along one or more of the coordinate curves so as to form an orthogonal representation. (This point will be discussed further in section IV).

vii) Introduce the following transformation of the angle variables, preserving the $\bar{x}^i$ spatial coordinates.

$$T_2: \quad \begin{aligned} \bar{\bar{x}}^1 &= \bar{x}^1 \\ \bar{\bar{x}}^2 &= \bar{x}^2 \\ \bar{\bar{x}}^3 &= \bar{x}^3 \\ \bar{\bar{x}}^4 &= \tan^{-1}\left(\frac{\bar{\lambda}_i}{\bar{\lambda}_j}\right) \\ \bar{\bar{x}}^5 &= \bar{\lambda}_k \quad , \end{aligned}$$

where it is understood that i,j and k are any permutation of the indicies 1,2,3 (i.e. if i=3 and k=1, j=2).

ix) Transform the contravariant components of $\underline{\Omega}$.

The transformation of a contravariant vector is according to,

$$\bar{\bar{\Omega}}^i = \bar{\Omega}^j \frac{\partial \bar{\bar{x}}^i}{\partial \bar{x}^j} \quad . \tag{15}$$

x) The gradient form of the equation is given by,

$$\bar{\bar{\Omega}}^i \frac{\partial \Psi}{\partial \bar{\bar{x}}^i} + \sigma\Psi = S \quad .$$

xi) To form the divergence in $\bar{\bar{x}}^i$ it is necessary to know the determinant of the metric tensor, $\bar{\bar{g}}_{ij}$. This determinant, $|\bar{\bar{g}}|$, is obtained from the transformation rule,(5)

$$|\bar{\bar{g}}| = |g| \; J^2 \quad , \tag{16}$$

where J is the Jacobian of the transformation,

$$x^i = x^i \; (\bar{x}^j(\bar{\bar{x}}^k)) \quad . \tag{17}$$

The inner transformation is the inverse of T_2 and the outer one is T_1 consequently,

$$J = \frac{J_1}{J_2} \quad , \tag{18}$$

where J_1 is the Jacobian of T_1 and J_2 is the Jacobian of T_2.

xii) The conservation law form of the transport equation is given by,

$$\frac{1}{\{\bar{\bar{g}}\}^{\frac{1}{2}}} \frac{\partial}{\partial \bar{\bar{x}}^i} (\{\bar{\bar{g}}\}^{\frac{1}{2}} M^i) + \sigma\Psi = S \quad . \tag{19}$$

III. Application of the Tensor Transformation Technique to A Toroidal Coordinate System

A toroidal coordinate system, frequently used by plasma physicists concerned with tokamaks, and of possible application in the study of neutronic and photonic problems in future toroidal fusion devices, is formed by rotating a nest of concentric circles about an axis which does not intersect the nest (see Fig. 1). Pomraning and Stevens[3] have derived the transport equation in gradient form and the diffusion equation, by application of the chain rule. As an example of the application of the tensor transform technique we will derive the gradient form of the transport equation as well as the divergence form, the later form being more directly applicable to the construction of finite difference equations by the integration technique. We will also derive the diffusion equation in the same manner. Transformation T_1 is given by,

$$T_1: \quad \begin{aligned} x^1 &= \bar{x}^1 \cos \bar{x}^2 \\ x^2 &= (\bar{x}^1 \sin \bar{x}^2 + R) \cos \bar{x}^3 \\ x^3 &= (\bar{x}^1 \sin \bar{x}^2 + R) \sin \bar{x}^3 \\ x^4 &= \bar{x}^4 \\ x^5 &= \bar{x}^5 \quad , \end{aligned}$$

where ($x^1 = x$, $x^2 = y$, $x^3 = z$, $x^4 = \omega$, $x^5 = \delta$) and ($\bar{x}^1 = r$, $\bar{x}^2 = \Theta$, $\bar{x}^3 = \phi$, $\bar{x}^4 = \omega$, $\bar{x}^5 = \delta$). The transformation of Drawbaugh's metric is accomplished by evaluation of the derivatives in equation 10. As an example,

$$\bar{g}_{11} = \left(\frac{\partial x^1}{\partial \bar{x}^1}\right)^2 + \left(\frac{\partial x^2}{\partial \bar{x}^2}\right)^2 + \left(\frac{\partial x^3}{\partial \bar{x}^3}\right)^2$$

$$= \cos^2(\bar{x}^2) + \sin^2(\bar{x}^2)\cos^2(\bar{x}^3) + \sin^2(\bar{x}^2)\sin^2(\bar{x}^3)$$

$$= 1 \quad .$$

The metric tensor in the $\bar{x}^i$ coordinates is

$$\bar{g}_{ij} = \left\| \begin{matrix} 1 & & & & \\ & r^2 & & & \\ & & (R + r\sin\Theta)^2 & & \\ & & & (1-\delta^2) & \\ & & & & (1-\delta^2)^{-1} \end{matrix} \right\|$$

