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**A NONINTERFERENCE METHOD FOR DETERMINING
TEMPERATURE AND WATER VAPOR CONCENTRATION
PROFILES IN CYLINDRICALLY SYMMETRICAL
COMBUSTION SYSTEMS**

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L. E. Brewer

ARO, Inc.

July 1971

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PROFILES IN CYLINDRICALLY SYMMETRICAL
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FOREWORD

The work reported herein was sponsored by the Arnold Engineering Development Center (AEDC), Air Force Systems Command (AFSC), Arnold Air Force Station, Tennessee, under Program Element 65701F, Project 4344.

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This technical report has been reviewed and is approved.

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ABSTRACT

An optical method to determine radial temperature and water vapor concentration profiles from a radiating combustion source is presented. Equations for radiance and transmissivity using the random band model with constant line widths and a delta-function distribution for line strengths are written for a hypothetical cylindrically symmetrical source. A numerical iterative technique of solution of these equations for temperature and water vapor concentration from measured radiance and transmittance profiles is presented, utilizing band model parameter data from the literature. Experimental data from a small hydrogen-air burner are used to verify the analytical treatment.

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SECTION I INTRODUCTION

Systems involving flow of a gas through a nozzle in which combustion has occurred or is occurring present a formidable, if not impossible, problem to the theorist attempting to calculate the properties of the effluent in all but ideal cases. Generally, any real system deviates considerably from the ideal because of combustion inefficiencies, boundary layers, radiative cooling, etc. Therefore, measurements of some of the effluent properties become a necessity to fully understand the flow process. Considerable effort has been expended at AEDC in recent years to develop experimental techniques for determining certain of the chemical, physical, and flow parameters of these complicated systems. An area in which the efforts have culminated in a successful measurement technique is one of using infrared radiance and transmissivity data to determine water vapor concentration and temperature profiles across a plane in the effluent. That technique is the subject of this report.

The method presented herein consists of representing molecular radiance and transmissivity using a mathematical band model rather than using expressions from quantum theory which require the knowledge of fundamental molecular constants, many of which are either not available or not sufficiently accurate for some of the more prevalent combustion product molecules. The band model equations, first developed by astrophysicists (Ref. 1) for calculating atmospheric transmissivities have been extensively utilized in the past few years for calculations of the radiative heat transfer from rocket exhausts. In the typical radiative heat transfer application, the temperature and partial pressure distributions of each molecular radiator are assumed, and the radiance (which requires a knowledge of the transmissivity) is calculated. The inverse problem, that of calculating temperature and partial pressure distributions from a knowledge of the gas radiance and transmissivity, is treated herein. The method utilizes experimentally verified expressions for the radiance and transmissivity of the $2.7\text{-}\mu$ water vapor band using a random band model with constant line widths and a delta-function distribution for line strengths. These expressions, in conjunction with measured radiance and transmissivity data, are then used to calculate the water vapor partial pressure and temperature profiles through a procedure which involves an inversion of temperature and pressure rather than emission coefficient and absorptivity as is usually done for optically thin inhomogeneous gases. Also included are experimental data from a hydrogen-air burner having known properties which are used to validate the calculative procedure presented.

SECTION II THEORY

For most applications of diagnostics using emitted radiation from an optically thin, inhomogeneous, axisymmetric gas stream, the measured intensity profile is inverted by the Abel Integral Transform to a radial profile of emission coefficients which are directly relatable to local densities and temperature (Ref. 2). For cases where the gas is not optically thin but the Beer-Lambert law of absorption holds, the measured intensities can still be inverted to emission coefficients using a more complicated inversion technique. When the diagnostics are performed from the measured transmittance of an external source through the gas stream, the Abel inversion can also be done if the Beer-Lambert law holds, and the resulting transmittance related to temperature and density. Unfortunately, the Beer-Lambert law, which simply relates the attenuation through a path to a geometrical factor, does not hold when the spectral interval encompasses several lines within a band (Ref. 3). The closely packed line structure of molecules like H₂O and CO₂ which make up the bulk of most combustion gases are cases in point, and direct inversion techniques cannot be used. This report is concerned with the use of spectral band models which were designed to handle the transmission of radiation through inhomogeneous paths.

The use of models to represent individual or composite bands of structurally complex molecular species such as H₂O or CO₂ is necessary because of the large number of lines which are overlapping or superimposed. The models, referred to as band models, provide a mathematical means of averaging over the fine structure, without distorting the band contour, by assuming combinations of randomly or evenly spaced lines with a constant or varying distribution of intensities. For the H₂O molecule in the 2.7- μ band, experimental verification has been provided in Ref. 4 for the use of the random band model with constant line widths and a delta function distribution of line strengths.

