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Optimal Gain in CO_2-N_2-H_2O Gasdynamic Lasers with Shock Free Active Medium

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In this paper, the method of calculus of variation is used for finding the supersonic part of the nozzle of a gasdynamic laser with optimal gain in which Mach lines intersect at some points outside the active medium. This will control the position of shock occurrence and also will ensure the optical uniformity of the active medium. The interesting result is that the supersonic part of such a nozzle consists of a wedge and channel joined by a smooth surface characterized by the geometric locus of points, whose Mach lines are concurrent at a certain point. It is also shown that, overlooking minor differences in gain, the nozzle can be chosen to be shock free with ultimate optical uniformity.

INTRODUCTION

Gain optimization in carbon dioxide Gasdynamic Lasers (GDLs) has been studied by several investigators [1-12]. The optimization problem depends on some numerical variables such as molar fractions, stagnation pressure and temperature as well as some functional variables such as the shape of the subsonic and supersonic parts of the nozzle. In these papers, special families of parametric functions were selected for the shape of the supersonic part and gain was optimized by solving a parametric optimization problem. In particular, to postpone shocks, the authors of [9-11] studied smooth and convex curves whose second derivatives were bounded below. As a result, they showed that the supersonic part consists of a wedge and channel joined by a parabolic surface.

In this paper, z_1, the first point at which the two different Mach lines meet will be also controlled. (For detail see Appendix II.) This is the point after which the non-uniformity of the media begins. A new parameter $\alpha = z_f/z_1$ is defined as an index of the uniformity of the media. Here, the variable z_f denotes the length of the supersonic part of the nozzle. To have uniformity throughout the media, it is necessary to have $0 \leq \alpha \leq 1$. The calculation shows that if $\alpha = 1$, the highest gain is obtained but, instead, the optical uniformity is disturbed; on the other hand, if $\alpha = 0$, then $z_1 = \infty$ and perfect optical uniformity is reached. Further calculation reveals that the difference between optimal gains for various values of α is insignificant. Under the new assumptions, for each α, the optimal shape of the supersonic part consists of a wedge and channel joined by a smooth surface, along which Mach lines are concurrent at z_1. In the case of $z_1 = \infty$, the optimal nozzle shape is the well-known shock free nozzle [13,14].

FORMULATION OF THE STATE VARIABLE EQUATIONS

Throughout this paper, the gas mixture will be CO_2, N_2 and H_2O. It is assumed that the nozzle has a non-equilibrium quasi one-dimensional steady-state inviscid ideal gas flow with no change in its chemical composition. Following Anderson bimodal model for the relaxation of the vibrational phenomena, the governing equations of the flow are as follows [1,9]:

$$p = \rho \, R \, T \text{ (State equation of an ideal gas)}, \quad (1)$$

$$\rho \, v \, A = q \text{ (Conservation law of mass)}, \quad (2)$$

$$dp/\rho + dv = 0 \text{ (Conservation law of momentum)}, \quad (3)$$

$$H_0 = v^2/2 + R\gamma(\gamma-1)^{-1}T + e_1(T_1) + e_2(T_2)$$
$$\text{(Conservation law of energy)}, \quad (4)$$

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$$\frac{de_i}{dz} = \frac{e_i(T_i) - e_i(T)}{\tau_i}, \quad (i = 1, 2)$$

$$\text{(Relaxation equations).} \tag{5}$$

Here q, γ and R denote, respectively, net flux of mass, specific heat capacity ratio and universal gas constant. Also, p, ρ, v, T, A, e_i, T_i and τ_i are, respectively, pressure, density, velocity, translational temperature, cross sectional area (shape function), vibrational energy, temperature and relaxation life time of the ith mode, at a point in the supersonic part of horizontal distance z from the throat plane [11]. By introducing a state vector $x \in \mathbb{R}^5$, one can write the state equations as follows:

$$\begin{aligned}\dot{x}^T &= (\dot{x_1}, \dot{x_2}, \dot{x_3}, \dot{x_4}, \dot{x_5}) \\ &= \left(x_4^{-1} f_1, x_4^{-1} f_2, x_4^{-1}(f_4 x_5 + f_3), x_5, 0\right) \\ &+ (0, 0, 0, 0, 1)\, u = F(x)^T + b^T u,\end{aligned} \tag{6}$$

