

OPTIMAL NOZZLE SHAPES OF CO₂-N₂-H₂O GASDYNAMIC LASERS

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Abstract

In an axisymmetric CO₂-N₂-H₂O gas dynamic laser, let Γ denote the intersection of the vertical plane of symmetry with the upper part of the (supersonic) nozzle. To obtain a maximal small signal gain, some authors have tested several families of curves for Γ . To find the most general solution for Γ , an application of Pontryagin's principle led to the conjecture that the optimal Γ must consist of two straight lines of slopes m and 0 smoothly joined by a parabolic arc. (The parabolic section will vanish if nonsmooth Γ is allowed.) The conjecture was settled in the affirmative for special cases. The present work extends these results in the following directions. (i) For the nonsmooth case, Pontryagin's principle produces no singularity and Γ consists of k straight lines of certain slopes m and 0. (ii) A "semi-uncoupled" approximation is used to show, in (i), that $k=2$. ("coupled" stands for the dynamic coupling between vibrational temperatures and translational temperature.) (iii) An uncoupled approximation is used in the smooth case to show that the general Γ consists of a line segment of slope m , a parabolic arc and a horizontal line. (iv) The small signal gain increases whenever the slope m and/or the curvature of the parabolic section increase. However, the latter two quantities must be bounded to reduce gas detachment from the walls or oblique shock waves in the active media. (v) Finally, the optimal shapes and gains are numerically calculated for several values of the stagnation pressure and molar fractions of the gas mixture.

1. Introduction

Let x_i be the vibrational temperature of mode i ($i = 1,2$), in Anderson's bimodal model [1] of a CO₂-N₂-H₂O or He gas dynamic laser whose supersonic part is axisymmetric with a quasi 1-dimensional steady state

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flow. (For a geometrical schematics of a gasdynamic laser, see Fig. 1) Let x_3 denote the translational temperature and let A denote the cross sectional area of the supersonic part by planes perpendicular to the nozzle axis. Let $x_4 = A/A^*$, where A^* is the throat area. It is assumed that x_1 , x_2 , and x_3 of a gas molecule are functions of s , the distance of the gas molecule in the

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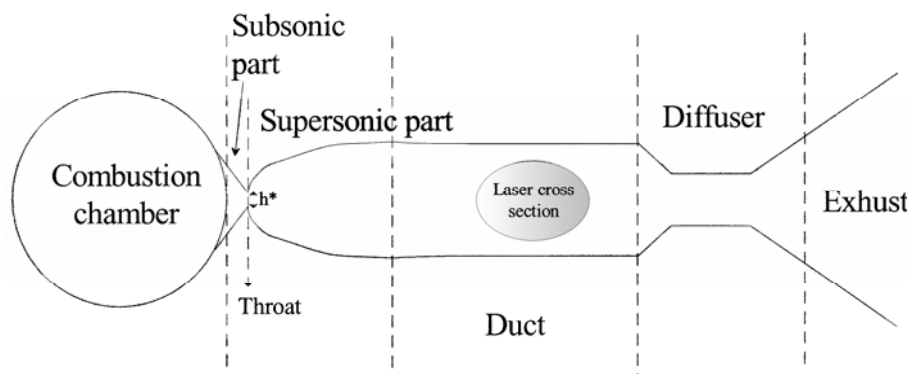


Figure 1. Simplified schematic of a gasdynamic laser.

supersonic part from the throat plane. Our interest is, for given reservoir conditions, to study the optimal shape of the supersonic part of a laser yielding a maximal small signal gain. i.e., knowing the stagnation parameters (reservoir temperature, pressure, and molar fractions), as well as the temperatures

$$x_i(0) = T_{0i}, \quad (i = 1,2,3), \quad (1)$$

at the throat $s_0 = 0$, we must find an interval $[0, s_1]$ and functions $x_i: [0, s_1] \rightarrow \mathbb{R}^+$, ($i = 1,2,3,4$), such that $g_0(x_1(s_1), x_2(s_1), x_3(s_1))$ is maximal and that $x_i(s)$ ($i = 1,2,3,4$) as above represent the various temperatures and the normalized cross sectional area at a point of distance s from the throat plane. (The unknown positive number s_1 denotes the length of the supersonic part.) Note that if Γ is the intersection of the vertical plane of symmetry with the upper part of the (supersonic) nozzle, then $y(s) = (h^*/2)x_4(s)$ where h^* is the throat height and $(s, y(s))$ denotes a point of Γ in the coordinate system consisting of the (horizontal) axis of symmetry and a vertical axis in the throat plane.

Such problems were studied before in [2-14] by examining various families of functions for x_4 . In [15] it was assumed an uncoupled approximation of Anderson's model and was shown that an optimal nozzle must consist of a wedge and a channel smoothly joined by parabolic sheets. (If sharp corners are allowed, then the parabolic sheets vanish.) In the present work these results are extended in the following directions. For the nonsmooth case, Pontryagin's principle produces no singularity and nozzle shape consists of k straight lines of certain slopes m and 0. A "semi-uncoupled" approximation is used to show that $k = 2$. An uncoupled approximation is used in the smooth case to show that the general Γ consists of a line segment of slope m , a parabolic arc and a horizontal line. The small signal gain increases whenever m and/or the curvature of the parabolic section increase. However, the latter two quantities must be bounded to avoid gas detachment

from the walls or oblique shock waves in the active media. Finally, the optimal shapes and gains are numerically calculated for several values of the stagnation pressure and molar fractions of the gas mixture.