Equations (1) through (6) below (derived in detail in Ref. 4) are expressions for radiance and transmissivity using the band model, which is formulated for the homogeneous case, and the Curtis-Godson approximation, which allows extension from the homogeneous to the inhomogeneous case.

The equation for radiance (N) from a gas is

$$N = \sum_i N_B(T_i) \left[\tau_{(i-1)} - \tau_i \right] \quad (1)$$

where $N_B(T_i)$ = Planck's blackbody radiance at temperature, (T_i) and a particular frequency

τ_i = Transmissivity of zones 1, 2, . . . , i

τ_{i-1} = Transmissivity of zones 1, 2, . . . , i-1

The equation for transmissivity of a single zone of constant temperature and pressure derived using the random band model with constant line widths and a delta-function distribution for line strengths is

$$-\ln \tau = 2\pi \left(\frac{\gamma}{d}\right) f(x) \quad (2)$$

where

$$x = \frac{\left(\frac{S}{d}\right) \ell}{2\pi \left(\frac{\gamma}{d}\right)} \quad (3)$$

Use of the Curtis-Godson approximation (Ref. 4) allows an immediate extension of Eq. (2) to the many-zone (inhomogeneous) case:

$$-\ln \tau = \frac{\sum_h x_h \left[\frac{-\ln \tau_h}{f(x_h)}\right]^2}{\sum_h x_h \frac{-\ln \tau_h}{f(x_h)}} f \left(\frac{\left[\sum_h x_h \frac{-\ln \tau_h}{f(x_h)}\right]^2}{\sum_h x_h \left[\frac{-\ln \tau_h}{f(x_h)}\right]^2} \right) \quad (4)$$

The symbols in Eqs. (2), (3), and (4) are as follows:

τ = transmissivity

γ = line half-width at half height, cm

S = line strength

d = line spacing, cm

$S/d, \gamma/d$ = band model parameters

ℓ = zonal path length, cm

h = reference to a single zone

The terms $(\gamma/d)_h$ and $(S/d)_h$ for a particular zone are further defined as follows:

$$\left(\frac{\gamma}{d}\right)_h = \left(\frac{\gamma_a^0}{d}\right)_h P_h^a + \left(\frac{\gamma_b}{d}\right)_h P_h^b \quad (5)$$

$$\left(\frac{S}{d}\right)_h = \left(\frac{S^0}{d}\right)_h P_h^{a^*} \quad (6)$$

where:

$\gamma^0/d, S^0/d$ = experimentally determined tabular functions of temperature (Ref. 5)

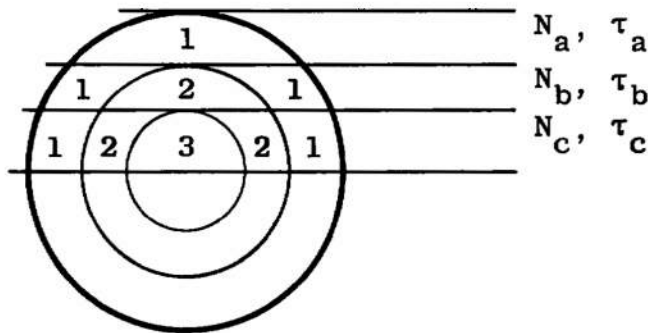
p_h^a = pressure of the absorbing gas in zone h, atm

p_h^b = pressure of a broadening gas (s), atm

$f(x)$ = Ladenburg and Reiche (L-R) function (tabular functions of x) (Ref. 6)

As previously noted, transmission of band radiation through combustion gases does not obey Beer's law. Therefore, the radiance (N) and the transmissivity (τ) cannot be scanned laterally outside the gas and inverted to radial positions using geometrical methods such as that provided by the Abel integral. However, Eqs. (1) and (4) are expressions for the radiance and transmissivity in the inhomogeneous gas in four unknowns, T_h and p_h and the measurable quantities N and τ , and therefore are, in principle, solvable for the T_h and p_h quantities.

In order to demonstrate a method of solution, consider a barometrically and thermally inhomogeneous, axisymmetric, three-zone case, such as:



N_a, N_b, N_c and τ_a, τ_b, τ_c are measured quantities; T_1, T_2, T_3 and p_1, p_2, p_3 are the unknown quantities. The effective zonal path length (ℓ) is defined by the geometry and is, therefore, a known quantity.

