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DEPARTMENT OF MATHEMATICAL SCIENCES
COLLEGE OF SCIENCES
OLD DOMINION UNIVERSITY
NORFOLK, VIRGINIA 23529

Old Dominion University Research Foundation

THEORETICAL STUDIES OF SOLAR LASERS AND CONVERTERS

By

John H. Heinbockel, Principal Investigator

Progress Report
For the period January 1988 to July 1988

Prepared for the
National Aeronautics and Space Administration
Langley Research Center
Hampton, Virginia 23665

Under
Research Grant NAG-1-757
Dr. Robert C. Costen, Technical Monitor
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ABSTRACT.

The previously constructed one dimensional model for the simulated operation of an iodine laser assumed that the perflouroalkyl iodide gas $n - C_3F_7I$ was incompressible. The present study removes this simplifying assumption and considers $n - C_3F_7I$ as a compressible fluid.

Introduction.

The iodine laser being modeled uses the gas $n - C_3F_7I$ flowing in a cylindrical tube. As a first approximation to the chemical kinetics and flow it was assumed that the gas was incompressible and operating at a constant temperature. To remove these simplifying assumptions we consider the effects of fluid density variation as a function of both pressure and temperature in the flow. In particular we have added to our previous model:

(i) An equation of state.

We assume the equation of state of an ideal gas and write

$$P = \eta RT \tag{1}$$

where P is the gas pressure $[Pa]$, η is the gas density $[Kg/m^3]$, T is the temperature $[^\circ K]$, and $R = R^*/296\,[J/Kg^\circ K]$, and R^* is the gas constant, $R^* = 8.317\ [J/mole\ ^\circ K]$. For $n - C_3F_7I$ we use the value of 296 $Kg/mole$ to convert R^* to R.

(ii) Continuity equation.

The continuity equation expressing the conservation of mass flow can be represented

$$\frac{\partial \eta}{\partial t} + div\,(\eta \vec{V}) = 0 \tag{2}$$

where η is the fluid density $[Kg/m^3]$, and $\vec{V}$ is the fluid velocity $[m/s]$. For steady state conditions and a flow in the axial direction we let $\vec{V} = \omega \hat{k}$ and reduce the continuity equation to the form

$$\frac{\partial}{\partial z}(\eta\omega) = 0 \tag{3}$$

An integration of this equation gives

$$\eta\omega = c_1 \tag{4}$$

where c_1 is a constant of integration.

(iii) Momentum equation.

The momentum equation for a control volume having a mass $\eta d\tau$, where $d\tau$ is an element of volume, is given by

$$\vec{M} = \iiint \vec{V}\eta \, d\tau \tag{5}$$

From Newton's second law we have

$$\vec{F} = \frac{D\vec{M}}{Dt} = \frac{D}{Dt}\iiint \vec{V}\eta \, d\tau \tag{6}$$

where D/Dt is the material derivative. We have

$$\frac{D\vec{M}}{Dt} = \iint \vec{V}\left(\eta\vec{V}\cdot d\vec{\sigma}\right) + \frac{\partial}{\partial t}\iiint \vec{V}\eta \, d\tau \tag{7}$$

where $d\vec{\sigma}$ is an element of surface area. The surface integral term in (7) represents the efflux of momentum through the control volume and the volume integral term in (7) represents the change in momentum inside the control volume. Using the Gauss–divergence theorem we can change the surface integral to a volume integral and write

$$\iint_S \vec{V}(\eta\vec{V}\cdot d\vec{\sigma}) = \iiint \left[\nabla\cdot\eta\vec{V}\vec{V}\right] d\tau \tag{8}$$

Then the momentum equation becomes

$$\vec{F} = \frac{D\vec{M}}{Dt} = \iiint div\,(\eta\vec{V}\vec{V})\, d\tau + \frac{\partial}{\partial t}\iiint (\eta\omega\hat{k})\, d\tau \tag{9}$$

where $\vec{V}\vec{V}$ is the dyadic $\omega^2\hat{k}\hat{k}$ for $\vec{V} = \omega\hat{k}$, and

$$\nabla\cdot\eta\vec{V}\vec{V} = \frac{\partial}{\partial z}\left(\eta\omega^2\right)\hat{k} \tag{10}$$

We also make the substitution $\vec{F} = \iiint \vec{f}\, d\tau$ where $\vec{f}$ is the average force per unit volume

as this allows the momentum equation to be written in the form

$$\vec{F} = \iiint \vec{f}\, d\tau = \frac{D\vec{M}}{Dt} = \iiint \left[\frac{\partial}{\partial t}(\eta\omega)\hat{k} + \frac{\partial}{\partial z}(\eta\omega^2)\hat{k}\right] d\tau \tag{11}$$

Neglecting viscosity and using $\vec{f} = -\nabla P$ as the average force per unit volume which is due to the fluid pressure P , we have

$$-\frac{\partial P}{\partial z} = \frac{\partial}{\partial t}(\eta\omega) + \frac{\partial}{\partial z}(\eta\omega^2) \tag{12}$$

From equation (4) we use $\eta\omega = c_1$ and examine the steady state form of the equation (12) to obtain

$$-\frac{\partial P}{\partial z} = c_1\frac{\partial \omega}{\partial z} \tag{13}$$

Integrating this equation gives

$$P + c_1\omega = c_2 \tag{14}$$

where c_2 is a constant of integration.

(iv) Energy Equation.

In terms of the specific enthalpy h per unit mass, the energy equation for the fluid flow is

$$\eta \frac{Dh}{Dt} = \frac{DP}{Dt} + \kappa \nabla^2 T + q \tag{15}$$

where P is the pressure, T is the temperature, κ is the thermal conductivity and $q = q(z)$ is the radiation heat flux. In one dimension this can be written

$$\eta \frac{\partial h}{\partial t} + \eta\omega \frac{\partial h}{\partial z} = \frac{\partial P}{\partial t} + \omega \frac{\partial P}{\partial z} + \kappa \frac{d^2T}{dz^2} + q \tag{16}$$

The specific enthalpy h can be expressed in terms of the specific heat at constant pressure and

$$h = C_p T \tag{17}$$

Using the relation

$$C_p^* - C_v^* = R^* \tag{18}$$

where $R^* = 8.317\ [J/mole - {}^\circ K]$ is the universal gas constant.

The specific heat at constant pressure C_p^* can be expressed in terms of the specific heat at constant volume C_v^*. We use the numerical data

Temperature $^\circ K$	C_v^* *for* $C_3F_7I\ [J/mole\,^\circ K]$
298.15	146
400.00	169
500.00	186

(19)

and assume that C_v^* can be obtained from the relation

$$C_v^* = C_v^*(T) = \alpha_v \exp(\beta_v (T - 300)), \qquad 298.15 \le T \le 500 \tag{20}$$

By applying a least square's fit of the data with the exponential curve in (20) we obtain the best fit parameter values of

$$\alpha_v = 147.23 \qquad \beta_v = 0.0012 \tag{21}$$

This gives the steady state energy equation

$$\eta\omega[C_v(T) + R]\frac{dT}{dz} = \omega \frac{dP}{dz} + \kappa \frac{d^2T}{dz^2} + q(z) \tag{22}$$

where $C_v(T)$ is the correct dimensional form of C_v^*.