2. Governing Equations

Let t denote the time, with which we will have a very short encounter. The main independent variable here is the spatial coordinate s and hence the notation \dot{f} is reserved only for df/ds if f is considered as a function of s . Let p, ρ , and v denote the gas pressure, density, and velocity, respectively. Also, let e_i and τ_i denote, respectively, the vibrational energy and the characteristic relaxation time for mode i , ($i = 1,2$). The following relations between the above variables as well as the Mach number M and the small signal gain g_0 are needed in our arguments:

$$p = R\rho x_3, \quad \rho v x_4 = q, \quad v dv = -(1/\rho)dp, \quad (2)$$

$$v^2 = 2H - 2\gamma(\gamma - 1)^{-1}R x_3 - 2e_1 - 2e_2, \quad (3)$$

$$M^2 = v^2/(\gamma R x_3),$$

$$e_1 = E_1(x_1) :=$$

$$\delta_1 \left[\frac{1999}{\exp(1999/x_1) - 1} + \frac{1920}{\exp(960/x_1) - 1} \right], \quad (4)$$

$$e_2 = E_2(x_2) :=$$

$$\delta_1 \left[\frac{3383}{\exp(3383/x_2) - 1} + \frac{X_{N_2}}{X_{CO_2}} \frac{3357}{\exp(3357/x_2) - 1} \right], \quad (5)$$

$$\dot{e}_i := de_i / ds = (1/\nu) de_i / dt = -\frac{q(E_i(x_i) - E_i(x_3))}{\gamma M^2 p \tau_i x_4}, \quad (6)$$

(i=1,2),

$$\dot{x}_3 := dx_3 / ds = \frac{\gamma - 1}{x_4(M^2 - 1)} \left[-M^2 x_3 \dot{x}_4 + \frac{q(\gamma M^2 - 1)}{\gamma^2 R M^2} \times \sum_{i=1}^2 \frac{E_i(x_i) - E_i(x_3)}{p \tau_i} \right], \quad (7)$$

$$g_0(x_1, x_2, x_3) = \delta_3 \frac{\exp(-3383/x_2) - \exp(-1999/x_1)}{x_3 \exp(\eta/x_3)}, \quad (8)$$

$$[1 - \exp(-1999/x_1)][1 - \exp(-960/x_1)]^2 \times [1 - \exp(-3383/x_2)]$$

$$\frac{\partial g_0}{\partial x_1} < 0 \text{ and } \frac{\partial g_0}{\partial x_2} > 0, \quad (9)$$

$$\frac{\partial g_0}{\partial x_3} > 0 \text{ for } x_3 < \eta, \quad (10)$$

and some constants $q > 0$, $R > 0$, $\gamma > 1$, $\delta_i > 0$ ($i = 1, 2, 3$), $0 < \eta < 290$, whose more precise values are not needed in our arguments. X_{CO_2} , X_{N_2} , and X_{H_2O} are the mass fractions.

The above relations are taken from [1,5,10,16,17]. In particular, (4)-(6) are from [1, pp. 41-43]. Also, (8) is taken from [1, p. 63] where $\eta=234$ in the room temperature. The expressions $p \tau_i$ ($i = 1, 2$) are functions of x_3 . (See [1, pp. 41-42 & 170].)

In view of (4)-(6),

$$\dot{x}_i := dx_i / ds = (dx_i / de_i) \dot{e}_i = \dot{e}_i / E'_i(x_i) = -\frac{1}{x_4} \left[\frac{q(E_i(x_i) - E_i(x_3))}{\gamma M^2 p \tau_i E'_i(x_i)} \right], \quad (i = 1, 2). \quad (11)$$

(Here E'_i denotes the derivative of the function E_i .)

We conclude the section by verifying a key result, which support the well known fact that the value of dx_1/dx_2 is large enough to produce population inversion in the supersonic part. The result asserts that if the gas

mixture is fixed and the translational temperature x_3 in the supersonic part is cooled down due to an admissible deformation of the nozzle or change of reservoir temperature and pressure, then x_1 accelerates with respect to x_2 .

Observe that dx_1/dx_2 , computed from (11), is a function of x_1, x_2, x_3 , and does not depend explicitly on any other variable. In fact

$$\frac{dx_1}{dx_2} = \frac{p \tau_2}{p \tau_1} \cdot \frac{E'_2(x_2)}{E'_1(x_1)} \cdot \frac{E_1(x_1) - E_1(x_3)}{E_2(x_2) - E_2(x_3)} \quad (12)$$

Fact 2.1. If dx_1/dx_2 is regarded as an explicit function of x_1, x_2 , and x_3 , then

$$\frac{\partial}{\partial x_3} (dx_1 / dx_2) < 0, \quad x_3 < x_1 < x_2. \quad (13)$$

One way to see this is to rely on numerical computation. Here is a direct justification. Since E_1 and E_2 are strictly increasing functions, it follows that, for fixed values of $x_1 < x_2$, the expression $[E_1(x_2) - E_1(x_1)] / [E_2(x_3) - E_2(x_2)]$ is a strictly decreasing function with respect to x_3 whenever $x_3 < x_1 < x_2$. Also, since the planner curve Γ with the parametric equations $x = E_2(u)$ and $y = E_1(u)$ is strictly increasing and concave downward for $0 < u < \infty$, it follows that the expression

$$\frac{E_1(x_3) - E_1(x_2)}{E_2(x_3) - E_2(x_2)} \left(= \frac{E'_1(c)}{E'_2(c)} \right)$$

is a strictly decreasing function of x_3 when x_2 is fixed and $0 < x_3 < x_2$. (The point c of the mean-value theorem strictly increases with x_3 .)

From a physical point of view, it is obvious that the expression $p \tau_2 / (p \tau_1)$ is a strictly decreasing function of x_3 . (This can be mathematically justified by choosing, for instance, $p \tau_i = \delta_i \exp(\gamma_i x_3^{-1/3})$, $i = 1, 2$ [11,17].) Thus the expression

$$K(x_1, x_2, x_3) = (p \tau_2 / p \tau_1) \left[\frac{E'_1(c)}{E'_2(c)} + \frac{E_1(x_2) - E_1(x_1)}{E_2(x_3) - E_2(x_2)} \right] \quad (14)$$

is strictly decreasing in x_3 .

3. Constraints and End Conditions

The domain in which the governing equations are defined lies in the set

$$x_3 < x_1 < x_2, \quad (15)$$

which, being an open set, imposes no constraint on the

trajectories

$$x(s) = \begin{bmatrix} x_1(s) \\ x_2(s) \\ x_3(s) \\ x_4(s) \end{bmatrix}, \quad (0 \leq s \leq s_1). \quad (16)$$

Note that in Pontryagin’s principle, the existence of an optimal solution is assumed and the task is to describe it. Since, without (15), the population inversion is impossible, thus we assume it is satisfied automatically. We further reduce the domain by assuming

$$M > 1 \quad (17)$$

at the throat and all the points in the supersonic part. (The validity of (17) guarantees the continuity of the functions defining the governing equations at the throat as well as the rest of the supersonic part.)