For any orthogonal coordinate system, as this one is, it is necessary that each of the off diagonal elements of the metric tensor be zero. When this is so, the associated contravariant tensor $\bar{g}^{ij}$ is formed by inverting each element of $\bar{g}_{ij}$. For example,

$$\bar{g}^{33} = (R + r\sin\Theta)^{-2}$$

The components of $\underline{\Omega}$ are given by

$$\underline{\Omega} = \{\delta, (1-\delta^2)^{\frac{1}{2}} \cos\omega, (1-\delta^2)^{\frac{1}{2}} \sin\omega\} \quad ,$$

and substituting in equation 11 we find,

$$\bar{\Omega}_1 = (1-\delta^2)^{\frac{1}{2}} \cos(\omega-\Phi) \sin\Theta + \delta\cos\Theta$$

$$\bar{\Omega}_2 = r\{(1-\delta^2)^{\frac{1}{2}} \cos(\omega-\Phi) \cos\Theta - \delta\sin\Theta\}$$

$$\bar{\Omega}_3 = (1-\delta^2)^{\frac{1}{2}} (R + r\sin\Theta) \sin(\omega-\Phi) \quad .$$

Equation 13 gives the values of $\bar{\Omega}^i$,

$$\bar{\Omega}^1 = (1-\delta^2)^{\frac{1}{2}} \cos(\omega-\Phi) \sin\Theta + \delta\cos\Theta$$

$$\bar{\Omega}^2 = \frac{1}{r} \{(1-\delta^2)^{\frac{1}{2}} \cos(\omega-\Phi) \cos\Theta - \delta\sin\Theta\}$$

$$\bar{\Omega}^3 = \{(1-\delta^2)^{\frac{1}{2}} \sin(\omega-\Phi)\} \left\{\frac{1}{R + r\sin\Theta}\right\} \quad ,$$

and using equation 14 we see that,

$$\bar{\lambda}_1 = \bar{\Omega}^1$$

$$\bar{\lambda}_2 = r\,\bar{\Omega}_2$$

$$\bar{\lambda}_3 = (R + r\sin\Theta)\bar{\Omega}^3 \quad .$$

The transformation T_2 will be,

$$T_2: \quad \begin{aligned} \bar{\bar{x}}^1 &= \bar{x}^1 \\ \bar{\bar{x}}^2 &= \bar{x}^2 \\ \bar{\bar{x}}^3 &= \bar{x}^3 \\ \bar{\bar{x}}^4 &= \tan^{-1}\frac{\bar{\lambda}_3}{\bar{\lambda}_2} \\ \bar{\bar{x}}^5 &= \bar{\lambda}_1 \quad . \end{aligned}$$

Equation 15 will then give the contravariant components of $\underline{\Omega}$ in the $\bar{\bar{x}}^i$ coordinates,

$$\bar{\bar{\Omega}}^1 = \bar{\Omega}^1$$

$$\bar{\bar{\Omega}}^2 = \bar{\Omega}^2$$

$$\bar{\bar{\Omega}}^3 = \bar{\Omega}^3$$

$$\bar{\bar{\Omega}}^4 = \bar{\Omega}^2\frac{\partial\bar{\bar{x}}^4}{\partial\bar{x}^2} + \bar{\Omega}^3\frac{\partial\bar{\bar{x}}^4}{\partial\bar{x}^3}$$

$$\bar{\bar{\Omega}}^5 = \bar{\Omega}^2\frac{\partial\bar{\bar{x}}^5}{\partial\bar{x}^2} + \bar{\Omega}^3\frac{\partial\bar{\bar{x}}^5}{\partial\bar{x}^3} \quad .$$

Evaluating the derivatives and simplifying,

$$\bar{\bar{\Omega}}^4 = -\frac{\lambda_\Theta}{r} + \frac{\lambda^2_\Phi}{\lambda_r^2 + \lambda^2_\Theta} \frac{\lambda_r \cos\Theta - \lambda_\Theta \sin\Theta}{(R + r \sin\Theta)}$$

and

$$\bar{\bar{\Omega}}^5 = \frac{-\lambda\Phi}{(R + r \sin\Theta)} (\lambda_r \sin\Theta + \lambda_\Theta \cos\Theta) \quad .$$