Having neglected the viscosity terms, we also neglect the effect of thermal conductivity and integrate the equation

$$c_1[C_v(T) + R]dT + \omega c_1 d\omega - q(z)dz = 0 \tag{23}$$

to obtain

$$c_1 \int C_v(T)dT + c_1 R(T - 300) + \frac{c_1}{2}\omega^2 - Q(z) = c_4 \tag{24}$$

where

$$Q(z) = \int q(z)\,dz$$

and c_4 is a constant of integration.

Implementation of Model.

In order to compare and verify the computer model with laboratory data it is assumed that we are given the boundary conditions as $z = 0$ and $z = L$. We use the subscript 0 to denote values at $z = 0$ and subscript L to denote the values at $z = L$. By setting $z = 0$ we obtain:

$$from\,(4) \quad c_1 = \eta_0 \omega_0$$
$$from\,(14) \quad c_2 = P_0 + c_1 \omega_0$$

from (24) we have

$$c_4 = c_1 \left[R(T_0 - 300) + \int C_v(T)\, dT \right] + \frac{c_1}{2}\omega_0^2$$

Assuming that $q = q(z)$ can be represented by a constant, at $z = L$ we obtain from the equation (24) the relation

$$q_0 = \frac{1}{z_1} \left\{ c_1 \left[R(T_L - 300) + \int C_v(T)\, dT \right] + \frac{c_1}{2}\omega_L^2 - c_4 \right\}$$

Knowing the values of the above constants the temperature, density, pressure and flow rate as a function of distance z can be calculated as follows:

From the equation of state we can write

$$P = \eta RT$$

and multiplication by ω gives

$$P\omega = \eta \omega RT = c_1 RT$$

Using the relation (14) in the above equation gives

$$(c_2 - c_1 \omega)\omega = c_1 RT$$

or

$$T = \frac{c_2 \omega - c_1 \omega^2}{c_1 R} \tag{25}$$

We also use the scale factors

$$SF_1 = \frac{10^3}{296} \quad mole/Kg \qquad \text{and} \qquad SF_2 = \frac{1.01325(10^5)}{760} \quad (N/m^2)/Torr \tag{26}$$

where applicable to insure all equations balance dimensionally.

For

$$Q(z) = \begin{cases} q_0 z, & 0 < z < z_1 \\ q_0 z_1, & z_1 < z < L \end{cases} \tag{27}$$

We may then solve for $\omega = \omega(z)$ such that the energy equation

$$F(\omega) = c_1 \int C_v(T)\, dT + c_1 R(T - 300) + \frac{c_1}{2}\omega^2 - Q(z) - c_4 = 0 \tag{28}$$

is satisfied where T is determined by the relation (25). Since this is a nonlinear equation, the method of interval halving is used. The value of ω is changed until $F(\omega)$ changes sign and then interval halving is used until the desired solution accurracy is obtained. The temperature T is then determined from (25), the density is obtained from the relation (4) and the pressure is obtained from the relation (1). We then have the flow rate, temperature, pressure and density as functions of distance z.

Reaction Rates.

The reaction rate coefficients

$$k_1, k_2, k_3, k_43, k_5, k_6, k_7, k_8,$$
$$c_1, c_2, c_3, c_4, c_5, c_6,$$
$$Q_1, Q_2, Q_3, Q_4, Q_5$$

which occur in the chemical kinetics associated with the iodine laser can be assumed to vary with temperature. Various assumptions can be made concerning the effects of temperature on these rate coefficients. Various Arrenius type temperature variation effects can be modeled using one or more of the following expressions:

$$K = k_0 e^{\beta(T-T_0)}$$
$$K = k_0 e^{\beta/T}$$
$$K = k_0 T^{-N}$$
$$K = k_0 k T^{-N} e^{\beta/T}$$
$$K = k_0 T^{-N} e^{\beta/T^m}$$

Since the coefficients in these expressions are not known, as a first approximation to temperature on the rate coefficients, we will keep most of the rate coefficients constant.

Incompressible flow model.

The incompressible flow model was presented in the previous progrsss report (reference 2). Nominal results from that model are illustrated in the figures 1 through 5 for various values of the flow rate ω. Values of ω used in these graphs are:

$$\omega = 750., 1750., 2750., 5500. \quad cm/s$$

while other parameters were held constant. These other parameters were:

$$P = 23.5 \text{ Torr},$$
$$R_1 = .95848 \text{ reflectivity at left end of the tube},$$
$$R_2 = .81634 \text{ reflectivity at right end of the tube},$$
$$\text{concentration} = 1267 \text{ (peak concentration in solar constants.)}$$

Both the incompressible and compressible flow models are being modified to include temperature effects. Also an analysis by R.C. Costen of the pumping photon density is being studied and incorporated into the model. This analysis is given in the Appendix A along with figures of the results therein.