where $x_1 = T_1$, $x_2 = T_2$, $x_3 = T$, $x_4 = a$, $x_5 = da/dz$ and $u = d^2 f/dz^2$. Here, a is the normalized shape function A/A^*, where A^* is the throat area. The variable $u = d^2 f/dz^2$ is taken as the control function. The functions f_i $(i = 1, 2, 3, 4)$ are differentiable and their exact forms are given in Appendix I. The initial values of the state variables x_1, x_2 and x_3 are denoted by $x_1(0)$, $x_2(0)$ and $x_3(0)$, which are determined by the reservoir conditions and the subsonic structure of the nozzle and that of x_4 by $x_4(0) = 1$. The initial value for x_5 is $x_5(0) = (2/h^*) \tan(\Theta/2)$, where h^* is the throat height and Θ is the opening angle. The value of $x_5(0)$, depending on Θ, will be determined in the optimization process. To avoid gas detachment from the walls, it is assumed that $x_5(0) \leq \beta$, where β is a positive constant depending on the fluid parameters [15]. Also, to terminate the nozzle into a channel, it is further assumed that $x_5 \geq 0$ and

$$u \leq 0. \tag{7}$$

In particular,

$$0 \leq x_5 \leq \beta. \tag{8}$$

Shock waves introduce discontinuity or rapid changes in not only the thermodynamic variables such as the density of the gas mixture, but also in the optical refraction coefficient of the gas. Therefore, occurrence of shock waves in the active and immediate areas destroys the optical uniformity and gain coefficient. Hence, to maintain a more uniform active media, it is necessary to postpone the formation of such waves to a region faraway enough from the end of the nozzle. It follows from approximation of the characteristic curves by Mach lines that curved shock waves occur at each point $z_s = z_s(z, x, u) = z + 1/\left[h_1(z, x)u + h_2(z, x)\right]$ at which two close Mach lines intersect. (See Appendix II for the exact form of $z_s(z, x, u)$.)

To avoid occurence of curved shock waves in the active media, $z_s(z, x, u)$ must be either less than z or greater than $(1/\alpha)\, z_f$ for each z $(0 \leq z \leq z_f)$ and a certain constant $0 \leq \alpha < 1$ not depending on z. This can be achieved by setting a constraint of the form:

$$h(z, x, u, z_f) = (z_s - z)\left(\alpha^{-1} z_f - z_s\right) \leq 0. \tag{9}$$

The problem is now to optimize the small signal gain $g_0 = g_0(x_1, x_2, x_3)$ (see Appendix I for detail), where x_1, x_2 and x_3 satisfy state Equation 6 with Constraints 7, 8 and 9 and the initial conditions:

$$x_1(0) = x_{10}, \tag{10}$$

$$x_2(0) = x_{20}, \tag{11}$$

$$x_3(0) = x_{30}, \tag{12}$$

$$x_4(0) = x_{40} = 1. \tag{13}$$

Since Constraint 9 depends on u, it is not possible to imitate the method of [9-11] to solve the optimization problem via Pontryagin's principle. To avoid this difficulty, the calculus of variation is applied directly.

GAIN OPTIMIZATION WITH RESPECT TO NOZZLE SHAPE

By introducing new variables q_1, q_2 and q_3, the inequality Constraints 7 to 9 can be rewritten as follows:

$$y = \left(x_5\,(x_5 - \beta) + q_1^2, h(z, x, u, z_f) + q_2^2, u + q_3^2\right) = 0. \tag{14}$$

Let $p \in \mathbb{R}^5$ and $\lambda \in \mathbb{R}^3$ be Lagrange multipliers corresponding to state Equation 6 and Constraint 14, respectively. Now, the optimization problem is reduced to optimizing the following generalized cost function without any constraints,

$$\begin{aligned} g_a &= g_0\left(x\left(z_f\right)\right) \\ &+ \int_0^{z_f} \left[p^T\left(F(x) + bu - \dot{x}\right) + \lambda^T y\right] dz. \end{aligned} \tag{15}$$