The reservoir conditions are assumed to be fixed throughout the experiment. Thus, we have the end conditions

$$x_3(0) = T_{03} < x_1(0) = T_{01} < x_2(0) = T_{02}, \quad (18)$$

as well as

$$x_4(0) = 1, \quad (19)$$

where the constants T_{01} , T_{02} , and T_{03} are the various temperatures of the gas at the throat $s = 0$. We also assume there exists no interval $(0, \varepsilon)$ on which \dot{x}_4 is identically zero; otherwise, it follows from (7), as well as the relations,

$$\left[\frac{d(M^2)}{ds} = \frac{(\gamma - 1)M^2}{x_4(M^2 - 1)} \times \left(M^2 + \frac{2}{\gamma - 1} \dot{x}_4 - \frac{q(\gamma M^2 + 1)}{\gamma^2 R x_3 M^2} \sum_{i=1}^2 \frac{E_i(x_i) - E_i(x_3)}{p \tau_i} \right) \right] \quad (20)$$

and

$$\left[\frac{d(v^2)}{ds} = \frac{2\gamma R x_3}{x_4(M^2 - 1)} \times \left[M^2 \dot{x}_4 - \frac{q(\gamma - 1)}{\gamma^2 R x_3} \sum_{i=1}^2 \frac{E_i(x_i) - E_i(x_3)}{p \tau_i} \right] \right], \quad (21)$$

that the translational temperature x_3 increases and the speed v as well as the Mach number M decrease; something not expected from a nozzle throat. Also, to avoid gas detachment from the walls, it is assumed in

[6, pp. 782-83] that

$$0 \leq \dot{x}_4 \leq \beta = 2m/h^*, \quad (22)$$

where h^* is the throat height and m is the maximum allowable slope of the curve Γ . (See section I.) This will define the set U of the control values in the forthcoming section.

4. Optimization in Fully Coupled Models (nonsmooth case)

In this section we ignore oblique shock waves and find a vector-valued function $x(s)$ on some interval $[0, s_1]$ satisfying the above governing equations and end conditions such that $g_0(x_1(s_1), x_2(s_1), x_3(s_1))$ is maximal. The first theorem shows that x_4 is obtained by joining finitely many lines of slopes β and 0. In the next section, a semi-uncoupled model is introduced to show the number of line segments is at most 2.

Theorem 4.1. *Assume x_i ($i = 1, 2, 3, 4$) are functions defined on some interval $[0, s_1]$ satisfying the governing equations as well as the end conditions defined in sections II and III. Moreover, assume $g_0(x_1(s_1), x_2(s_1), x_3(s_1))$ is maximal and that \dot{x}_4 is piecewise continuous and left continuous. (The right limits of \dot{x}_4 are assumed to exist at points of discontinuity.) Then \dot{x}_4 is piecewise constant with values β and 0. In particular, $\dot{x}_4 = \beta$ on the first interval.*

Proof. Let $u = \dot{x}_4$ and $U = [0, \beta]$. Then, following the version of Pontryagin’s principle stated in [18, pp. 23-28], and replacing the independent variable t by our spatial coordinate s , we further define

$$e = \begin{bmatrix} s_0 \\ s_1 \\ x(s_0) \\ x(s_1) \end{bmatrix} \in [0, \infty)^{10}, \quad (23)$$

$$\phi(e) = \begin{bmatrix} -g_0(x_1(s_1), x_2(s_1), x_3(s_1)) \\ s_0 \\ x_1(s_0) - T_{01} \\ x_2(s_0) - T_{02} \\ x_3(s_0) - T_{03} \\ x_4(s_0) - 1 \end{bmatrix},$$

where $x(s)$ is as in (16), and s_0 and s_1 denote the throat and the end of the supersonic part, respectively. So, the optimal pair (x, u) minimizes $\phi_1(e)$, and satisfies the system

$$\dot{x}_4 = x_4^{-1} F_i(x_1, x_2, x_3) \tag{24}$$

$$\dot{x}_3 = x_4^{-1} [u F_3(x_1, x_2, x_3) + F_4(x_1, x_2, x_3)], \tag{25}$$

where

$$F_i := -\frac{q(E_i(x_i) - E_i(x_3))}{\gamma M^2 p \tau_i E_i'(x_i)}, \quad (i = 1, 2),$$

$$F_3 := -\frac{(\gamma - 1) M^2 x_3}{(M^2 - 1)},$$

$$F_4 := \frac{q(\gamma - 1)(\gamma M^2 - 1)}{\gamma^2 R M^2 (M^2 - 1)} \sum_{i=1}^2 \frac{E_i(x_i) - E_i(x_3)}{p \tau_i},$$

along with the end conditions $\phi_i(e) = 0$ ($i = 2, 3, 4, 5, 6$).

Thus, there exist a nonzero vector $\lambda \in \mathbb{R}^6$ with $\lambda_1 = 0$ or -1 and a function $P : [0, s_1] \rightarrow \mathbb{R}^4$ such that, for $s \in (0, s_1)$,

$$\dot{P}_i = -x_4^{-1} \left[P_1 \frac{\partial F_1}{\partial x_i} + P_2 \frac{\partial F_2}{\partial x_i} + u P_3 \frac{\partial F_3}{\partial x_i} + P_4 \frac{\partial F_4}{\partial x_i} \right], \tag{26}$$

$(i = 1, 2, 3),$

$$\dot{P}_4 = x_4^{-2} [P_1 F_1 + P_2 F_2 + u P_3 F_3 + P_4 F_4]. \tag{27}$$

where (x, u) is the optimal solution of (24)-(25). Additional equations are obtained via the Hamiltonian

$$H(s, y, w) := y_4^{-1} \left(\sum_{i=1}^2 P_i(s) F_i(y_1, y_2, y_3) \right) + y_4^{-1} w P_3(s) F_3(y_1, y_2, y_3) + y_4^{-1} P_4(s) F_4(y_1, y_2, y_3) + P_4(s) w, \quad y \in \mathbb{R}^4, w \in U, \tag{28}$$

as follows:

$$\max \{H(s, x(s), u) : 0 \leq u \leq \beta\} = H(s, x(s), u(s)), \tag{29}$$

$0 \leq s \leq s_1,$

$$0 = H(s_1, x(s_1), u(s_1)), \tag{30}$$

$$H(s, x(s), u(s)) = \lambda_2, \quad (0 \leq s \leq s_1). \tag{31}$$

The principle also implies that the system of differential equations (24)-(27) involving $(x, P) \in \mathbb{R}^8$ satisfies the

additional end conditions

$$P_i(s_1) = -\lambda_1 \frac{\partial g_0(x_1(s_1), x_2(s_1), x_3(s_1))}{\partial x_i}, \quad (i = 1, 2, 3), \tag{32}$$

$$P_1(0) = -\lambda_3, \quad P_2(0) = -\lambda_4, \quad P_3(0) = -\lambda_5, \tag{33}$$