a. First Zone

Since this is a single zone, the measurable quantities N_a and τ_a are directly substituted into Eq. (1); thus

$$N_a = N_B(T_1) [1 - \tau_a] \tag{a-1}$$

from which $N_B(T_1)$, a value for the Planck blackbody function, is directly obtained. This immediately yields T_1 . From tabulated values, $(S^o/d)_1$ and $(\gamma^o/d)_1$ for T_1 are obtained, and Eqs. (5) and (6) can be written for zone 1:

$$\left(\frac{\gamma}{d}\right)_1 = \left(\frac{\gamma_a^c}{d}\right)_1 p_1^a \quad (a-2)$$

$$\left(\frac{S}{d}\right)_1 = \left(\frac{S^o}{d}\right)_1 p_1^a \quad (a-3)$$

(Note that the foreign gas broadening term of Eq. (5) has been omitted here. This term can be represented by a constant multiplier or assumed to be zero depending on the constituents of the gas under observation.) Substitution of these expressions into Eq. (3) yields

$$x_1 = \frac{\left(\frac{S^o}{d}\right)_1 p_1^a \ell}{2\pi \left(\frac{\gamma_a^c}{d}\right)_1 p_1^a} \quad (a-4)$$

The p_1^a terms can be cancelled, and the value of x_1 is obtained and used in the Ladenburg and Reiche (L-R) function tabulation to obtain $f(x_1)$. Substitution into Eq. (2) then yields

$$-\ln \tau_1 = 2\pi \left(\frac{\gamma_a^c}{d}\right)_1 p_1^a f(x_1) \quad (a-5)$$

which can be immediately solved for p_1^a , the other desired quantity.

b. Second Zone

Because of the First Zone calculation just shown and the axis of symmetry of the gas source, p_1^a , T_1 , $(\gamma/d)_1$, $(S/d)_1$, and $N_B(T_1)$ are known for the zone in which N_b and τ_b are the measured quantities. Therefore, x_1 and $f(x_1)$ for the appropriate ℓ can be directly calculated using Eq. (3) and the L-R function.

Equation (1) for position b is

$$N_b = N_B(T_1) [1 - \tau_1] + N_B(T_2) [\tau_1 - \tau_{21}] + N_B(T_1) [\tau_{21} - \tau_{121}] \quad (b-1)$$

where $\tau_{121} = \tau_b$ and the unknowns are $N_B(T_2)$ and τ_{21} .

Equation (4) for position b is

$$-\ell_n \tau_b = \frac{2x_1 \left(\frac{-\ell_n \tau_1}{f(x_1)} \right)^2 + x_2 \left(\frac{-\ell_n \tau_2}{f(x_2)} \right)^2}{2x_1 \left(\frac{-\ell_n \tau_1}{f(x_1)} \right) + x_2 \left(\frac{-\ell_n \tau_2}{f(x_2)} \right)} f \left(\frac{\left[2x_1 \frac{-\ell_n \tau_1}{f(x_1)} + x_2 \frac{-\ell_n \tau_2}{f(x_2)} \right]^2}{2x_1 \left(\frac{-\ell_n \tau_1}{f(x_1)} \right)^2 + x_2 \left(\frac{-\ell_n \tau_2}{f(x_2)} \right)^2} \right) \quad (b-2)$$

Unknowns in this equation are $-\ell_n \tau_2$ and x_2 ($f(x_2)$ is also unknown but is determined through the L-R function from the value of x_2).

Equations (b-1) and (b-2) are two equations in two unknowns, p_2 and T_2 ; however, they cannot be written in terms of these two parameters and solved simultaneously because of the tabular nature of S^0/d , γ^0/d , and $f(x)$. Therefore, an iterative scheme is necessary for the solution of (b-1) and (b-2). Assume that the radiance and transmissivity can be written functionally:

$$\begin{aligned} N &= N(T_i, p_i) \\ r &= r(T_i, p_i) \end{aligned} \quad (b-3)$$

where the subscript "i" refers to the inner zone for which the properties are unknown. This functional form notes that, for all zones other than the i^{th} , the T's and p's are known and may be considered constant. Forming the differential of (b-3) then gives

$$\begin{aligned} dN &= \frac{\partial N}{\partial T_i} dT_i + \frac{\partial N}{\partial p_i} dp_i \\ dr &= \frac{\partial r}{\partial T_i} dT_i + \frac{\partial r}{\partial p_i} dp_i \end{aligned} \quad (b-4)$$

where Eqs. (b-1) and (b-2) can be used to obtain the partial derivatives.

