COMPUTER PROGRAM FOR CALCULATION OF A GAS TEMPERATURE PROFILE BY INFRARED EMISSION - ABSORPTION SPECTROSCOPY

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A computer program to calculate the temperature profile of a flame or hot gas is presented in detail. Emphasis is on profiles found in jet engine or rocket engine exhaust streams containing H₂O or CO₂ radiating gases. The temperature profile is assumed axisymmetric with an assumed functional form controlled by two variable parameters. The parameters are calculated using measurements of gas radiation at two wavelengths in the infrared. The program also gives some information on the pressure profile. A method of selection of wavelengths is given that is likely to lead to an accurate determination of the parameters. The program is written in FORTRAN IV language and runs in less than 60 seconds on a Univac 1100 computer.
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COMPUTER PROGRAM FOR CALCULATION OF A GAS TEMPERATURE PROFILE BY INFRARED EMISSION - ABSORPTION SPECTROSCOPY

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SUMMARY

A computer program to calculate the temperature profile of a flame or hot gas is presented in detail. Emphasis is on profiles found in jet engine or rocket engine exhaust streams containing H₂O or CO₂ radiating gases. The temperature profile is assumed axisymmetric with an assumed functional form controlled by two variable parameters. The parameters are calculated using measurements of gas radiation at two wavelengths in the infrared. The program also gives some information on the pressure profile. A method of selection of wavelengths is given that is likely to lead to an accurate determination of the parameters. The program is written in FORTRAN IV language and runs in less than 60 seconds on a Univac 1100 computer.

INTRODUCTION

Infrared emission and absorption measurements at two or more wavelengths provide a means of determining a gas temperature profile along a path through the gas by using a radiation source and receiver located only at the ends of the path (ref. 1). In the case of a jet engine or rocket engine exhaust stream, the instrumentation may be outside of the stream. The method has been termed the "spectral-scanning method." Practical instruments that permit use of this technique are described in references 1 through 4.

Tests of the method with heated pure gases in a furnace of 60 cm path length (ref. 2), and then with flames over a 22 cm path length
(ref. 3) gave good results. An analysis in reference 5 showed the effect of radiometric errors on the accuracy of the computed profile. The analysis assumed the partial pressure of the radiating gas was a constant over the entire path, with the constant determined from radiometric measurements. More recently, the feasibility of using only emission measurements and an estimated gas composition to determine industrial furnace temperature profiles over a 10-meter path length at atmospheric pressure has been shown (ref. 6).

The computer program presented herein involves an iterative, cyclic computation in which an initial assumed (arbitrary but realistic) temperature profile is altered in shape until the computed emission and absorption that it would yield agree as closely as possible with the actual instrumental measurements of emission and absorption. The procedure requires the use of a large-scale computer. These procedures have been outlined in principle in previous publications; but this report presents an actual program that has been found to produce useful results.

The present work also extends the work of reference 5 by providing greater latitude in the temperature-profile shape that can be treated and by relaxing restrictions on the shape of the associated pressure profile. Thus, whereas previous studies have principally treated profiles with a substantial temperature difference over the optical path, the present study also includes the equally important case of an almost isothermal profile; and whereas the work of reference 5 has assumed constant pressure over the path, the present work allows an additional degree of freedom in the description of the pressure profile.

The program presented provides a means of determining temperature from experimental measurements of emission and absorption at two or more wavelengths. But it also provides a means, before any experiments are performed, of selecting those wavelengths whose use will lead to the best attainable accuracy. This prior selection is very important, because a poor selection of wavelengths may lead to unacceptably high uncertainty in the temperature and may even lead to an erroneous solution of the equations. The existence and avoidance of this incorrect solution for the
temperature profile is demonstrated. Thus, this report provides the potential user with a means of determining whether this method will be sufficiently accurate for his particular application, as well as providing a means of finding the solution if the method is adopted. Symbols are listed in appendix A.

MATHEMATICAL ANALYSIS

Method of Determining Temperature and Pressure Profiles

The method is iterative with each iterative step consisting of three principal parts:

1. With current profiles of temperature and pressure, compute the gas radiance and transmittance at each wavelength of measurement.
2. Record the difference between computed and measured gas radiance and transmittance at each wavelength of measurement.
3. Correct the current profiles in (1) to reduce the differences in (2) to zero.

Functional forms of the temperature profile $T(x)$ and the partial pressure profile $p(x)$ of the absorbing gas are assumed in advance. The temperature profile is expressed in terms of two unknown parameters, and the pressure profile in terms of one unknown parameter. A minimum of one set of measurements, at each of two wavelengths, is required to yield a solution for the unknown parameters, each set actually involves four radiometric measurements (i.e., four instrument readings). The computational program then determines, from the simultaneous solution of equations containing actual radiometric measurements, the values of these parameters that make computed values of radiance and transmittance equal to measured values.

Additional wavelengths of measurement may improve accuracy, in such case, a least-squares method of solution is employed. The results obtained are the values of the parameters when the 'residual', which is the sum of the squares of the differences between measured and computed values of radiance, is a minimum.
The functions used in this program may be modified as desired for a particular application. However, tests during development of the program have shown that it is impractical to characterize the temperature profile by more than two unknown parameters because the accuracy of the solution becomes unacceptably low.