$P_4(0) = -\lambda_6, \quad P_4(s_1) = 0.$

It follows from (27), (30), and (31) that

$$\dot{P}_4 = -x_4^{-1} \dot{x}_4 P_4, \tag{34}$$

and hence

$$P_4(s) x_4(s) = P_4(s_1) x_4(s_1) = 0, \quad (0 \leq s \leq s_1). \tag{35}$$

Since $\dot{x}_4 \geq 0$, it follows from (19) that $P_4 = 0$. Now, by (29) and the fact that F_3 is negative,

$$u(s) = \begin{cases} 0, & \text{if } P_3(s) > 0, \\ \beta, & \text{if } P_3(s) < 0. \end{cases} \tag{36}$$

We show that u has no other value in its range; i.e., the solution is a bang-bang one. To prove this, it is sufficient to show that $P_3(s) = 0$ for at most finitely many points $s \in [0, s_1]$. Since u is piecewise continuous and left continuous, there exist a positive integer k and a partition $\{0 = c_0 < c_1 < \dots < c_{k-1} < c_k = s_1\}$ of $[0, s_1]$ such that $P_3(c_i) = 0$ for $1 \leq i \leq k-1$ and, on each subinterval $[c_{i-1}, c_i]$, P_3 is always nonnegative or always nonpositive $1 \leq i \leq k$. We claim $P_3(s) \neq 0$ for all $s \in (0, s_1) \setminus \{c_1, \dots, c_{k-1}\}$.

Assume $P_3(s^*) = 0$ for some $s^* \in (c_{i-1}, c_i)$. Then, in view of (30)-(31),

$$\sum_{i=1}^2 P_i(s^*) F_i(x_1(s^*), x_2(s^*), x_3(s^*)) = 0, \tag{37}$$

which implies in view of (26) that

$$\dot{P}_3(s^*) = \frac{-1}{x_4} P_1(s^*) F_2(x_1, x_2, x_3) \frac{\partial}{\partial x_3} \left(\frac{F_1(x_1, x_2, x_3)}{F_2(x_1, x_2, x_3)} \right), \tag{38}$$

where x_i ($i = 1, 2, 3, 4$) are evaluated at $s = s^*$. Since s^* is a relative extremum of P_3 , it follows that $\dot{P}_3(s^*) = 0$. Hence, in view of Fact 2.1 and the fact that $F_2 < 0$, we conclude that $P_1(s^*) = 0$ and thus $P_2(s^*) = 0$. Therefore,

$P(s^*)=0$. Now, by the uniqueness of the solution of the system (26), $P=0$ on $[c_{i-1}, c_i]$ and by continuity of P on all of $[0, s_1]$. In view of (9) and (32)-(33), $\lambda=0$; a contradiction.

The above argument yields the following facts:

$$P(s) \neq 0, \text{ for all } s \in [0, s_1], \tag{39}$$

$$\lambda_1 = -1, \tag{40}$$

$$P_3(s) \neq 0 \text{ for all } s \in [0, s_1] \setminus \{c_1, \dots, c_{k-1}\}, \tag{41}$$

$$|P_3(s)| + |\dot{P}_3(s)| \neq 0 \text{ for all } s \in (0, s_1). \tag{42}$$

By omitting those c_i 's at which u is continuous (or, equivalently, at which P_3 does not change sign), we can assume without loss of generality that $u=\beta$ on subintervals (c_{i-1}, c_i) for all odd integers i , and $u=0$, otherwise.

5. Uncoupled and Semi-Uncoupled Approximations

To find the optimal shape of the supersonic part of a gas-dynamic laser by means of Theorem 4.1, one has to find the partition nodes $c_1 < c_2 < \dots < c_k = s_1$. To find c_i 's, one has to solve the system (24)-(26) in terms of c_i 's and determine a set $\{c_1, \dots, c_k\}$ for which $g_0(x_1(c_k), x_2(c_k), x_3(c_k))$ is maximal. To simplify the computation, the number k of the nodes must be reduced. Anderson [1, pp. 48-52] suggests an uncoupling of the variables by assuming a zero rate or an equilibrium for the vibrational energies in the calculation of v from (2)-(3). Here we introduce a semi-uncoupled approximation of the model in which only *one* of the vibrational energies is uncoupled and that the approximation is used only in a *portion* of the duct.

In fact, all experiments show that the vibrational temperature and energy of mode 2 have a rapid fall shortly after the throat and soon become almost flat along the remainder of the duct. (See, for example, [1].) Thus it is better to assume there exists $s_2 < c_1$ with $c_1 - s_2$ small enough such that the vibrational energy e_2 is constant on $[s_2, s_1]$ only for the purpose of calculating v from (2)-(3). An alternative approximation model is to assume the vibrational temperature of mode 1 equals the translational temperature on $[s_2, s_1]$. By Pontryagin's principle, the restriction of (x, u) to the interval $[s_2, s_1]$ is

a solution of (24)-(25) satisfying appropriate new end conditions, and optimizing the small signal gain. Thus if x_2 is assumed to be constant (resp. if x_1 is assumed to be equal to x_3) on $[s_2, s_1]$, then one of the variables x_1 or x_2 is uncoupled in the following sense. For some $i=1$ or 2 the variable x_i disappears in the calculation of v and thus the functions $F_j (j \neq i, j=1,2,3,4)$ are now independent of x_i . The new function P_i satisfies

$$\dot{P}_i = -x_4^{-1} P_i \partial F_i / \partial x_i. \tag{43}$$

Thus

$$P_i(s) = P_i(s_1) \exp \int_s^{s_1} \frac{1}{x_4(\theta)} \frac{\partial F_i(x_1(\theta), x_2(\theta), x_3(\theta))}{\partial x_i} d\theta \tag{44}$$

which implies that P_i never changes the sign. Assume without loss of generality that $i=2$. If $k \geq 3$, then $P_3(c_1) = P_3(c_2) = 0$ and hence in view of (37), $P_1(c_1)$ and $P_1(c_2)$ have the same sign opposite to that of P_2 . (Note that $P(s) \neq 0$ for all $s \in [s_2, s_1]$. See (39).) Now, it follows from (38) that both $\dot{P}_3(c_1)$ and $\dot{P}_3(c_2)$ have the same sign; a contradiction. This implies that $k \leq 2$. The case $k=1$ is rejected by numerical observations. It remains $k=2$.