Now, let some T_i , p_i be assumed. Call these $T_i^{(0)}$, $p_i^{(0)}$, and use these to calculate radiance, transmittance, and the partial derivatives in the system (b-4) or

$$\begin{aligned} N^{(0)} &= N(T_i^{(0)}, p_i^{(0)}) \\ r^{(0)} &= r(T_i^{(0)}, p_i^{(0)}) \\ N_x - N^{(0)} &= \left. \frac{\partial N}{\partial T_i} \right|_{T_i^{(0)}, p_i^{(0)}} (T_i^{(1)} - T_i^{(0)}) + \left. \frac{\partial N}{\partial p_i} \right|_{T_i^{(0)}, p_i^{(0)}} (p_i^{(1)} - p_i^{(0)}) \\ \tau_x - r^{(0)} &= \left. \frac{\partial r}{\partial T_i} \right|_{T_i^{(0)}, p_i^{(0)}} (T_i^{(1)} - T_i^{(0)}) + \left. \frac{\partial r}{\partial p_i} \right|_{T_i^{(0)}, p_i^{(0)}} (p_i^{(1)} - p_i^{(0)}) \end{aligned} \quad (b-5)$$

where the subscript x refers to the experimentally measured values, and the identification of dN with $N_x - N^{(0)}$, dT_i with $T_i^{(1)} - T_i^{(0)}$, etc., is obvious. Since the values for $T_i^{(0)}$ and $p_i^{(0)}$ were assumed, the only unknowns in the system (b-5) are $T_i^{(1)}$ and $p_i^{(1)}$; they occur in a 2 by 2 linear system, and the solution for them is immediate.

The $T_i^{(1)}$, $p_i^{(1)}$ is a first approximation to the true value T_i , p_i for the unknown zone. However, the Eqs. (b-1) and (b-2) are quite non-linear in T_i , p_i , and the process must be repeated using $T_i^{(1)}$, $p_i^{(1)}$ to calculate a new $N^{(1)}$, $\tau^{(1)}$, which in turn will lead to a $T_i^{(2)}$, $p_i^{(2)}$. The technique is iterated until the values of N and τ , calculated, agree with the experimentally measured values within predetermined limits. The converged value is then the T , p ascribed to that zone of the gas.

Hence, for the second zone, since any reasonable guess is satisfactory for the zeroth approximation, start with $T_2^{(0)} = T_1$ and $p_2^{(0)} = p_1$. The values calculated from (b-1) and (b-2) are compared with N_b , τ_b which suggests the $T_2^{(1)}$, $p_2^{(1)}$, and the process is iterated until the convergence criteria are satisfied.

c. Third Zone

The extension to the third zone (and subsequent zones) where N_c and τ_c are the measured quantities follows the method outlined above for the second zone. Equations (1) and (4) are written with additional known terms for the two p_2 and T_2 zones resulting in two equations in two unknowns, p_3 and T_3 , which are then solved by the iterative computer solution discussed above.

SECTION III APPLICATION OF METHOD

To apply the calculative method discussed in the previous section to a real system, a knowledge of the band model parameters is necessary. For the water vapor molecules the parameters K , absorption coefficient, and $\frac{1}{d_{LR}}$, the fine structure parameter, are given in Ref. 5 as a function of wave number (ν) and temperature. For pure collision broadening (Lorentz) the absorption coefficients and the fine structure

parameters are related to the band model parameters through the following two equations:

$$\frac{S^{\circ}}{d} = K \frac{T_0}{T}$$

and

$$\frac{\gamma^{\circ}}{d} = \gamma^* \frac{T_0}{T} \frac{1}{d_{LR}}$$

where

$$T_0 = 273^{\circ}\text{K}$$

$$\gamma^* = 0.44 \text{ (an empirical constant from Ref. 5)}$$

The tabulated values of K are listed for temperatures of 300, 600, 1000, 1500, 2000, 2500, and 3000°K and for $\nu = 50$ to 9300 cm^{-1} at intervals of 25 cm^{-1} . The values of $1/d_{LR}$ are listed at the same temperature and the same wave number intervals from $\nu = 1150$ to 7500 cm^{-1} .

Utilization of the parameters was accomplished by means of fifth-degree polynomial curve fits in the computer program. In order to use a spectral interval greater than 25 cm^{-1} , as was done in the experiment described below, it was necessary to check the variation of the parameters with ν for the expected temperature range over the spectral interval to be used. If necessary, adjustment of the parameters must be made such that they represent average values for the spectral interval. For the case described herein, however, no adjustment of the parameters was necessary since the values given for 4000 cm^{-1} represented average values from 3900 to 4100 cm^{-1} over the temperature range expected.

To demonstrate the applicability of the analytical approach described in the previous section and to provide a check on the computer program, radiance and transmissivity data were obtained using a small hydrogen-air burner which had previously been studied quite extensively using thermocouple probes.