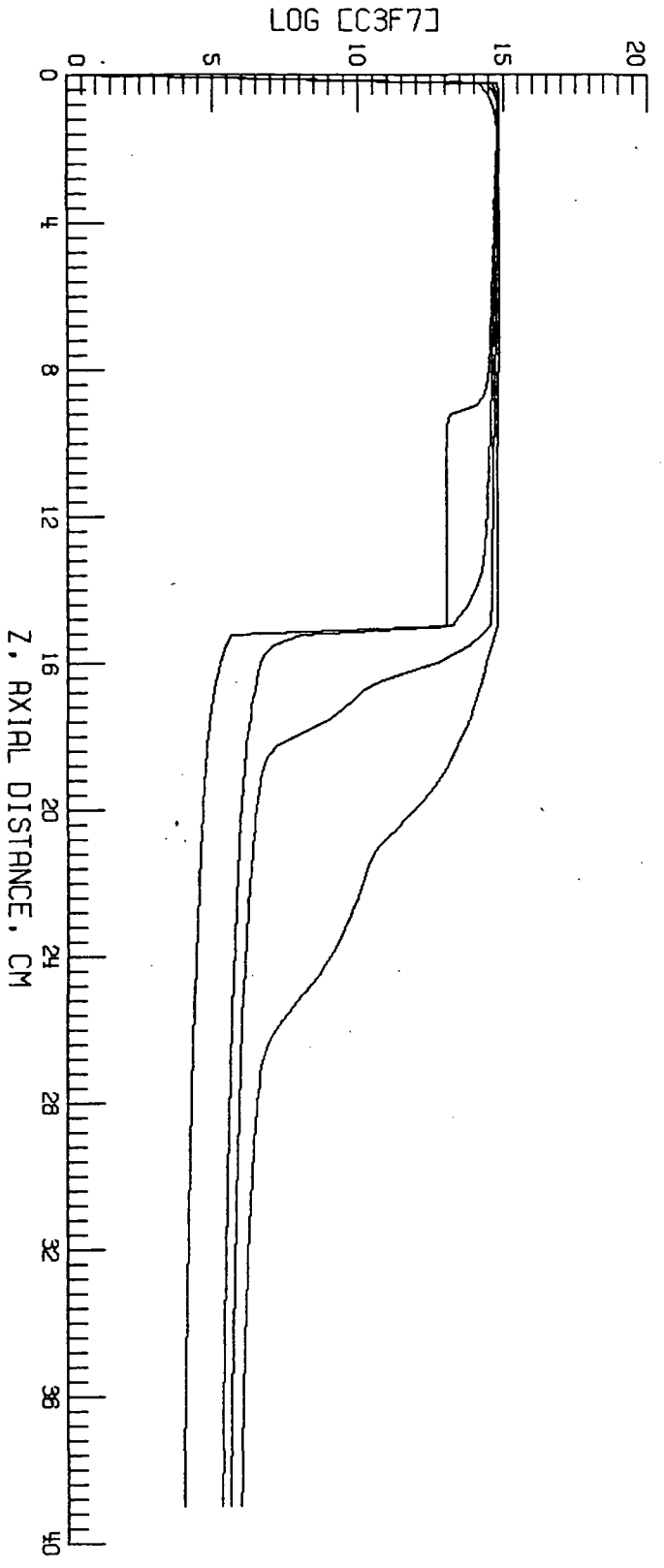
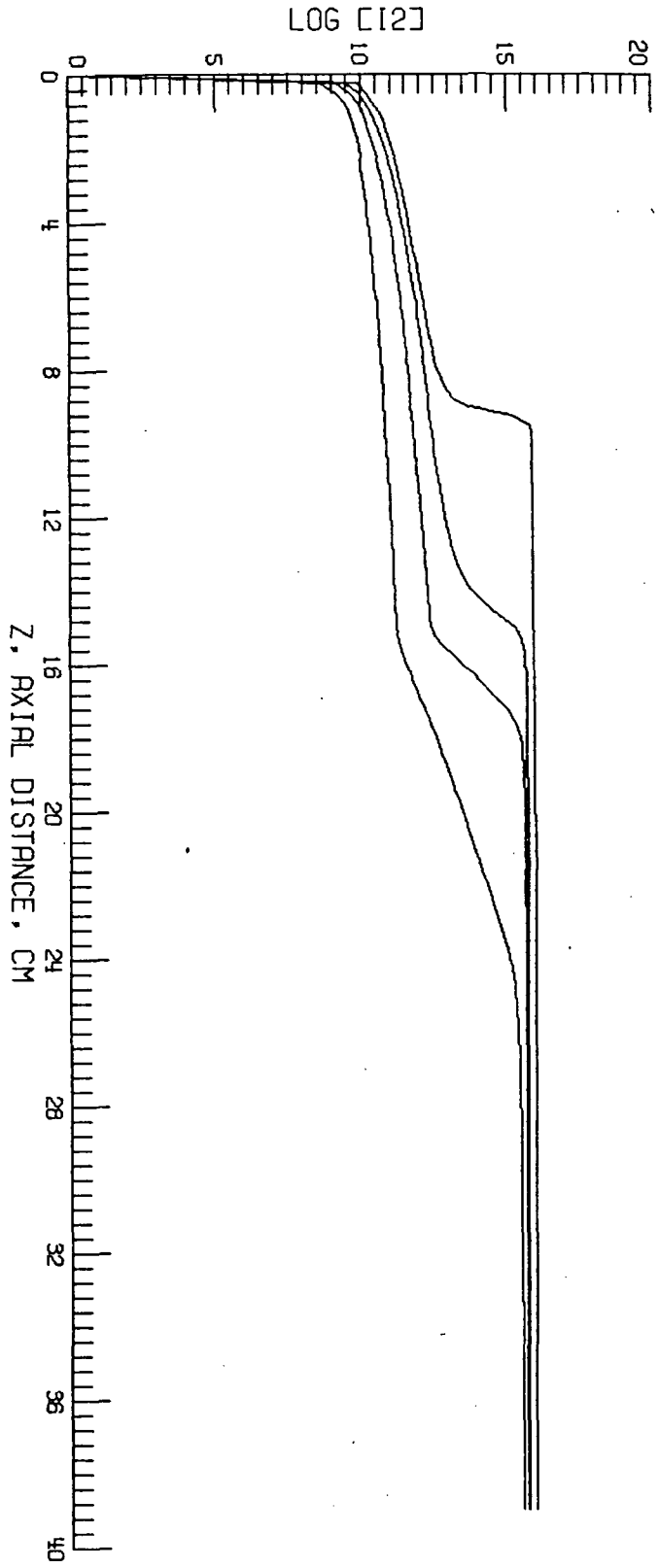
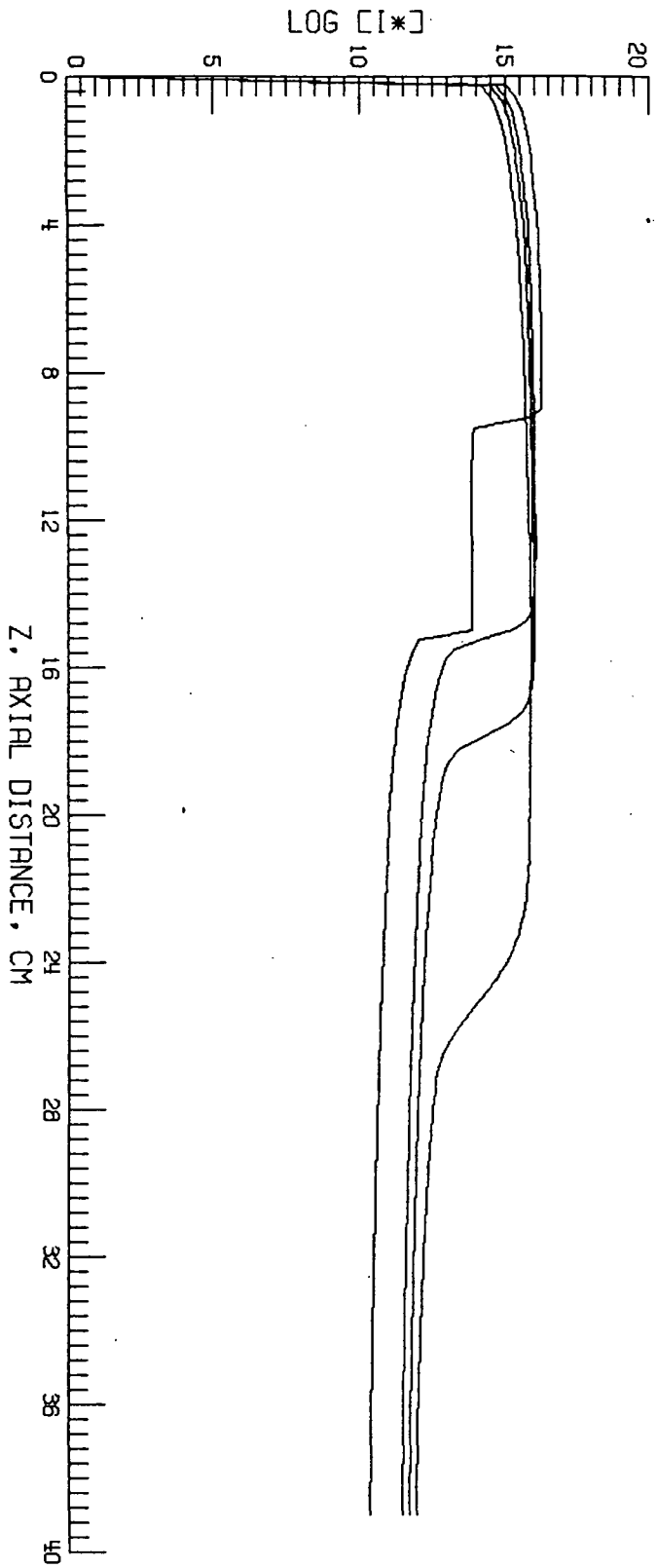