Assuming $k=2$, we have

$$x_4(s) = \begin{cases} \beta s + 1 & \text{if } 0 \leq s \leq c_1 \\ \beta c_1 + 1 & \text{if } c_1 \leq s \leq c_2 = s_1. \end{cases} \tag{45}$$

Note that, in view of (45), the gain increases with the opening angle Λ which, due to the gas detachment from the walls, is limited via (22). Thus, substituting x_4 in (24)-(25) yields $g(x_1(c_2), x_2(c_2), x_3(c_2))$ as a function of parameters c_1 and c_2 provided that the percentages X_{CO_2} , X_{N_2} and X_{H_2O} in the gas mixture as well as the reservoir temperature T_0 and pressure p_0 are known. However, one may let all these parameters vary to search for those values yielding higher small signal gains.

6. Oblique Shock Waves

The authors of [16, pp. 427-430] assume

$$-\alpha \leq \ddot{x} \leq 0 \tag{46}$$

to reduce the effect of oblique shock waves. The constraint turns \dot{x}_4 into a differentiable function and hence can be no longer obtained as a control function via Pontryagin's principle. Hence we define a new

variable

$$x_5 := \dot{x}_4 \tag{47}$$

and choose

$$u = \dot{x}_5 \tag{48}$$

as our new control function. Thus, x is augmented to a vector in \mathbb{R}^5 , and the problem becomes constrained by

$$0 \leq x_5 \leq \beta. \tag{49}$$

however, since $\dot{x}_5 \leq 0$, we will replace this constraint by end conditions

$$x_5(0) = \beta, \tag{50}$$

and

$$x_5(s_1) = 0 \tag{51}$$

if necessary. In fact we have replaced the problem with four independent problems as follows: Problem (i), $0 < x_5 < \beta$; Problem (ii), $0 < x_5$ and $x_5(0) = \beta$; Problem (iii), $x_5 < \beta$ and $x_5(s_1) = 0$; Problem (iv), $x_5(0) = \beta$ and $x_5(s_1) = 0$. The defining set for the new control u is $U = [-\alpha, \alpha]$. The end vector e now belongs to $[0, \infty)^{12}$ and the transversal function P has values in \mathbb{R}^5 . Here $\phi(e)$ is the same as in (23) for Problem (i). For Problem (ii), $\phi(e)$ has an additional component $x_5(s_0) - \beta$; for Problem (iii), $\phi(e)$ has an additional component $x_5(s_1)$; finally, for Problem (iv), $\phi(e)$ has additional components $x_5(s_0) - \beta$ and $x_5(s_1)$. The vector λ has the same number of components as $\phi(e)$ in each case. Equations (24)-(27) remain valid, except of course, u must be replaced by x_5 . The component P_5 satisfies

$$\dot{P}_5 = -x_4^{-1} P_3 F_3 - P_4. \tag{52}$$

The Hamiltonian H is accordingly modified, and (32)-(33) still hold. Moreover, $P_5(0) = P_5(s_1) = 0$ for Problem (i); $P_5(0) = -\lambda_7$ and $P_5(s_1) = 0$ for Problem (ii); $P_5(0) = 0$ and $P_5(s_1) = -\lambda_7$ for Problem (iii); $P_5(0) = -\lambda_7$ and $P_5(s_1) = -\lambda_8$ for Problem (iv). However, (34)-(36) are changed to

$$\dot{P}_4 = -x_4^{-1} \dot{x}_4 P_4 - u P_5, \tag{53}$$

$$x_4(s) P_4(s) = \int_s^{s_1} u(\theta) P_5(\theta) d\theta, \tag{54}$$

and

$$u(s) = \begin{cases} 0, & \text{if } P_5(s) > 0, \\ -\alpha, & \text{if } P_5(s) < 0. \end{cases} \tag{55}$$

Again, here, there exists a partition $\{0 = c_0 < c_1 < \dots < c_k = s_1\}$ such that on each subinterval $(0, s_1]$, either $P_5 = 0$ or u has one of the constant values 0 or $-\alpha$. (We assume without loss of generality that u does not have the same constant values on adjacent subintervals.) All we can show in this case, without any uncoupling approximation, is that the normalized area x_4 is either linear or parabolic on the last subinterval, and if it is linear on $(c_{k-1}, s_1]$, then it must be parabolic on $(c_{k-2}, c_{k-1}]$. To show this, assume $P_5 = 0$ on $(c_{k-1}, s_1]$. By (52)-(54), $P_3 = P_4 = 0$ on $(c_{k-1}, s_1]$. Now, the argument leading to (39), implies that $P = 0$ on $(c_{k-1}, s_1]$ and hence everywhere. This, again, implies that $\lambda = 0$; a contradiction. Next, assume $u = 0$ on $(c_{k-1}, s_1]$. If $P_5 = 0$ on $(c_{k-2}, c_{k-1}]$, $u P_5 = 0$ on $(c_{k-1}, s_1]$ and hence $P_4 = 0$ on $(c_{k-2}, s_1]$. Thus, $P_3 = 0$ and, again, $P = 0$ on $(c_{k-2}, c_{k-1}]$, which leads to the contradiction $\lambda = 0$. Hence, $u = -\alpha$ on $(c_{k-2}, c_{k-1}]$.