A schematic diagram of the experimental apparatus is shown in Fig. 1, and details of the burner are shown in Fig. 2. The apparatus consists of a burner and an emission-absorption spectroradiometer. The burner is a premixed, flat flame type in which the reactant gas mixture issues from the burner grid with a uniform velocity distribution across the grid, resulting in a uniform temperature profile across most of the grid when the premixed effluent is burned. The spectroradiometer consists of source and receiver units. A variable temperature globar in the source unit generated a beam of infrared radiation which was modulated by a mechanical chopper at a frequency of 300 cps and focused through the burner flame to the receiver unit

using a pair of matched focusing mirrors. A second chopper operating at a frequency of 13 cps was located inside the receiver unit prism monochromator which was set to pass radiation at a wavelength of 2.5μ with an equivalent slit width of 193 cm^{-1} . The radiation was detected by a lead sulfide detector. A blackbody was used at the same location as the burner to calibrate the receiver unit in order to make absolute intensity measurements. Absorption measurements were made by observing the attenuation of the modulated global radiation passing through the flame with the receiver chopper stopped in an open position. To make the flame emission measurements, the global radiation was blocked by a shutter, and the receiver chopper was started. The absorption and emission signals were recorded on a strip-chart recorder after amplification, using synchronous amplifiers tuned to the chopper frequencies.

The burner is mounted on a traversing mechanism which allows movement normal to the optical path to obtain data from parallel adjacent paths through the flame. Both the source and receiver units of the spectroradiometer were enclosed and purged continuously with dry nitrogen to eliminate the effects of atmospheric water vapor absorption in the optical path of the instrument.

Experimental radiance and transmissivity data are shown in Fig. 3. The data were obtained across a plane located a distance of 6.4 mm above the burner grid with the hydrogen-air burner operating at stoichiometric conditions.

The results of using the data in Fig. 3 to determine temperature and water vapor concentration profiles by the techniques presented in Section II are shown in Fig. 4. The band model parameters S^0/d and γ^0/d were obtained from Ref. 5. For comparison purposes, a thermodynamic calculation of the flame temperature, considering the burner cooling water enthalpy increase and the inlet gas temperatures but ignoring radiative losses, predicted a temperature of 2270°K , which compares favorably (5 percent) with the measured temperature near the flame center (Fig. 4). As a further comparison, the water vapor mole fraction was also determined using the same program. The calculated value of 0.34 atm agrees extremely well with the measured value for the water vapor pressure (Fig. 4) near the 1-atm flame center.

It should be noted, however, that, for the experimental test case, the value of x (see Eq. (3)) fell below or very near 0.1, thus resulting in $f(x) = x$ (within 5 percent). When $f(x) = x$, Eq. (4) reduces to

$$-\ln \tau = \sum (-\ln \tau_h) \quad (7)$$

which is equivalent to an expression of Beer's law.

SECTION IV CONCLUSIONS

A noninterference optical method was developed for determining the radial profiles of temperature and water vapor concentration in a radiating, cylindrically symmetrical gas flow. Radiance and transmissivity measurements through several path lengths are required. Based on the experimental results obtained by applying the method to an H₂-Air flame at 1-atm pressure, the technique developed herein has been satisfactorily validated by comparison with thermodynamic calculations. Although a simpler calculative procedure could have been used to obtain temperature and concentration (Eq. 7 rather than Eq. 4), the general equations and iterative procedures described in Section II were used to obtain the results shown in Fig. 4, thus validating the use of the equations and the computer program.

Extension of the theory is possible to other combustion product molecules such as CO and CO₂ as well as to cases where the source shape is known but different from the cylindrically symmetric case presented here.