Introducing the notation $\zeta = \bar{\bar{x}}^5$ and $\nu = \bar{\bar{x}}^4$ the gradient form of the equation is now obtained directly as

$$\lambda_r \frac{\partial\Psi}{\partial r} + \frac{\lambda_\Theta}{r} \frac{\partial\Psi}{\partial\Theta} + \frac{\lambda_\Phi}{(R + r \sin\Theta)} \frac{\partial\Psi}{\partial\Phi}$$

$$+ \left\{ \frac{\lambda^2_\Phi}{\lambda_r^2 + \lambda^2_\Theta} \frac{\lambda_r \cos\Theta - \lambda_\Theta \sin\Theta}{(R + r \sin\Theta)} - \frac{\lambda_\Theta}{r} \right\} \frac{\partial\Psi}{\partial\nu} \tag{20}$$

$$- \frac{\lambda\Phi}{(R + r \sin\Theta)} (\lambda_r \sin\Theta + \lambda_\Theta \cos\Theta) \frac{\partial\Psi}{\partial\zeta} + \sigma\Psi = S \quad .$$

Equation 20 can be compared directly to Pomraning and Stevens' result by observing in their figure 2 that,

$$\lambda_r = \sin\theta\cos\phi$$

$$\lambda_\Phi = \cos\theta$$

$$\lambda_\Theta = \sin\theta\sin\phi \quad .$$

The Jacobian of T_1 is given by equation 16,

$$J_1 = r(R + r\sin\Theta) \quad ,$$

and, as will be shown in the next section of this paper, if $\overline{\lambda}_1$, $\overline{\lambda}_2$ and $\overline{\lambda}_3$ form an orthogonal triad $J_2 = 1$, which is the case for the example being considered. Consequently,

$$J = r(R + r\sin\Theta) \quad .$$

Substituting in equation 19 gives the divergence form of the transport equation,

$$\frac{1}{r(R + r\sin\Theta)} \left\{ \frac{\partial}{\partial r} \left\{ r(R + r\sin\Theta)\lambda_r \Psi \right\} + \frac{\partial}{\partial \Theta} \left\{ (R + r\sin\Theta)\lambda_\Theta \Psi \right\} \right.$$
$$+ \frac{\partial}{\partial \Phi} \left\{ r\, \lambda_\Phi \Psi \right\} - \frac{\partial}{\partial \zeta} \left\{ r\, \lambda_\Phi (\lambda_r \sin\Theta + \lambda_\Theta \cos\Theta) \right\}$$
$$\left. + \frac{\partial}{\partial \nu} \left\{ r \frac{\lambda_\Phi^{2}}{\lambda_r^{2} + \lambda^{2}_\Theta} (\lambda_r \cos\Theta - \lambda_\Theta \sin\Theta) - \lambda_\Theta (R + r\sin\Theta) \right\} \right\}$$
$$+ \sigma\Psi = S \quad . \tag{21}$$

The diffusion approximation results when one assumes Fick's law,

$$\frac{1}{3} \nabla \chi + \sigma \underline{J} = 0 \quad , \tag{22}$$

where $\underline{J}$ is the current and χ the total flux, to be valid.[6] Integration over the angle variables in the transport equation yields a conservation law for $\underline{J}$,

$$\nabla \cdot \underline{J} + \sigma_a \chi = S \quad . \tag{23}$$

From equation 22 we see that the current,

$$\underline{J} = - \frac{1}{3\sigma} \nabla \chi \quad ,$$

is a gradient. Consequently, $\underline{J}$ is a covariant vector which may be written in the $\bar{x}^i$ spatial coordinates as

$$J_i = - \frac{1}{3\sigma} \frac{\partial \chi}{\partial \bar{x}^i} \quad .$$

Equation 23 is then,

$$\frac{1}{\{\bar{g}\}^{\frac{1}{2}}} \frac{\partial}{\partial \bar{x}^i} \left(\sqrt{\bar{g}} \; \bar{g}^{ij} J_j \right) + \sigma_a \chi = S \quad , \tag{24}$$

and substituting for $\bar{g}$ and summing over j gives,

$$\frac{-1}{r(R + r \sin\Theta)} \left\{ \frac{\partial}{\partial r} \left\{ r(R + r \sin \;) D \frac{\partial \chi}{\partial \Theta} \right\} + \frac{1}{r} \frac{\partial}{\partial \Theta} \left\{ (R + r \sin\Theta) D \frac{\partial \chi}{\partial \Theta} \right\} \right.$$

$$\left. + \frac{\partial}{\partial \Phi} \left\{ \frac{r}{(r + R \sin\Theta)} D \frac{\partial \chi}{\partial \Phi} \right\} \right\} + \sigma_a \chi = S \quad , \tag{25}$$

which is the desired diffusion equation.