Figure 1. Log (C_3F_7) vs axial distance.



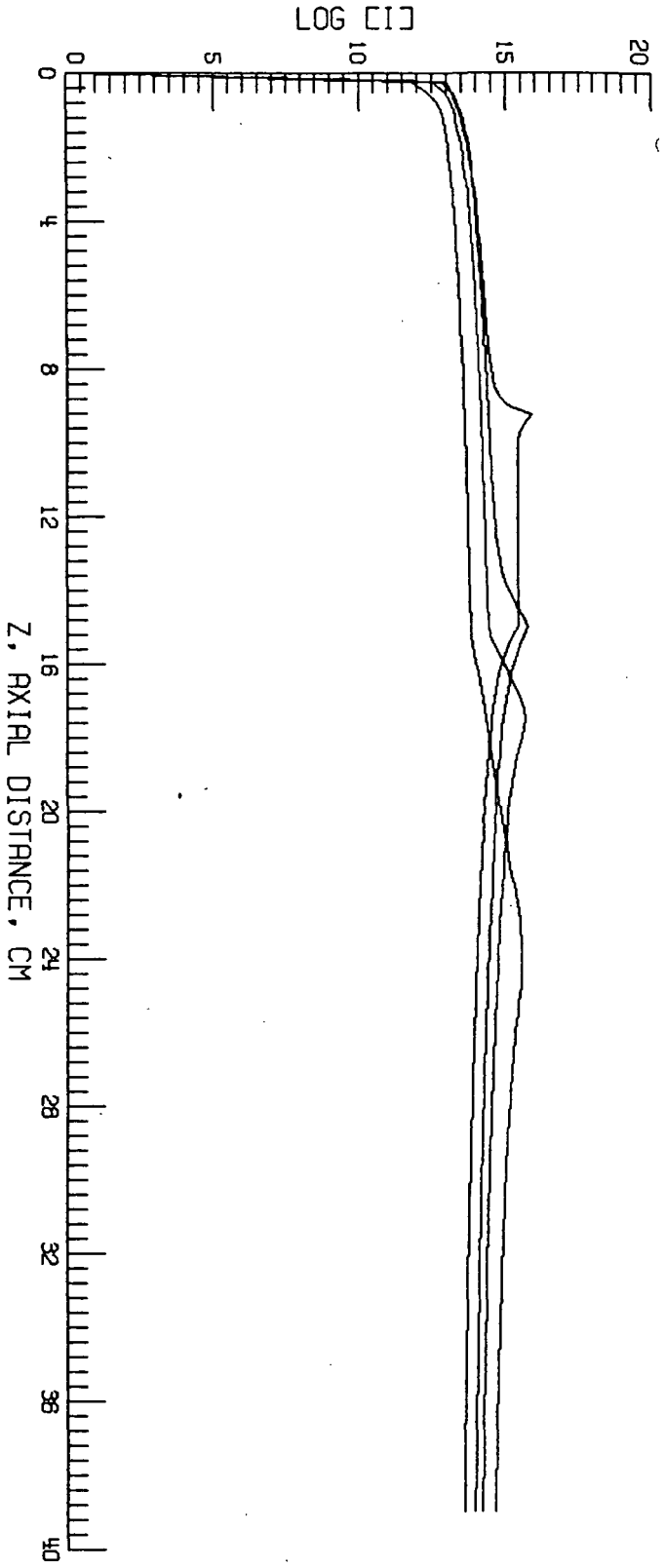
INFOPLT 2.

Figure 2. Log (I_2) vs axial distance.