To simplify the problem, we use an uncoupled approximation, but this time on both vibrational energies e_1 and e_2 throughout the interval $[s_0, s_1]$. The exact nature of the uncoupling is not important to be known; the whole idea is to assume the speed v and the pressure p can be calculated from (2)-(3) explicitly in terms of x_3 . To do this, we may, for example, assume throughout the supersonic part that x_2 , or equivalently e_2 , is constant, and that x_1 is in equilibrium, or equivalently $e_1 = E_1(x_3)$. This is justified by the fact that the vibrational temperature of mode 2 has a very slow equilibration while that of mode 1 equilibrates fast. (See the various experiments in [1].) Then one can calculate v and x_4 in terms of x_3 and substitute in the governing equations. The new governing equations will be of the following forms:

$$\dot{x}_i = F_i(x_i, x_3), \quad (i = 1, 2) \tag{56}$$

$$\dot{x}_3 = x_5 F_3(x_3), \tag{57}$$

$$\dot{x}_5 = u, \tag{58}$$

and the transversal vector \mathcal{P} satisfies

$$\dot{\mathcal{P}}_i = -\mathcal{P}_i \frac{\partial \mathcal{F}_i}{\partial x_i}(x_i, x_3), \quad (i=1,2), \quad (59)$$

$$\dot{\mathcal{P}}_3 = -\mathcal{P}_1 \frac{\partial \mathcal{F}_1}{\partial x_3}(x_1, x_3) - \mathcal{P}_2 \frac{\partial \mathcal{F}_2}{\partial x_3}(x_2, x_3) \quad (60)$$

$$- \mathcal{P}_3 x_3 \mathcal{F}'_3(x_3),$$

$$\dot{\mathcal{P}}_5 = -\mathcal{P}_3 \mathcal{F}'_3(x_3). \quad (61)$$

As it is seen, the components x_4 and \mathcal{P}_4 are not present in the equations and one can continue by an argument similar to the one given in the proof of Theorem 4.1 that u is either 0 or $-\alpha$ on each subinterval $(c_{i-1}, c_i]$, $(i=1,2,\dots,k)$. Assume $\mathcal{P}_3(\theta) = 0$ for some $\theta \in [0, s_1]$. By (32) and (59), \mathcal{P}_1 is always negative and hence, in view of (38), $\mathcal{P}_3(\theta) > 0$. This implies that θ is unique. Now, if $k \geq 3$, then $\mathcal{P}_3(c_{i-1}) = \mathcal{P}_3(c_i) = \dot{\mathcal{P}}_3(\theta) = \mathcal{P}_3(\theta) = 0$ for some $i = 1, 2, \dots, k$ and some $\theta \in (c_{i-1}, c_i)$. (See (61).) Since θ is unique, k must be 3 and then $\mathcal{P}_5(0) \neq 0$ and $\mathcal{P}_5(s_1) \neq 0$. This means that $x_5(0)$ and $x_5(s_1)$ are not free and hence $x_5(0) = \beta$ and $x_5(s_1) = 0$ (i.e., Problem (iv)). Moreover, \mathcal{P}_3 is negative on $[0, \theta)$ and positive on $(\theta, s_1]$. Thus, \mathcal{P}_3 is decreasing on $[0, \theta]$ and increasing on $[\theta, s_1]$. This, in turn, implies that \mathcal{P}_3 is positive on $[0, c_1) \cup (c_2, s_1]$ and negative on (c_1, c_2) . Hence, it follows from (55) that

$$x_4(s) = \begin{cases} \beta s + 1, & \text{if } 0 \leq s \leq c_1, \\ -\frac{1}{2} \alpha (s - c_1)^2 + \beta (s - c_1) + \beta c_1 + 1, & \text{if } c_1 \leq s \leq c_2, \\ -\frac{\beta^2}{2\alpha} + \beta c_1 + 1, & \text{if } c_2 \leq s \leq s_1, \end{cases} \quad (62)$$

and $c_2 = c_1 + \beta/\alpha$.

Next, if $k = 2$, it can be verified that x_4 consists of either a line of slope β followed by a parabola or a parabola followed by a horizontal line. Finally, if $k = 1$, then x_4 is a portion of a parabola.

However, our numerical observations reveal that $k = 3$ and x_4 is of the form (62). (See Fig. 2.)

7. Discussion

We showed that, given a fixed reservoir condition and gas mixture, to obtain a greater small signal gain, one must increase the nozzle opening angle. However, due to the gas detachment from the walls, there is an upper bound on the opening angle. We also showed that for a given opening angle Λ and a throat height h^* , the shape of the supersonic part of a GDL yielding a maximal small signal gain is described via its normalized cross sectional area $x_4(s) = A(s)/A^*$ as follows: The length of the duct is partitioned into k subintervals on which $x_4(s)$ is linear with slopes $\beta (= (2/h^*) \tan(\Lambda/2))$ and 0, alternatively. Then a semi-uncoupled approximation model was introduced in which it was assumed that either the vibrational temperature of mode 1 is in equilibrium, or the vibrational energy of mode 2 is constant on some interval containing the last $k-1$ subintervals as well as a small portion of the first subinterval. (This means that we did not assume any zero vibrational rate or infinite-rate vibrational equilibrium in the area close to the throat. Also, only one of these approximations is assumed on the last $k-1$ subintervals.) Using such approximating models, we showed that $k \leq 2$. Based on the above theoretical observations, we have calculated the small signal gain g_0 and the area ratio x_4 for opening angle 80° , $h^* = 0.25$ mm, $p_0 = 20$ atm, $T_0 = 1220^\circ\text{K}$, $X_{CO_2} = 0.1$, $X_{H_2O} = 0.05$, $X_{N_2} = 0.85$. We notice that $k = 2$; that is, the nozzle consists of a wedge of opening angle 80° and a channel of area ratio 107. The same general shape can be obtained if the above initial conditions are changed reasonably. If the optimal gain and final area ratio are drawn against the various values of the opening angle, one can observe that the optimal gain increases with the opening angle.

To remove sharp points for oblique shock wave considerations, we showed, theoretically, that, in the fully uncoupled approximating models, the nozzle is the same except that the wedge and the channel are joined smoothly by parabolic surfaces. Figure 2 shows the small signal gain g_0 along the nozzle with opening angle 80° , $h^* = 0.25$ mm, $p_0 = 20$ atm, $T_0 = 1220^\circ\text{K}$, $X_{CO_2} = 0.1$, $X_{H_2O} = 0.05$, $X_{N_2} = 0.85$ and $\alpha = 20$. Also Figure 3 shows the optimal gain and final area ratio vs. the opening angle with the same parameters. The effect of the various parameters p_0 , and the opening angle on the optimal gain is shown in Figures 4 and 5. (Here, again, $\alpha = 20$.) We note that the optimal gain decreases as the stagnation pressure and/or X_{H_2O} increases. In Figure 6, the effect of α on the final area ratio is demonstrated. For values of $\alpha \geq 10$, one can assume that $\alpha = +\infty$ and the parabolic surfaces virtually disappear.