IV. On the Evaluation of Jacobians

As we noted earlier, it is necessary to evaluate the Jacobian of both transformation groups T_1 and T_2, to be able to transform the determinant of the metric tensor necessary to forming the divergence in $\bar{\bar{x}}^i$. J_1 can be evaluated by using the transformation rule expressed in equation 16,

$$|\bar{g}| = |g| J_1^2 \quad , \tag{26}$$

and since the determinant $|g|$ which appears on the right hand side of equation 26 equals 1, J_1^2 is given by the determinant $|\bar{g}|$. Applying Laplace's rule for the development of a determinant we see that,

$$|\bar{g}| = |A| \quad ,$$

where $|A|$ is the determinant of the 3x3 submatrix defined in section 2.

The Jacobian determinant of the transformation T_2 will be of the form,

$$J_2 \equiv \left| \frac{\partial \bar{\bar{x}}^i}{\partial \bar{x}^j} \right| = \left| \begin{array}{ccc|cc} 1 & & & & \\ & 1 & & & \\ & & 1 & & \\ \hline x & x & x & \frac{\partial \bar{\bar{x}}^4}{\partial \bar{x}^4} & \frac{\partial \bar{\bar{x}}^4}{\partial \bar{x}^5} \\ x & x & x & \frac{\partial \bar{\bar{x}}^5}{\partial \bar{x}^4} & \frac{\partial \bar{\bar{x}}^5}{\partial \bar{x}^4} \end{array} \right| .$$

where the vacant locations are zero. Applying Laplace's rule again,

$$J_2 = \left| \begin{array}{cc} \frac{\partial \bar{\bar{x}}^4}{\partial \bar{x}^4} & \frac{\partial \bar{\bar{x}}^4}{\partial \bar{x}^5} \\ \frac{\partial \bar{\bar{x}}^5}{\partial \bar{x}^4} & \frac{\partial \bar{\bar{x}}^5}{\partial \bar{x}^5} \end{array} \right| . \tag{27}$$

For clarity we will consider the specific case in which $\bar{\bar{x}}^4$ and $\bar{\bar{x}}^5$ are defined by

$$\bar{\bar{x}}^4 = \tan^{-1}\left(\frac{\bar{\lambda}_3}{\bar{\lambda}_2}\right)$$

$$\bar{\bar{x}}^5 = \bar{\lambda}_1 \quad . \tag{28}$$

Evaluating the derivatives indicated in equation 27 gives

$$J_2 = \frac{1}{(\bar{\lambda}_3)^2 + (\bar{\lambda}_2)^2} \left\{ \bar{\lambda}_2 \begin{vmatrix} \frac{\partial \bar{\lambda}_3}{\partial \bar{x}^4} & \frac{\partial \bar{\lambda}_3}{\partial \bar{x}^5} \\ \frac{\partial \bar{\lambda}_1}{\partial \bar{x}^4} & \frac{\partial \bar{\lambda}_1}{\partial \bar{x}^5} \end{vmatrix} - \bar{\lambda}_3 \begin{vmatrix} \frac{\partial \bar{\lambda}_2}{\partial \bar{x}^4} & \frac{\partial \bar{\lambda}_2}{\partial \bar{x}^5} \\ \frac{\partial \bar{\lambda}_1}{\partial \bar{x}^4} & \frac{\partial \bar{\lambda}_1}{\partial \bar{x}^5} \end{vmatrix} \right\} . \tag{29}$$

The evaluation of the derivatives in the determinants in equation 29 requires first replacing the $\bar{\lambda}_i$ by λ_i which are functions of $\bar{x}^4$ and $\bar{x}^5$ only. Using the definition of and the transformation rule for covariant vectors,

$$\bar{\lambda}_i = \frac{\lambda_j}{\sqrt{\bar{g}_{i|i}}} \frac{\partial x^j}{\partial \bar{x}^i} \quad . \tag{30}$$