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**APPENDIX
ILLUSTRATIONS**

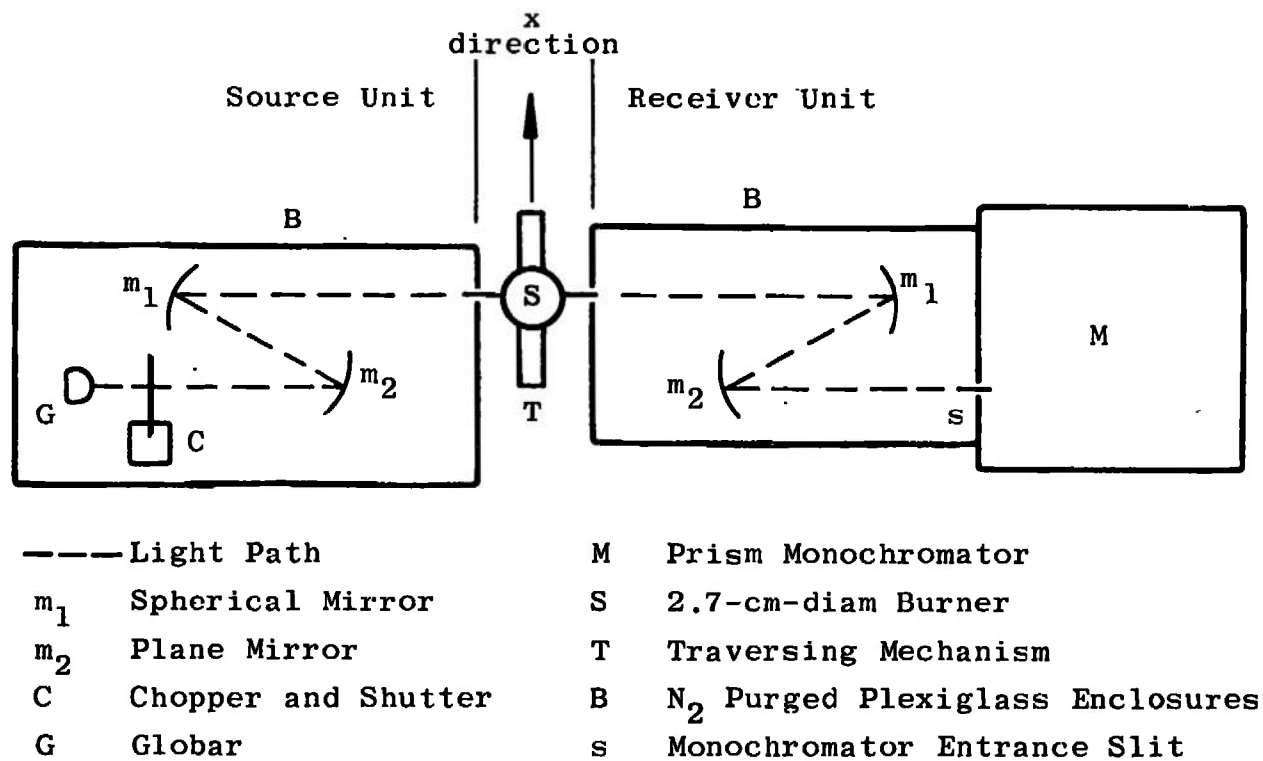


Fig. 1 Schematic Diagram of Experimental Apparatus

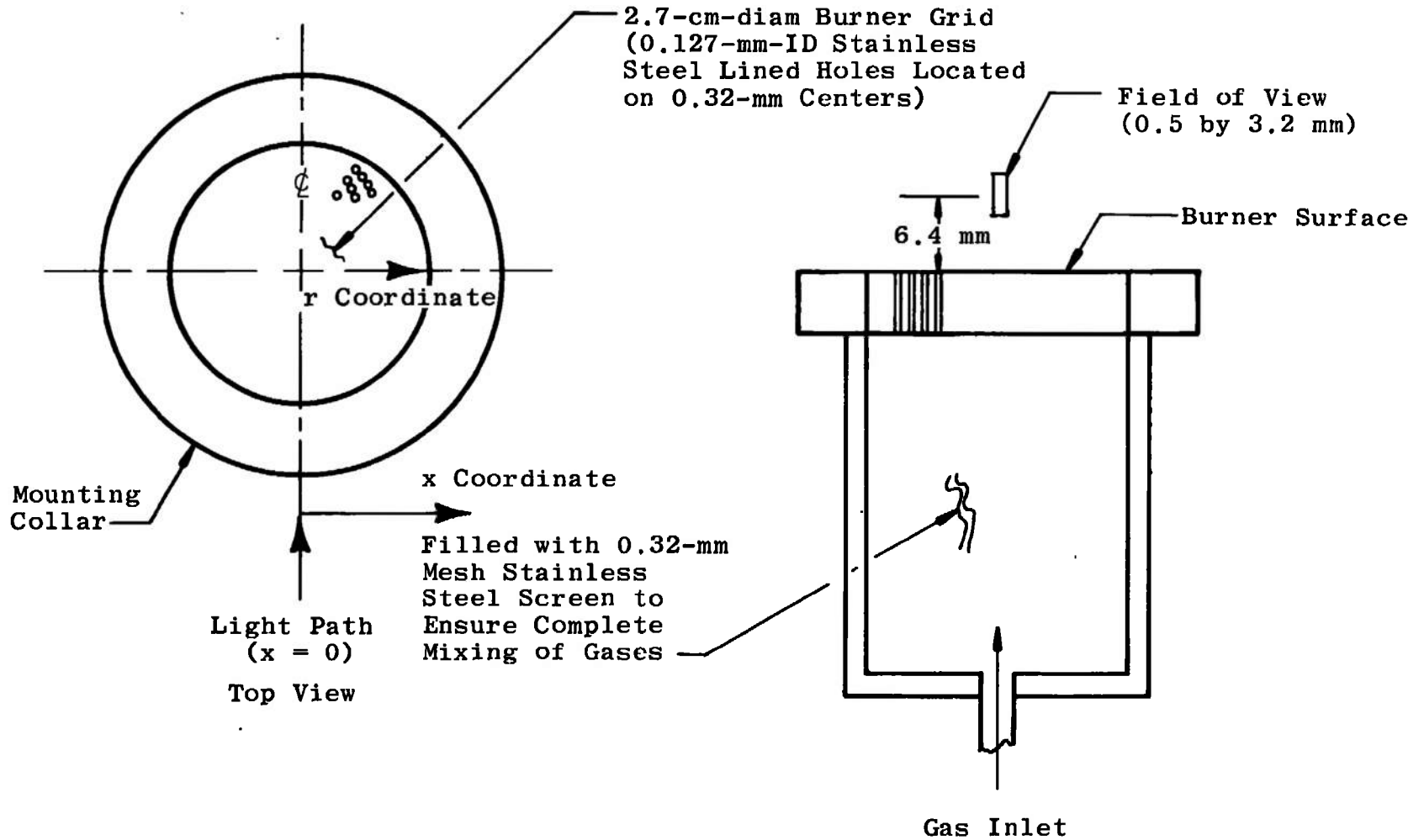