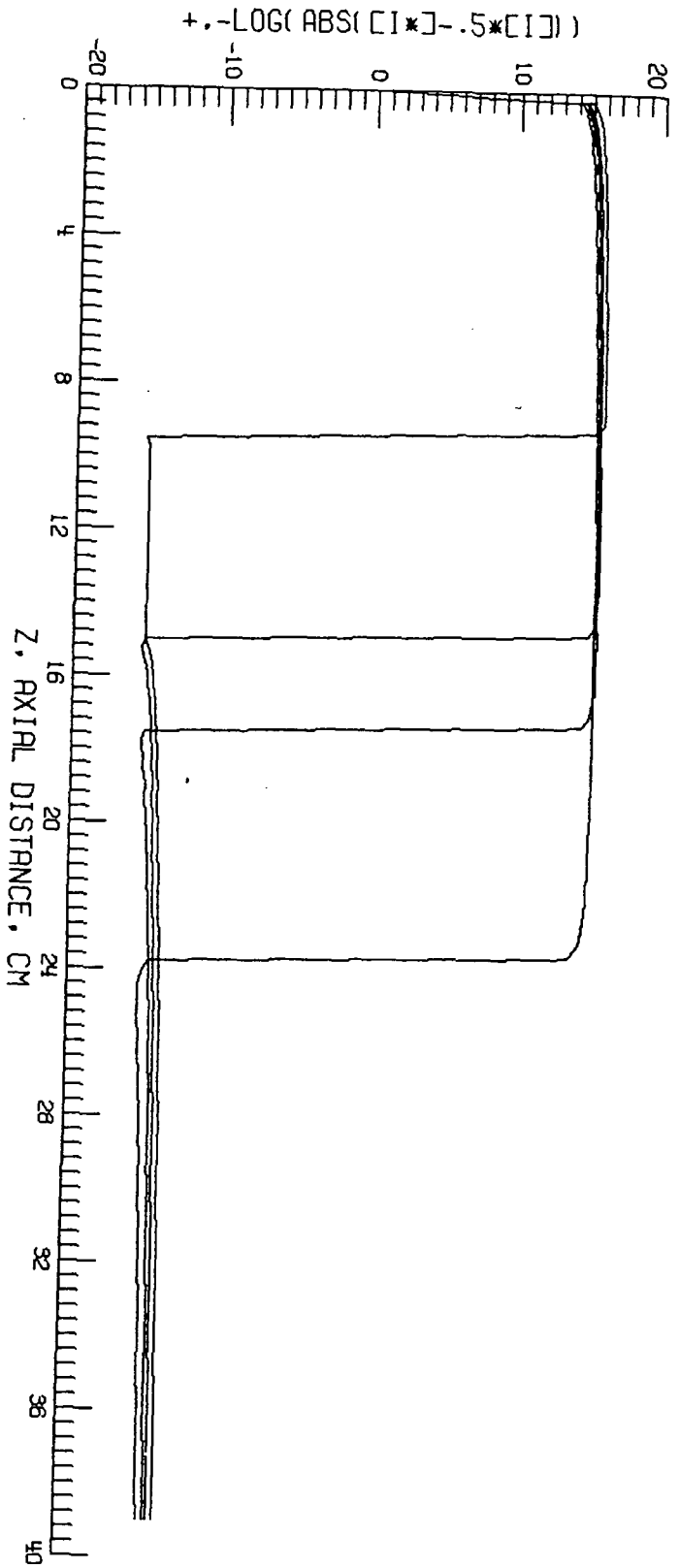
INFOPLT 3.

Figure 3. Log (I*) vs axial distance.



INFOPLT 4.

Figure 4. Log (I) vs axial distance.



INFOPLT 5.

Figure 5. $\pm\text{Log}|1*-\frac{1}{2}I|$ vs axial distance.

References

1. R.J. DeYoung, G.H. Walker, M.D. Williams, G.L. Schuster, E.J. Conway, Preliminary Design and Cost of a 1–Megawatt Solar Pumped Iodide Laser Space– to–Space Transmission Station, NASA TM 4002, September 1987.
2. J.H. Heinbockel, Theoretical Studies of Solar Lasers and Converters, Progrsss Report. Research Grant NAG–1–757, Old Dominion University Research Foundation, January 1988.

Appendix A

Pumping Photon Density within Absorbing Lasant Gas
by R.C. Costen

Assumptions: There is a 2-D cylindrical geometry which is treated as a black body cavity.

A. Consider the relation of 2-D surface brightness $B_2(W/m^2)$ to the 2-D surface flux $F_2(W/m^2)$. Consider a one meter depth of a cylindrical cavity of arbitrary shape as illustrated in the figure. A.1

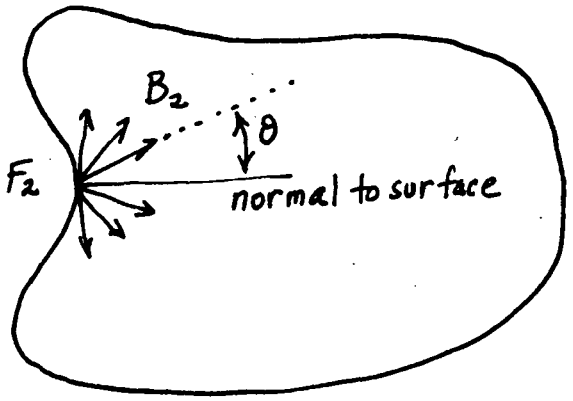


Figure A.1 Cylindrical geometry

We have

$$F_2 = \int_{-\frac{\pi}{2}}^{\frac{\pi}{2}} B_2 \cos\theta \, d\theta = 2B_2$$

W per m of perimeter entering the cavity per m of depth.

B. Determination of the pumping photon density at an interior point resulting from a length dL of perimeter.

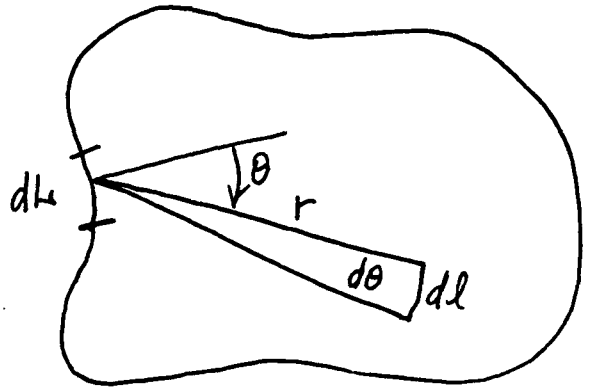


Figure A.2 Density at an interior point

The power in $d\theta$ due to a length dL is given by

$$B_2 \cos\theta \, dL \, d\theta$$

W in $d\theta$ per unit depth. This power (J/s) is due to the photons moving at the velocity of light c (m/s) The energy density in $d\theta$ per m of depth is

$$\frac{B_2}{c} \cos\theta \, dL \, d\theta \qquad (J/m)$$

Using $d\theta = \frac{dL}{r}$ and noting that the photon energy density $d\rho_2$ due to dL is given by

$$d\rho_2 = \frac{B_2}{cr} \cos\theta \, dL \qquad (J/m^2)$$

per m depth. For an absorbing gas we have

$$d\rho_2 = \frac{B_2}{cr} \exp(-\frac{r}{\delta}) \cos\theta \, dL \qquad (J/m^2)$$

per m depth and where δ, (m) is the absorption length.