Substituting in the determinants in equation 29,

$$\begin{vmatrix} \frac{\partial\bar{\lambda}_3}{\partial\bar{x}^4} & \frac{\partial\bar{\lambda}_3}{\partial\bar{x}^5} \\ \frac{\partial\bar{\lambda}_1}{\partial\bar{x}^4} & \frac{\partial\bar{\lambda}_1}{\partial\bar{x}^5} \end{vmatrix} = \frac{1}{\sqrt{\bar{g}_{33}\,\bar{g}_{11}}} \quad \frac{\partial x^j}{\partial\bar{x}^3} \quad \frac{\partial x^k}{\partial\bar{x}^1} \begin{vmatrix} \frac{\partial\lambda_j}{\partial x^4} & \frac{\partial\lambda_j}{\partial x^5} \\ \frac{\partial\lambda_k}{\partial x^4} & \frac{\partial\lambda_k}{\partial x^5} \end{vmatrix} , \tag{31}$$

(Note that in the final determinant use is made of $\bar{x}^4 = x^4$, $\bar{x}^5 = x^5$) and analogously,

$$\begin{vmatrix} \frac{\partial\bar{\lambda}_2}{\partial\bar{x}^4} & \frac{\partial\bar{\lambda}_2}{\partial\bar{x}^5} \\ \frac{\partial\bar{\lambda}_1}{\partial\bar{x}^4} & \frac{\partial\bar{\lambda}_1}{\partial\bar{x}^5} \end{vmatrix} = \frac{1}{\sqrt{\bar{g}_{22}\,\bar{g}_{11}}} \quad \frac{\partial x^j}{\partial\bar{x}^2} \quad \frac{\partial x^k}{\partial\bar{x}^1} \begin{vmatrix} \frac{\partial\lambda_j}{\partial x^4} & \frac{\partial\lambda_j}{\partial x^5} \\ \frac{\partial\lambda_k}{\partial x^4} & \frac{\partial\lambda_k}{\partial x^5} \end{vmatrix} . \tag{32}$$

We now introduce the notation,

$$D(j,k) \equiv \begin{vmatrix} \frac{\partial\lambda_j}{\partial x^4} & \frac{\partial\lambda_j}{\partial x^5} \\ \frac{\partial\lambda_k}{\partial x^4} & \frac{\partial\lambda_k}{\partial x^5} \end{vmatrix} . \tag{33}$$

In terms of which the Jacobian may be written as,

$$J_2 = \frac{1}{(\bar{\lambda}_3)^2 + (\bar{\lambda}_2)^2} \left\{ \frac{1}{\sqrt{\bar{g}_{11}\ \bar{g}_{22}\ \bar{g}_{33}}} \quad \frac{\partial x^k}{\partial \bar{x}^1} \ D(j,k) \left\{ \lambda_e \frac{\partial x^e}{\partial \bar{x}^2} \ \frac{\partial x^j}{\partial \bar{x}^3} - \lambda_e \frac{\partial x^e}{\partial \bar{x}^3} \ \frac{\partial x^j}{\partial \bar{x}^2} \right\} \right\}$$

The λ_i are functions of x_4 and x_5 only,

$$\lambda_1 = (1 - (x^5)^2)^{\frac{1}{2}} \cos x^4$$

$$\lambda_2 = (1 - (x^5)^2)^{\frac{1}{2}} \sin x^4$$

$$\lambda_3 = x^5$$

Consequently the determinants, $D(j,k)$, are readily evaluated and we find;

$$D(1,2) = - D(2,1) = \lambda_3 \quad ,$$

$$D(1,3) = - D(3,1) = - \lambda_2 \quad ,$$

$$D(2,3) = - D(3,2) = \lambda_1 \quad ,$$

all other $D(j,k)$ being equal to zero. A typical term in J_2 involves the evaluation of

$$\begin{aligned} \frac{\partial x^k}{\partial \bar{x}^1} \ \frac{\partial x^j}{\partial \bar{x}^3} \ D(j,k) = D(2,1) & \left\{ \frac{\partial x^1}{\partial \bar{x}^1} \ \frac{\partial x^2}{\partial \bar{x}^3} - \frac{\partial x^1}{\partial \bar{x}^3} \ \frac{\partial x^2}{\partial \bar{x}^1} \right\} \\ + D(3,1) & \left\{ \frac{\partial x^1}{\partial \bar{x}^1} \ \frac{\partial x^3}{\partial \bar{x}^3} - \frac{\partial x^3}{\partial \bar{x}^1} \ \frac{\partial x^1}{\partial \bar{x}^3} \right\} \\ + D(3,2) & \left\{ \frac{\partial x^2}{\partial \bar{x}^1} \ \frac{\partial x^3}{\partial \bar{x}^3} - \frac{\partial x^3}{\partial \bar{x}^1} \ \frac{\partial x^2}{\partial \bar{x}^3} \right\} . \end{aligned} \tag{34}$$