Fig. 2 Diagram of Burner and Coordinates

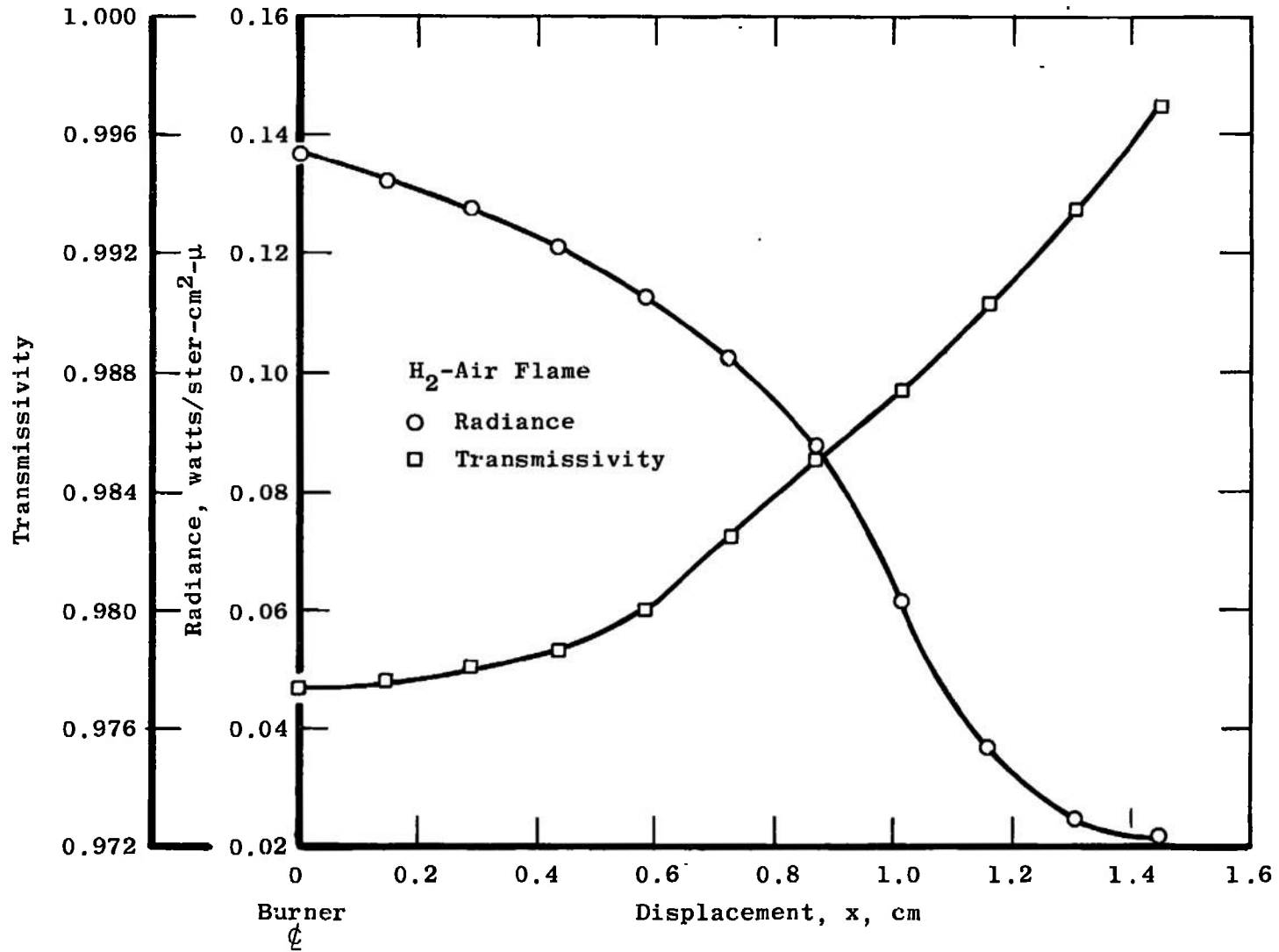


Fig. 3 Experimental Radiance and Transmissivity Measurements (6.44 mm above Burner Surface)