Applying the variational method [16], the equation $\delta g_a = 0$ for the optimal case yields:

$$\lambda_i q_i = 0 \quad (i = 1, 2, 3), \tag{16}$$

$$y = 0, \tag{17}$$

$$p^T b + \lambda_2 \frac{\partial h}{\partial u} + \lambda_3 = 0, \tag{18}$$

$$\dot{x} = F(x) + bu, \tag{19}$$

$$\dot{p}^T = -\left(p^T \frac{\partial F}{\partial x} + \lambda_2 \frac{\partial h}{\partial x} + \lambda_1 b^T (2x_5 - \beta)\right), \tag{20}$$

$$\left(p^T (F(x) + bu) + \lambda^T y\right)|_{z=z_f} + \int_0^{z_f} \frac{\alpha^{-1}\lambda_2}{(h_1 u + h_2)} dz = 0, \tag{21}$$

$$p(z_f) = \frac{\partial g_0}{\partial x}|_{z=z_f} . \tag{22}$$

The optimal solution is now obtained by solving Equations 16 to 22 for x, p, λ, q and u. If $q_1 = 0$ for all z in some interval, then it follows from Equation 14 that either $x_5 = \beta$ or $x_5 = 0$ which yields a wedge or a channel, accordingly. In both cases, $u = 0$. For the remainder of the nozzle, it is proceeded as follows. If λ_2 or λ_3 is non-zero on some interval, then u is determined by either $u = 0$ or $h(z, x, u, z_f) = 0$. The first conclusion implies that the concerned part of the nozzle is again either a wedge or a channel. The second conclusion implies that $z_s = \alpha^{-1} z_f$ and, hence, z_s is constant on that interval; i.e., all Mach lines pass through the same point. Finally, if λ_2 and λ_3 vanish simultaneously on an interval, then singularity is encountered and, hence, u cannot be determined directly. In this case, using Equation 18 and its first and second derivatives with respect to z, the optimal control u can be determined at each point of singularity as a function of the state variable x; i.e., $u = u_s(x)$ with $u \leq 0$ and $h(z, x, u, z_f) \leq 0$. (See Appendix III for detail.)

Summing up, in the absence of singularity and in view of the fact that $u \leq 0$, the following assertions are true in the optimal case:

- The channel part will occur only at the end part of the nozzle.
- Due to the smoothness of the shape function, the wedge and channel can not be adjacent.
- Since $\mu = \sin^{-1}(1/M)$ is decreasing and Mach lines initiating from the curved parts all pass through the same point $z_1 = \alpha^{-1} z_f$, it follows that disjoint wedge parts do not occur. (Here $M = v/\sqrt{\gamma RT}$ is the freezing Mach number and μ is the angle between the stream line and Mach line.)

Thus, the nozzle is divided into three distinct parts. The first part is a wedge, the second part is a curved surface with the property that all Mach lines concur at the point $\alpha^{-1} z_f$ and the third part is a channel. Theoretically, one may argue that the wedge part or the channel part may vanish. However, the nozzle shape depends on a set of numerical parameters c_1, z_f and $x_5(0)$, in which c_1 is the end of the wedge part. Note that the end of the curved part c_2 is not an independent parameter and is determined by equation $x_5(c_2) = 0$. To find the exact shape of the optimal nozzle, it is necessary now to solve a multi-factor optimization problem through numerical methods [5].

It should be noticed that throughout the paper, the smoothness of the shape function is guaranteed by enforcing the existence of $\dot{x_4}$.

NUMERICAL RESULTS

The optimal nozzle parameters are determined by numerical solution of Equations 16 to 22, since the exact solution of the governing non-linear system of differential equations of the gasdynamic laser is not possible. For example, choose $\Theta = 40^0$ and $h^* =$ 0.3 mm and assume the GDL of the C_6H_6-O_2-N_2 combustion-driven type. Then, $\beta = 6720$, $X_{CO_2} =$ 0.1, $X_{N_2} = 0.85$ and $X_{H_2O} = 0.05$. Arrange the stagnation condition in such a way that $p_0 = 20$ atm and $T_0 = 1220$ k. The optimal shape corresponding to $\alpha = 0.5$ is given in Figure 1. As shown in this figure, the nozzle shape has no singular part and its curved part is in the interval $[c_1, c_2]$=[0.18, 45] cm and the nozzle terminates at $z_f = 8.3$ cm. In Figure 2, the corresponding gain function is shown. To verify the existence of the singular branches, the singular control function u_s is obtained in Appendix III. If singularity begins at z, then $u_s(z)$ is calculated for the above example, for which the values are shown in Figure 3. Now, $u_s(z)$ being positive contradicts Statement 7. Hence, singular branches do not occur and the shape function has a definite structure as described in the preceding section. To determine the effect of variation of α on the optimal gain, the maximum of the optimal gain function is plotted versus α in Figure 4. The variation of the maximum gain with respect to α is insignificant, as seen in Figure 4. Thus, by overlooking