C. 2–D Circular cylinder with absorbing gas and uniform incident flux F_2.

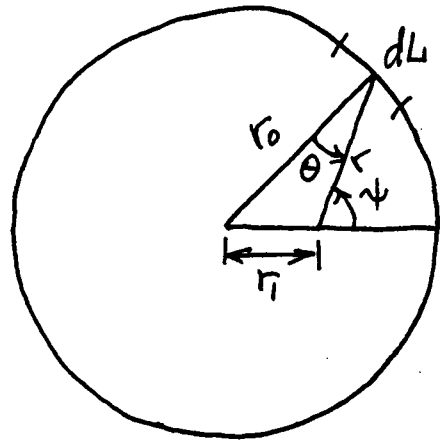


Figure A.3 Cylindrical geometry

At the point P we have due to dL that

$$d\rho = \frac{F_2}{2cr} e^{-\frac{r}{\delta}} \cos\theta \, dL \qquad (J/m^2)$$

per m of depth. Using

$$\frac{\cos\theta}{r} dL = d\psi$$

we can write

$$d\rho = \frac{F_2}{2c} e^{-\frac{r}{\delta}} \, d\psi$$

or

$$\rho = \frac{F_2}{2c} \int_0^{2\pi} e^{-\frac{r}{\delta}} \, d\psi = \frac{F_2}{c} \int_0^{\pi} e^{-\frac{r}{\delta}} \, d\psi \qquad (J/m^2)$$

per m of depth. Using the law of cosines

$$r = -r_1 \cos\psi + \sqrt{r_0^2 - r_1^2 \sin^2\psi}$$

we have

$$\rho = \frac{F_2}{c} \int_0^{\pi} \exp\left(\frac{1}{\delta}(r_1 \cos\psi - \sqrt{r_0^2 - r_1^2 \sin^2\psi})\right) d\psi$$

Changing r_1 to r the pumping photon density is given by:

$$\rho(r|r_0, \delta) = \frac{F_2}{c} \int_0^{\pi} \exp\left(\frac{1}{\delta}(r_1 \cos\psi - \sqrt{r_0^2 - r_1^2 \sin^2\psi})\right) d\psi$$

in J/m^2 per m of depth.

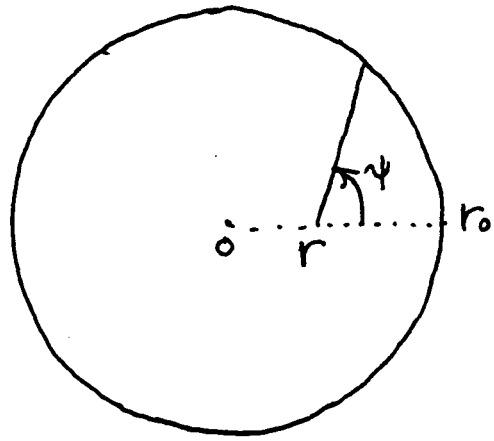


Figure A.4 Geometry

D. Average pumping photon density

The average pumping photon density is given by

$$< \rho(r_0, \delta) >= \frac{1}{\pi r_0^2} \int_0^{r_0} dr\, 2\pi r \rho(r|r_0, \delta)$$

Letting $s = r/\delta$ where $s_0 = r_0/\delta$ is the laser tube radius per absorption length, we have

$$\begin{aligned} \rho(r|r_0, \delta) &= \frac{f_2}{c} \int_0^{\pi} \exp(s\cos\psi - \sqrt{s_0^2 - s^2\sin^2\psi})\, d\psi \\ &= \rho(s, s_0) \end{aligned}$$

and

$$\begin{aligned} < \rho(r_0, \delta) > &= \frac{\delta^2}{\pi r_0^2} \int_0^{\frac{r_0}{\delta}} d\left(\frac{r}{\delta}\right) 2\pi \left(\frac{r}{\delta}\right) \rho(s, s_0) \\ &= \frac{2}{s_0^2} \int_0^{s_0} ds\, s\rho(s, s_0) \\ &=< \rho(s_0) > \end{aligned}$$

We define and compute

$$\rho'(s, s_0) = \frac{1}{\pi} \int_0^{\pi} \exp(s\cos\psi - \sqrt{s_0^2 - s^2\sin^2\psi})\, d\psi$$

with

$$< \rho'(s_0) >= \frac{2}{s_0^2} \int_0^{s_0} ds\, s\rho'(s, s_0)$$

which is the average pumping photon density.

Then

$$\rho(s, s_0) = \frac{\pi F_2}{c} \rho'(s, s_0)$$

and

$$\begin{aligned} < \rho(s_0) > &= \frac{2\pi F_2}{c s_0^2} \int_0^{s_0} ds\, s\rho'(s, s_0) \\ &= \frac{\pi F_2}{c} < \rho'(s_0) > \end{aligned}$$

Note:

$$\lim_{\delta\to\infty} \rho'(s, s_0) = 1 \qquad \lim_{\delta\to\infty} \rho(s, s_0) = \frac{\pi F_2}{c}$$

$$\lim_{s_0\to 0} < \rho'(s_0) > = 1 \qquad \lim_{s_0\to 0} < \rho(s_0) >= \frac{\pi F_2}{c}$$