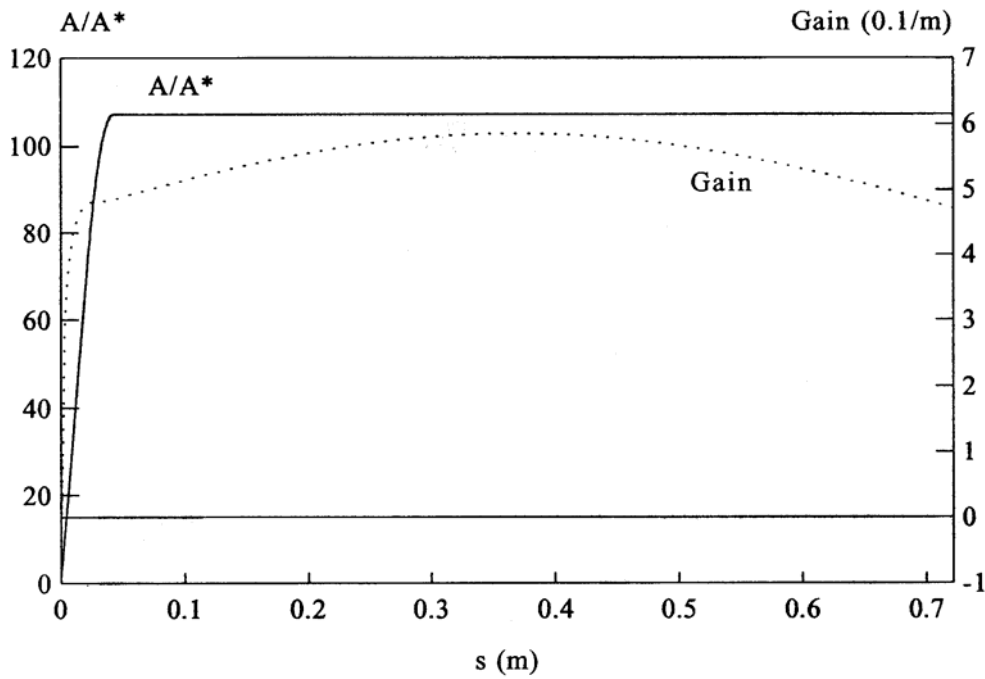


Figure 2. Optimal gain and nozzle shape in smooth case. ($p_0 = 20 \text{ atm}$, $T_0 = 1220^\circ\text{K}$, $X_{CO_2} = 0.1$, $X_{N_2} = 0.85$, $X_{H_2O} = 0.05$, Opening angle = 80° , $h^* = 0.25 \text{ mm}$, $\beta = 6712$.)

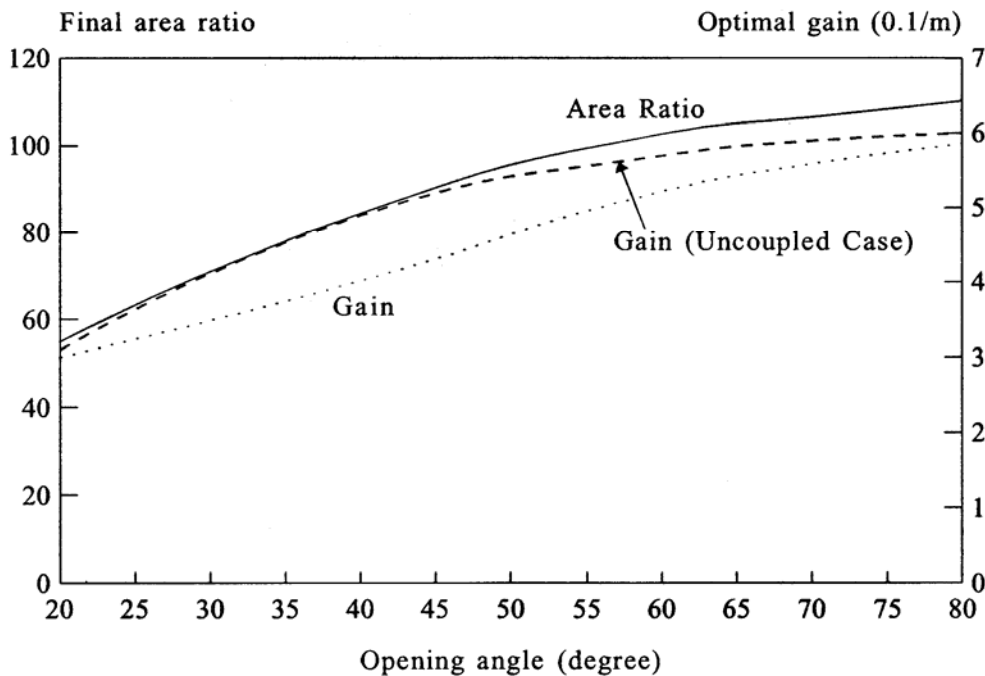


Figure 3. Optimal gain and final area ratio in smooth case versus opening angle. ($p_0 = 20 \text{ atm}$, $T_0 = 1220^\circ\text{K}$, $X_{CO_2} = 0.1$, $X_{N_2} = 0.85$, $X_{H_2O} = 0.05$.)