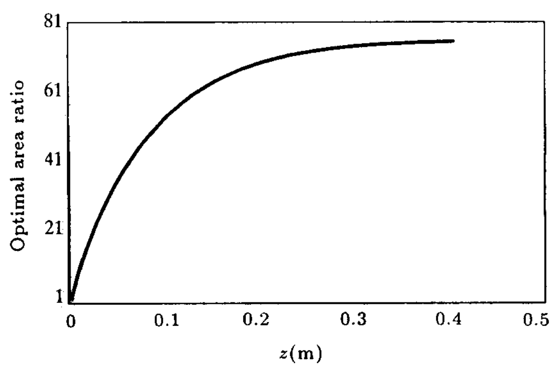

Figure 1. Optimal nozzle area ratio versus z, where z is the coordinate along the nozzle. The operation parameters of gasdynamic laser are: $p_0 = 20$ atm, $X_{CO_2} = 0.1$, $X_{H_2O} = 0.05$, $X_{N_2} = 0.85$, $c_1 = 0.0018$ m, opening angle $=17°$, $\alpha = 0.4$, $z_f = 0.8$ m and $c_2 = 0.45$ m.

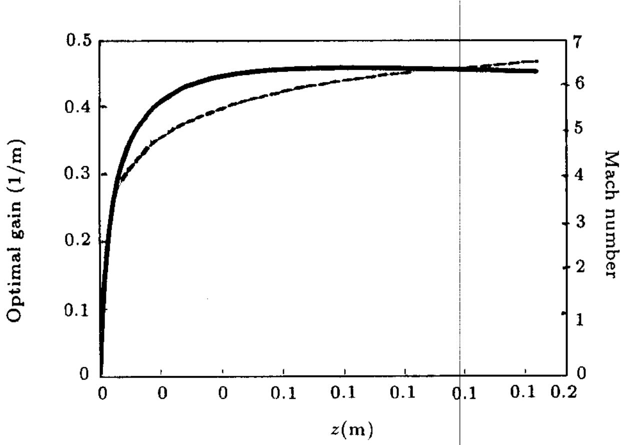

Figure 2. Gain and Mach number (dash line) profiles of the optimal nozzle versus z, where z is the coordinate along the gas flow axis. Operation parameters are: $p_0 = 20$ atm, $X_{CO_2} = 0.1$, $X_{H_2O} = 0.05$, $X_{N_2} = 0.85$, opening angle = 17° and $\alpha = 0.4$.

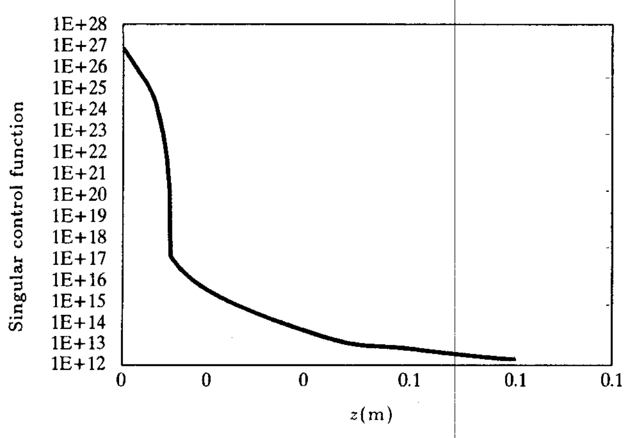

Figure 3. Control signal at the begining of the singular path. Since it is positive everywhere, no singular branch exists. $p_0 = 20$ atm, $T_0 = 1220$, $X_{CO_2} = 0.1$, $X_{H_2O} = 0.05$, $X_{N_2} = 0.85$, opening angle = 17° and $\alpha = 0.4$.