and at the center $s = 0$ we have

$$\rho'(0, s_0) = \frac{1}{\pi}\int_0^{\pi} e^{-s_0}\, d\psi = e^{-s_0}$$

and on the wall $s = s_0$ we have

$$\rho'(s_0, s_0) = \frac{1}{\pi}\int_0^{\pi} e^{0}\, d\psi = 1$$

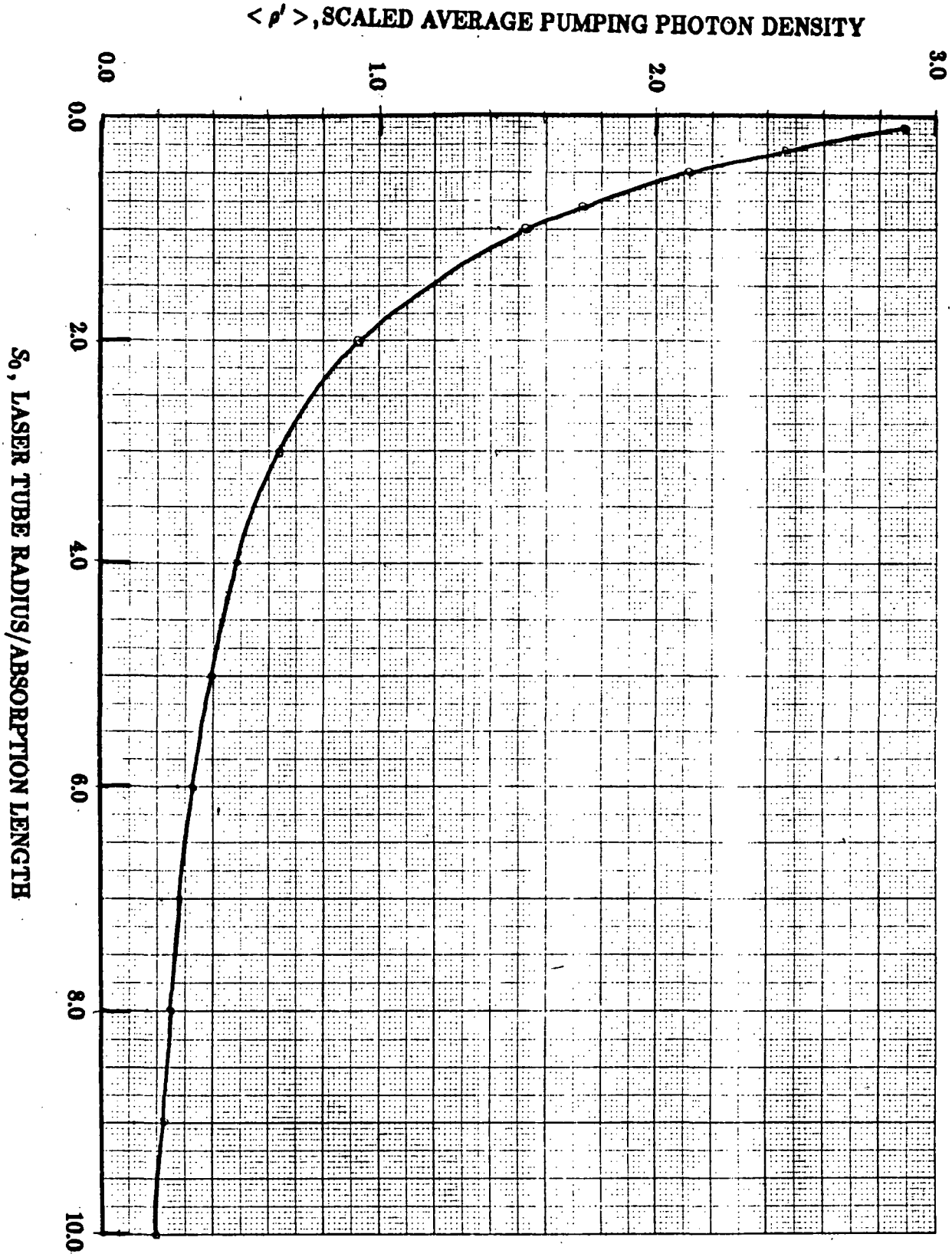


Figure A.5 <ρ'> vs S_0.

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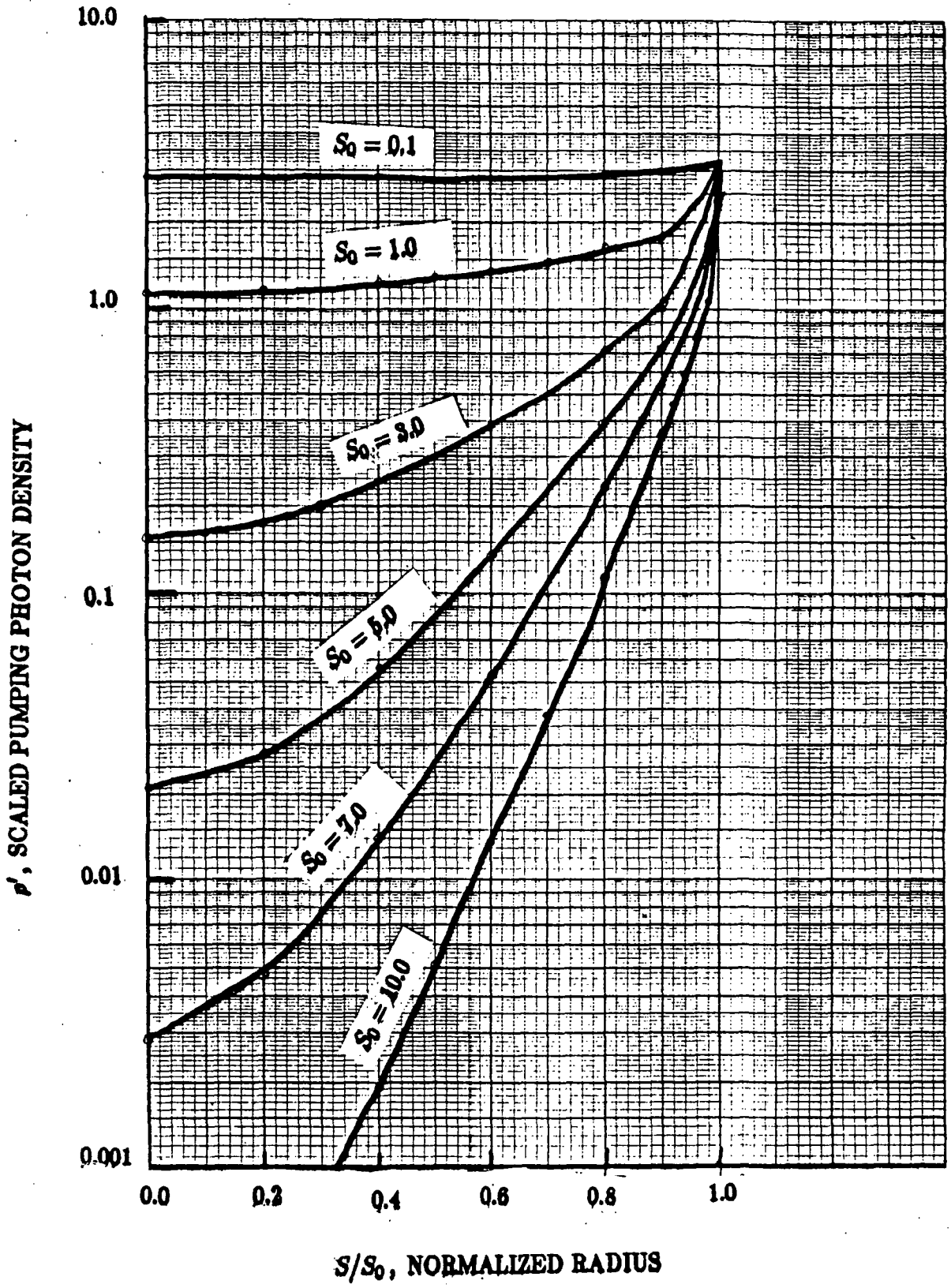


Figure A.6(a) ρ' vs S/S_0.