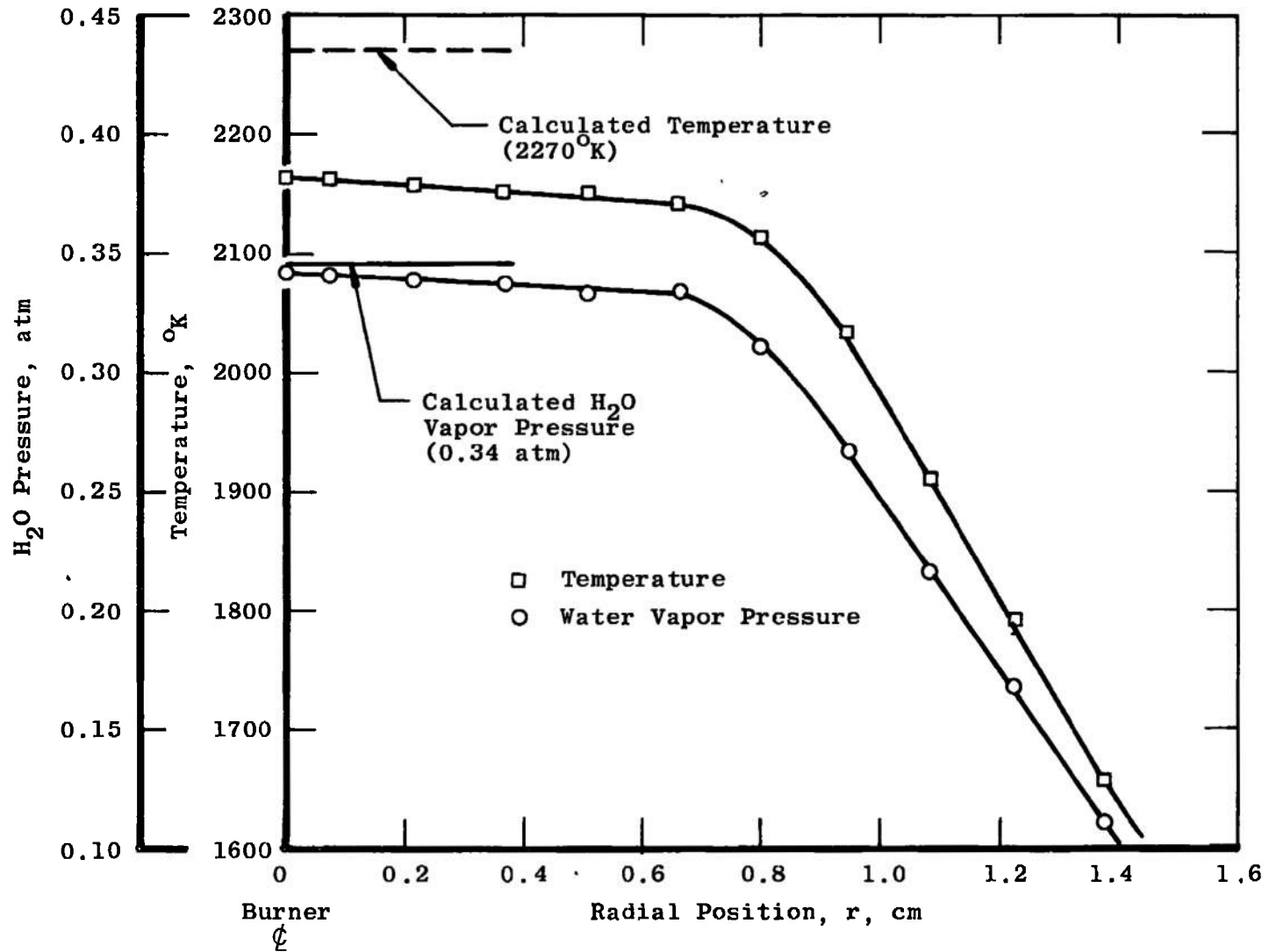


Fig. 4 Temperature and Water Vapor Pressure Profiles Determined from Data of Fig. 3

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14. KEY WORDS	LINK A		LINK B		LINK C	
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