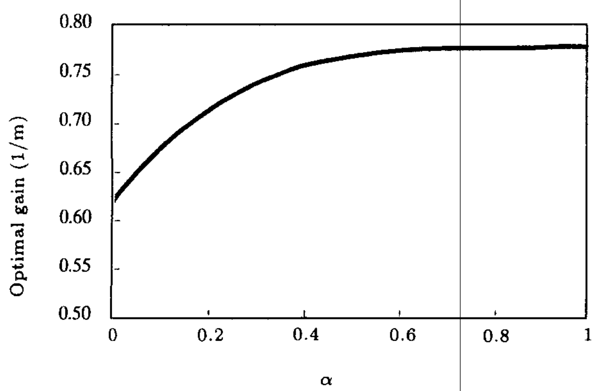

Figure 4. Maximum gain of the optimal nozzle versus dimensionless parameter a. The operating parameters of the gasdynamic laser are: $p_0 = 20$ atm, $X_{CO_2} = 0.1$, $X_{H_2O} = 0.05$, $X_{N_2} = 0.85$ and opening angle = 20°.

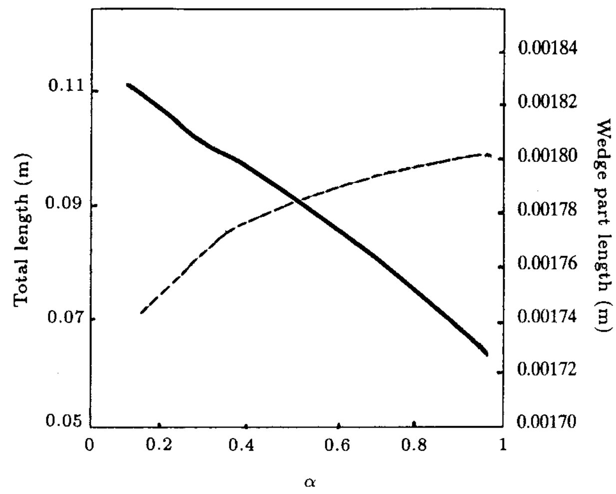

Figure 5. The total length of the maximum gain nozzle (dash line) and the length of its wedge part (solid line) as functions of the dimensionless parameter α. The operating parameters are: $p_0 = 20$ atm, $X_{CO_2} = 0.1$, $X_{H_2O} = 0.05$, $X_{N_2} = 0.85$ and opening angle = 20°.

minor differences in gain, the nozzle can be chosen to be shock free with the ultimate optical uniformity. Therefore, one can improve the optical uniformity of the active medium against a slight loss in gain. In Figure 5, the starting point of the curved part and the length of the nozzle are presented as functions of α. The case $\alpha = 0$ corresponds to the well-known shock free nozzles (SFNs) [13].

CONCLUSION

The optimal nozzle shape in a general gasdynamic laser consists of a wedge and channel joined by a smooth surface which is the geometrical locus of the points for which their Mach lines concur at a certain point. There exists a weak trade-off between the optical uniformity of the active medium and its maximum gain. In the case of highest optical uniformity, the nozzle has the shape of the well-known shock free nozzle. Finally, it has been shown that the gain optimization problem in gasdynamic lasers is reduced to a multi-parametric optimization problem.

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APPENDIX I

The vibrational model used in this work is Anderson bimodal model [1]. According to this model and the quasi one-dimensional inviscid non-chemical reacting ideal gas flow assumptions, the functions $f_i(i = 1,2,3,4)$ are as follows:

$$f_i = \frac{q\,(e_i(x_i) - e_i(x_3))}{\gamma M^2 p\tau_i e_i'(x_i)}, \quad (i = 1,2), \tag{A1}$$

$$f_3 = \frac{q(\gamma-1)(\gamma\ M^2-1)}{\gamma^2\ M^2\ R(M^2-1)} \sum_{i=1}^{2} \frac{e_i(x_i) - e_i(x_3)}{p\tau_i}, \tag{A2}$$

$$f_4 = -\frac{(\gamma-1)M^2\ x_3}{(M^2-1)}. \tag{A3}$$

The gain function for non-lasing operation is given by:

$$g_0 = \frac{e^{\frac{-3383}{x_2}} - e^{\frac{-1999}{x_1}}}{x_3^{3/2}\ e^{\frac{234}{x_3}}} \frac{0.0977}{Q} \cdot \frac{T_0^{3/2} X_{CO_2}}{X_{CO_2} + 0.7589 X_{N_2} + 0.3236 X_{H_2O}}, \tag{A4}$$

where the energy of the ith vibrational mode and its relaxation life time, as a function of the state variables and gas fractions, is given in [1].