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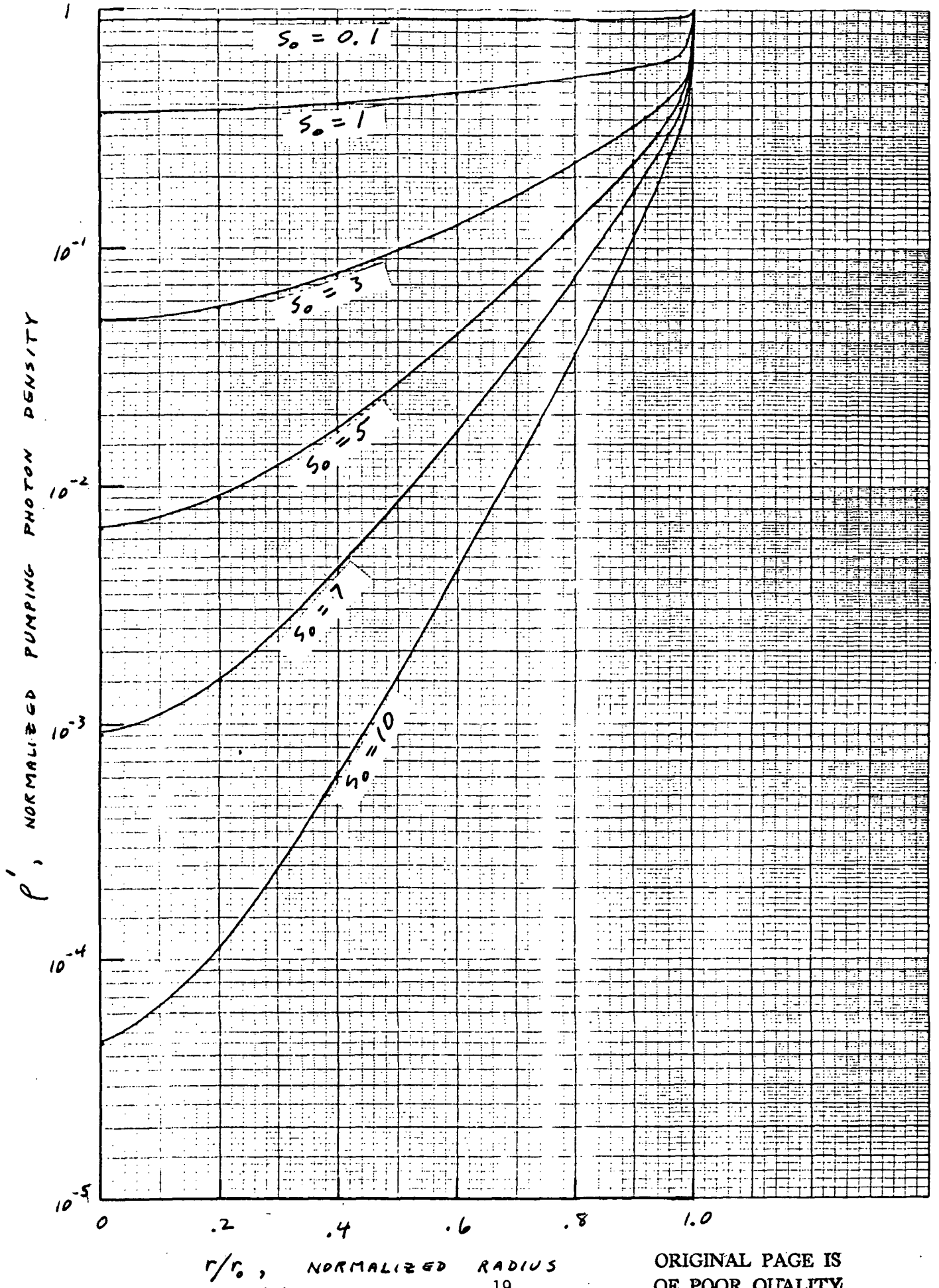


Figure A.6(b)

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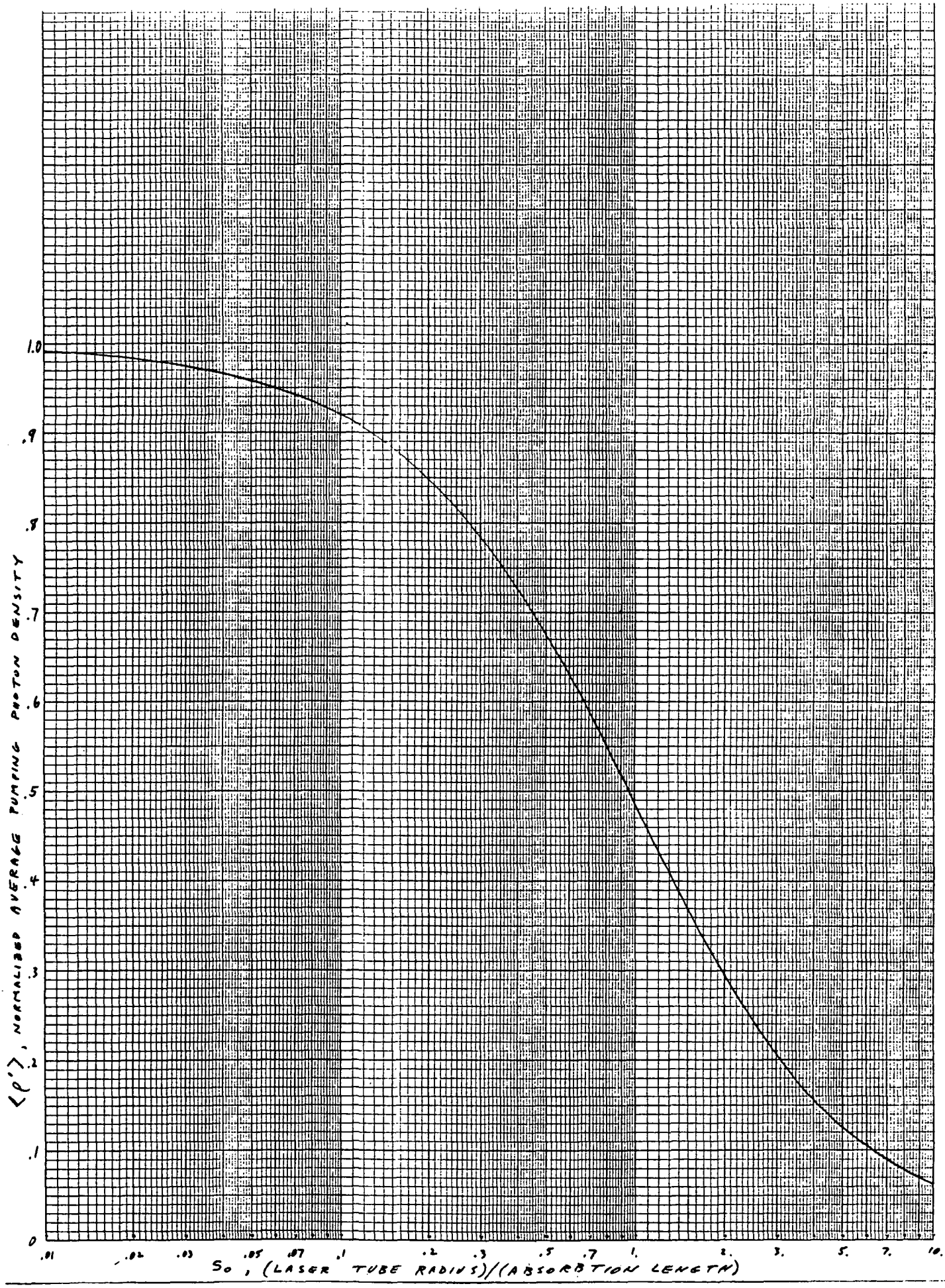


Figure A.7 $\langle \rho' \rangle$ vs S_0 011 semi-log scale.

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