The bracketed terms in equation 34 are the cofactors of the elements of the second column of the Jacobian of T_1, and consequently,

$$J_2 = \frac{J_1/\sqrt{\bar{g}_{11}\,\bar{g}_{22}\,\bar{g}_{33}}}{(\bar{\lambda}_3)^2 + (\bar{\lambda}_2)^2} \left\{ \lambda_e \frac{\partial x^e}{\partial \bar{x}^2} \left[D(1,2)\,\frac{\partial \bar{x}^2}{\partial x^3} + D(3,1)\,\frac{\partial \bar{x}^2}{\partial x^2} - D(3,2)\,\frac{\partial \bar{x}^2}{\partial x^1} \right] \right.$$

$$\left. + \lambda_e \frac{\partial x^e}{\partial \bar{x}^3} \left[D(1,2)\,\frac{\partial \bar{x}^3}{\partial x^3} + D(3,1)\,\frac{\partial \bar{x}^3}{\partial x^2} - D(3,2)\,\frac{\partial \bar{x}^3}{\partial x^2} \right] \right\}$$

This equation may be written as

$$J_2 = \frac{1}{(\bar{\lambda}_3)^2 + (\bar{\lambda}_2)^2} \left\{ \frac{J_1}{\sqrt{\bar{g}_{11}\,\bar{g}_{22}\,\bar{g}_{33}}} \left\{ \sqrt{\bar{g}_{22}}\;\bar{\lambda}_2\,\bar{\Omega}^2 + \sqrt{\bar{g}_{33}}\;\bar{\lambda}_3\,\bar{\Omega}^3 \right\} \right\} . \quad (35)$$

If the geometric coordinates, $\bar{x}^1 \ldots \bar{x}^3$, form an orthogonal coordinate system,

$$\bar{\lambda}_i = \sqrt{\bar{g}_{i|i}}\;\;\bar{\Omega}^i ,$$

and

$$|\bar{g}_{ij}| = \bar{g}_{11}\,\bar{g}_{22}\,\bar{g}_{33} \quad ,$$

Then,

$$J_2 = 1 \quad .$$

Any representation of $\underline{\Omega}$ in terms of its components in three mutually orthogonal directions, not necessarily the coordinate directions defined by $\bar{x}^1 \ldots \bar{x}^3$, will introduce a transformation T_2 having $J_2 = 1$. To demonstrate this, let us consider the transformation T_2 written in the form,[7]

$$G: \quad \begin{aligned} \bar{\bar{y}}^1 &= \bar{\bar{y}}^1\,(\bar{y}^1, \bar{y}^2; \bar{x}^1 .. \bar{x}^3) \\ \bar{\bar{y}}^2 &= \bar{\bar{y}}^2\,(\bar{y}^1, \bar{y}^2; \bar{x}^1 .. \bar{x}^3) \quad . \end{aligned} \qquad (36)$$

$\bar{y}^1$ and $\bar{y}^2$ are defined by

$$\bar{y}^1 = \frac{\bar{\lambda}_i}{\bar{\lambda}_j} \quad , \qquad (i \neq j \neq k = 1 \ldots 3)$$

$$\bar{y}^2 = \bar{\lambda}_k \quad .$$

and the spatial coordinates $\bar{x}^1 \ldots \bar{x}^3$ are parameters of the transformation group, G. Chose the $\bar{y}^i$ as coordinates of a 2-dimensional subspace of the 5-dimensional space having coordinates $\bar{x}^i$; the metric tensor of this subspace is,

$$\bar{A}_{\alpha\beta} = \bar{g}_{ij} \frac{\partial \bar{x}^i}{\partial \bar{y}^\alpha} \frac{\partial \bar{x}^j}{\partial \bar{y}^\beta} = \left\| \begin{matrix} \dfrac{[1 - (\bar{y}^2)^2]}{[1 + (\bar{y}^1)^2]^2} & \\ & \dfrac{1}{[1 - (\bar{y}^2)^2]^2} \end{matrix} \right\| . \qquad \begin{matrix} i,j = 1..5 \\ \alpha,\beta = 1...2 \end{matrix} \tag{37}$$