APPENDIX II

Curved Shock Waves Formation Position

Oblique shock waves are two-dimensional phenomena; their formation positions are the intersection points of the characteristic curves of the governing hyperbolic partial differential equations [13,17]. In this work, Mach lines are used as an approximation of the characteristic curves. The equations of Mach lines, which start from points $(z,\ x_4(z))$ and $(z + dz,\ x_4(z + dz))$ on the boundary of the nozzle, are as follows:

$$(Y - h^* x_4(z)) = (X - z)\tan(\theta - \mu), \tag{A5}$$

$$(Y - h^* x_4(z + dz)) = (X - z - dz)\tan(\theta - \mu + d\theta - d\mu), \tag{A6}$$

where $\tan\theta = A^* x_5$, $\sin\mu = 1/M$ and (X, Y) is a point on Mach line.

After some mathematical manipulations, the z-coordinate of the intersection point of the above lines (z_s) is given by:

$$z_s = z + \frac{1}{h_1(z,x)u + h_2(z,x)}, \tag{A7}$$

where,

$$h_1(z,x) = [-h^*] / \left[x_5\ h^*(\sqrt{M^2-1}+1) + 2(\sqrt{M^2-1}-1)\right],$$

$$h_2(z,x) = \frac{[-(4+(x_5 h^*)^2)]}{[2M\sqrt{M^2-1}(x_5 h^*(\sqrt{M^2-1}+1) + 2(\sqrt{M^2-1}-1))]} \cdot \left[1/(\sqrt{\gamma R x_3})\ dv/dz - v/(2\sqrt{\gamma R x_3^3})\ dx_3/dz\right]$$

z_s is an increasing function of z in the compression region and its positive minimum in this region is denoted by z_1.

APPENDIX III

The Singular Part of the Nozzle Shape

A singular part of the nozzle appears when $\lambda_1 = \lambda_2 = \lambda_3 = 0$ on some interval. In this case, it follows from Equation 18 that:

$$p_5 \equiv 0. \tag{A8}$$

It is obvious that $\dot{p_5}$ is also zero on that interval and hence, by Equation 20:

$$x_4\ x_5\ \dot{p_5} = x_5\ f_3\ p_3 + x_5\ x_4\ p_4 = A_1 p_1 + A_2 p_2 + A_3 p_3 \equiv 0 \tag{A9}$$

Obviously, the first and second derivatives of the above equation are also zero on that interval and thus:

$$B_1 p_1 + B_2 p_2 + B_3 p_3 \equiv 0, \tag{A10}$$

$$(C_1 + D_1 u_s) p_1 + (C_2 + D_2 u_s) p_2 + (C_3 + D_3 u_s) p_3 \equiv 0. \tag{A11}$$

The above homogeneous system of linear Equations A9 to A11 has non-zero solution if:

$$\begin{vmatrix} A_1 & A_2 & A_3 \\ B_1 & B_2 & B_3 \\ C_1 + D_1 u_s & C_2 + D_2 u_s & C_3 + D_3 u_s \end{vmatrix} = 0 \tag{A12}$$

Then, by solving the above equation with respect to u_s, the control function on the singular path, it is obtained that:

$$u_s = -\frac{\begin{vmatrix} A_1 & A_2 & A_3 \\ B_1 & B_2 & B_3 \\ C_1 & C_2 & C_3 \end{vmatrix}}{\begin{vmatrix} A_1 & A_2 & A_3 \\ B_1 & B_2 & B_3 \\ D_1 & D_2 & D_3 \end{vmatrix}}, \tag{A13}$$

where A_i, B_i, C_i and D_i ($i = 1,2,3$) are given as follows:

$$A_i = -f_i, \tag{A14}$$

$$B_i = \sum_{j=1}^{3} \frac{\partial A_j}{\partial x_j} F_j + \sum_{j=1}^{3} A_j \frac{\partial F_j}{\partial x_i}, \tag{A15}$$

$$C_i = \sum_{j=1}^{3} \frac{\partial B_j}{\partial x_j} F_j + \sum_{j=1}^{3} B_j \frac{\partial F_j}{\partial x_i} + \sum_{j=1}^{3} -f_j B_j \frac{\partial F_j}{\partial x_4}, \tag{A16}$$

$$D_i = \frac{\partial B_i}{\partial x_5}. \tag{A17}$$