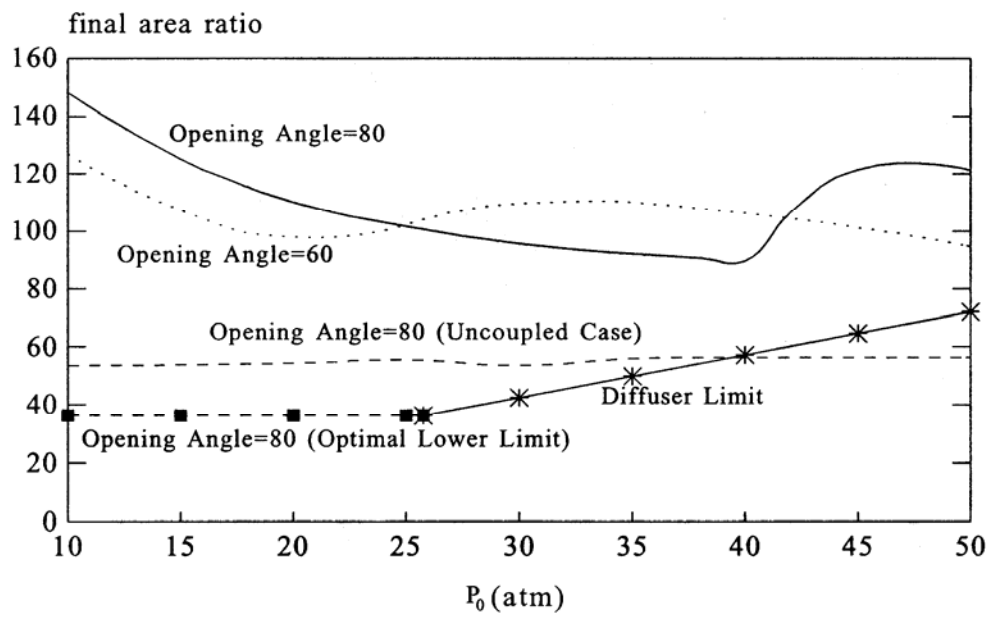


Figure 4. Effect of stagnation pressure on the final area ratio in smooth case. ($T_0 = 1220^\circ\text{K}$, $X_{CO_2} = 0.1$, $X_{N_2} = 0.85$, $X_{H_2O} = 0.05$.)

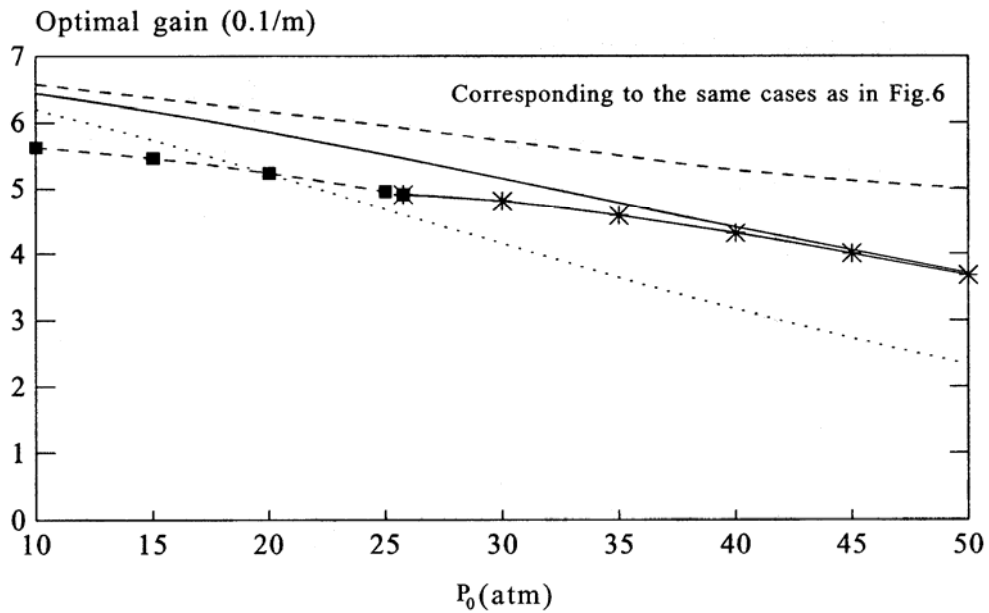


Figure 5. Effect of stagnation pressure on the optimal gain in smooth case. ($T_0 = 1220^\circ\text{K}$, $X_{CO_2} = 0.1$, $X_{N_2} = 0.85$, $X_{H_2O} = 0.05$.)

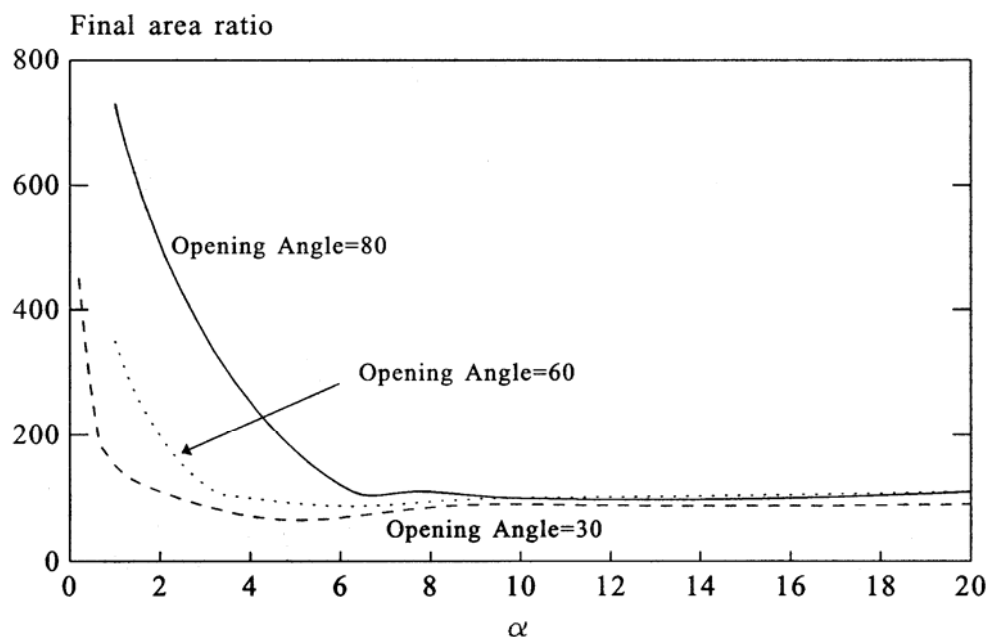


Figure 6. Effect of α on the final area ratio in smooth case. ($p_0 = 20$ atm, $T_0 = 1220^\circ\text{K}$, $X_{\text{CO}_2} = 0.1$, $X_{\text{N}_2} = 0.85$, $X_{\text{H}_2\text{O}} = 0.05$.)

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