This subspace has one non-vanishing Riemannian symbol of the first kind,

$$R_{1212} = \frac{1}{[1 + (y^1)^2]^2} \quad ,$$

and consequently the condition,

$$R_{\alpha\beta\gamma\delta} = K_o (A_{\alpha\gamma} A_{\beta\delta} - A_{\alpha\delta} A_{\beta\gamma}) \quad , \tag{38}$$

is satisfied indentially with $K_o = 1$. The subspace is said to have constant Riemannian curvature. For such a space there exists a set of (n+1) coordinates, (n = dimension of the space), Z^i, satisfying the condition,

$$\sum_i c_i \, (Z^i)^2 = \frac{1}{K_o}, \; i = 1, \ldots, n+1 \quad , \tag{39}$$

and in terms of which the metric of the sub-space may be written as,

$$\bar{A}_{\alpha\beta} = \sum_i c_i \, \frac{\partial Z^i}{\partial \bar{y}^\alpha} \, \frac{\partial Z^i}{\partial \bar{y}^\beta} \quad . \tag{40}$$

The relationship between the Z^i and $\bar{y}^\alpha$ is

$$\frac{\partial Z^i}{\partial \bar{y}^\alpha \partial \bar{y}^\beta} = - K_o \, \bar{A}_{\alpha\beta} Z^i \quad . \tag{41}$$

This system of equations is integrable and yields a family of solutions

$$\bar{Z}^i = a^i_j \, Z^j \quad , \tag{42}$$

in which the a^i_j are constants, n(n+1)/2 of which are independent, satisfying the conditions,

$$\sum_i c_i \left(a^i_j\right)^2 = c_j \qquad (43)$$

$$\sum_i c_i\, a^i_j\, a^i_k = 0 \quad . \qquad (44)$$

Choosing the Z^i to be

$$Z^1 = [1 - (\bar{y}^2)^2]^{\frac{1}{2}} \cos(\tan^{-1} \bar{y}^1)$$

$$Z^2 = [1 - (\bar{y}^2)^2]^{\frac{1}{2}} \sin(\tan^{-1} \bar{y}^1)$$

$$Z^3 = \bar{y}^2 \quad .$$

satisfies equations 41 and the conditions expressed by equations 39 and 40. Equation 42 is then the group of rotations about a point in the 3-dimensional Euclidean space having coordinates Z^i and maps any orthogonal representation of $\underline{\Omega}$ into another. Its Jacobian is equal to 1 and it will not alter the metric properties of the subspace using the Z^i as coordinates. Conversely a transformation of Z^i giving a non-orthogonal representation of $\underline{\Omega}$ will not satisfy equation 39 and therefore will not be an allowable choice of coordinates for the subspace with the metric $\bar{A}_{\alpha\beta}$. In other words such a transformation would alter the metric properties of the subspace.

V. Concluding Remarks

This paper has presented a tensor transformation technique, useful in representing the transport equation in an arbitrary spatial coordinate system. Both the gradient and divergence form of the equation are obtained, the latter being particularly suited to the derivation of finite difference equations by the integral method. The diffusion equation, applicable in the short mean free path limit, was obtained in a similar manner.

By recognizing the tensor character of the equation and introducing a suitable metric tensor in a five dimensional Riemannian space, Drawbaugh set the stage for the use of the tensor formalism. His work however was complicated by the need to invert a 5-dimensional matrix. For arbitrary and unusual coordinate systems this is a non-trivial undertaking. The current work should be viewed as an extension of Drawbaugh's effort. Recognizing that the transformation of the five coordinates could be constructed of two transformations, the first operating on the spatial coordinates alone and the second transforming the angle variable, we have reduced the problem to a set of tractable steps. Further, by first working with the covariant components of $\underline{\Omega}$ and later with the contravariant components of $\underline{\Omega}$, the necessity of forming the inverse transformation is replaced by the need of finding $\bar{g}^{ij}$, which involves forming the inverse of a 3x3 matrix.

Although the choice of spatial coordinate systems and variables has intentionally been left arbitrary a prescription for the selection of the representation of $\underline{\Omega}$, i.e. the choice of angular variables, has been given. In particular, if the choice of the $\overline{\lambda}_i$ is such that they are the projections of $\underline{\Omega}$ along the directions of an orthogonal triad, then T_2 will have a unit value Jacobian. Thus in dealing with coordinate systems which are spatially non-orthogonal a simplified equation may result from choosing an angular representation of $\underline{\Omega}$ along directions other than that of the coordinates.

The particular application of this technique is in the representation of the equation in coordinate systems other than the usual rectangular, cylindrical and spherical ones. A representation of this form allows one to choose coordinate surfaces along surfaces of physical interest (e.g. a surface of constant properties). Today's interest in the development a fusion reactors based on the tokamak provides an incentive to consider toroidal coordinate representations of the transport equation for the investigation of neutronic, photonic and neutral transport problems. We have illustrated the technique by applying it to the toroidal coordinate system previously treated by Pomraning and Stevens.

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7. The following discussion relies on materials to be found in Reference 5, section 16 and chapter 5.

Acknowledgment

The author wishes to express his gratitude to his colleagues at the Princeton Plasma Physics Laboratory for many helpful discussions during the course of this work. In particular I would like to acknowledge the contributions of Dr. R. G. Mills and Dr. W. G. Price, Jr.

This research was supported by the Energy Research & Development Administration, (formerly AEC) under contract E(11-1)-3073.

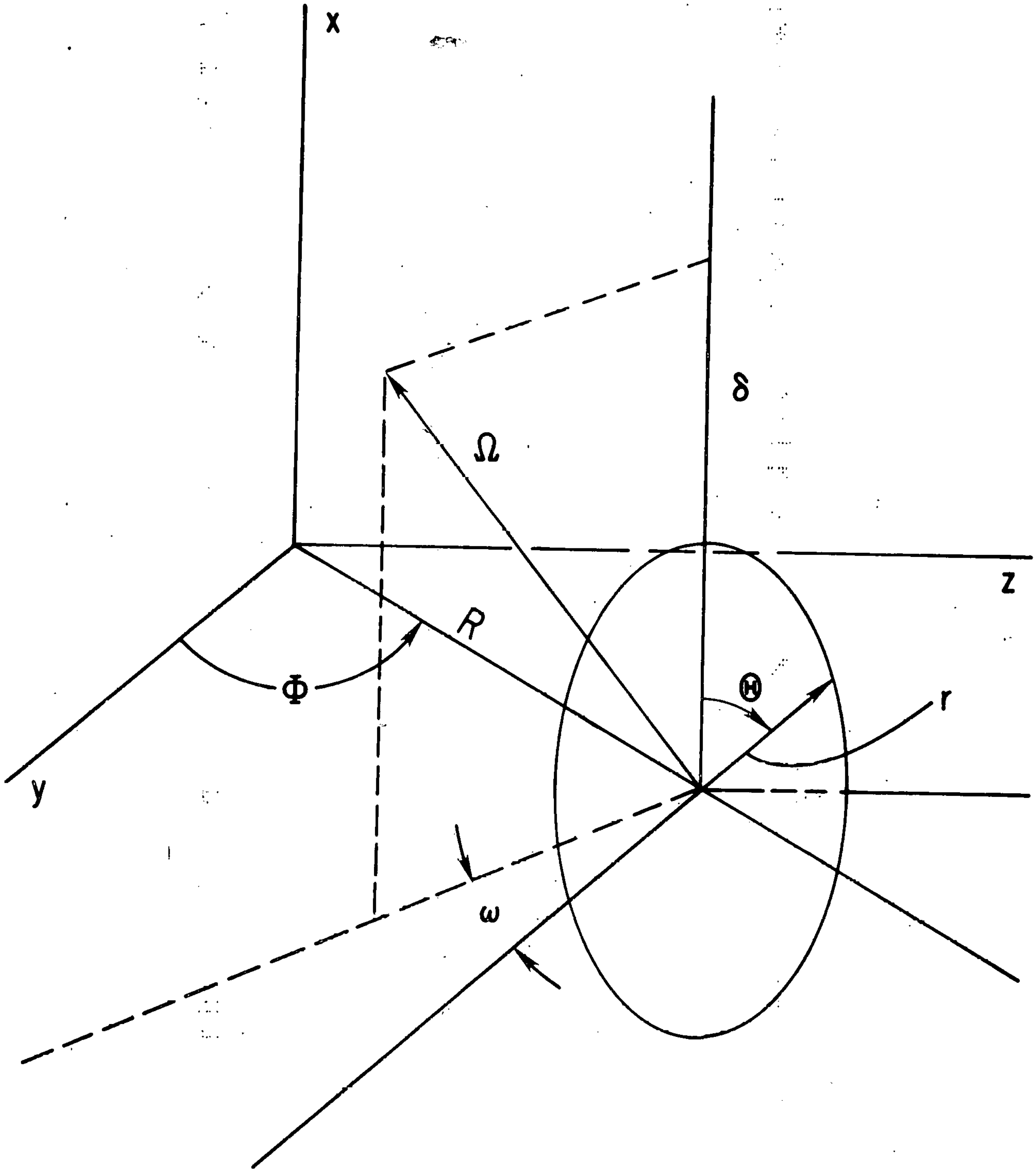

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Fig. 1. Toroidal coordinates r, Θ, Φ, generated by rotating a nest of concentric circles about an axis which does not intersect the nest.