The profiles. - In the present program, the profiles are taken to be axisymmetric, with shapes chosen to resemble the transverse pressure and temperature distributions often found in ducts. The functions are expressed in terms of values of the dependent variable at the axial, or centerline, position (subscript c) and at a wall position (subscript w), and the value of a shape parameter $\eta_T$ or $\eta_p$ for temperature or pressure, respectively.

1. When the temperature profile is far from isothermal, it is taken as

$$T(x) = T_c - (T_c - T_w) \left| \frac{y}{y} \right|^{1/\eta_T}$$  \hspace{1cm} (1)

where

$$y = (2x/L) - 1 \quad 0 \leq x \leq L$$

It is assumed that $T_w$ is measured independently. Parameters $T_c$ and $\eta_T$ are determined by the computational program. They are then termed the dependent parameters. This family of curves is shown in figure 1(a).

2. When the profile is nearly isothermal, except for a thin boundary layer at each end, the temperature profile is taken as

$$T(x) = T_c - (T_c - T_w^*) \left| \frac{y}{y} \right|^{1/\eta_T}$$  \hspace{1cm} (2a)

where

$$y = (2x/L) - 1 \quad x_1 \leq x \leq L - x_1$$
and

\[ T(x) = T_w + (T_1 - T_w)z + (mx_1 + T_w - T_1)z(z - 1) \quad 0 \leq z \leq 1 \quad (2b) \]

where

\[ z = x/x_1 \quad \text{for} \quad 0 \leq x \leq x_1 \]

\[ z = (L - x)/x_1 \quad \text{for} \quad L - x_1 \leq x \leq L \]

\[ T_1 = T(x_1) = T(L - x_1) \]

\[ m = (dT/dx)_{x=x_1} = 2(T_c - T_1)/[\eta_T(L - 2x_1)] \]

This definition of \( T(x) \) provides continuity of both temperature and temperature gradient at \( x = x_1 \) and at \( x = L - x_1 \). This family of curves is shown in figure 1(b). Using this definition, \( \eta_T \) and \( x_1 \) are preassigned some reasonable values and the computational program determines \( T_w \) and \( T_c \) as the dependent parameters. It is assumed that \( T_w \) is measured independently.

3. The partial pressure profile of each absorbing gas is assumed to be of the form

\[ p(x) = p_c - (p_c - p_w)|y|^{1/\eta_p} \quad (3) \]

where

\[ y = (2x/L) - 1 \quad 0 \leq x \leq L \]

The profile is shown in figure 1(c). Different initial values may be assumed for parameters \( p_c, p_w, \) and \( \eta_p \) for each gas. The choice of the initial values of the parameters may be aided by a computation of the partial pressure of the reaction products. These pressures can be computed for a range of reaction product temperatures and a range of partial pressures
and reactant composition using the computer program of reference 7. From these data a choice for initial values of the pressure parameters can be made. (The program of ref. 7 may be obtained from its authors, on written request, by sending a magnetic tape at least 1200 ft long and by specifying the type of computer. Parts of the program not used in this application may be removed after the program has been transferred from tape to cards.)

Tests during the development of the program for computing temperature and pressure profiles have shown that only one dependent pressure parameter can be determined with acceptable accuracy. This is best done by designating the parameter $p_{c,1}$ of the principal absorbing gas (subscript 1) as an independent parameter. The wall pressure $p_{w,1}$ is selected to be directly proportional to the center pressure, and the shape parameter $n_{p,1}$ is chosen judiciously and held constant. Assumed parameters for all other absorbing gases (subscript k) and all nonabsorbing gases (subscript j) determine the initial pressure profiles $[p_k(x)]_o$ and $[p_j(x)]_o$.

Next, these profiles are made dependent on the profile $p_1(x)$. The absorbing gases initially have profiles that determine ratios $[p_k(x)/p_1(x)]_o$. Then, as $p_1(x)$ is changed by the program, these other profiles are also changed by the linear relation

$$p_1(x)[p_k(x)/p_1(x)]_o$$

After the absorbing-gas pressure profiles are determined, the nonabsorbing-gas pressure profiles $p_j(x)$ are adjusted to make the sum of all gas pressures equal to the measured static pressure $p_S$ which is assumed to be independent of $x$, so that

$$p_S = \sum_k p_k(x) + \sum_j p_j(x)$$

An additional constraint is to maintain the relative amounts of each nonabsorbing gas as given by the initial profiles, that is, in the ratio
Thus the pressures of the nonabsorbing gases are given by

\[ p_j(x) = \left[ p_s - \sum_{k} p_k(x) \right] \frac{[p_j(x)]_0}{\sum_{j} [p_j(x)]_0} \]  

(5)

The residuals. - Initial values of all parameters of the profile functions are tabulated, and the resultant sets of values of gas radiance \( N_L \) and transmittance \( \tau_L \) are computed for two or more wavelengths from radiometric equations. The computed quantities are denoted by \( \text{c} N_L \) and \( \text{c} \tau_L \). The corresponding measured quantities at the same wavelengths are denoted by \( \text{m} N_L \) and \( \text{m} \tau_L \). The difference between the computed and measured quantities is called the "residual." The residual for gas radiance may be expressed as a fractional value

\[ R_N = (\text{c} N_L - \text{m} N_L)/\text{m} N_L \]  

(6)

It is preferable to use gas absorptance \( \alpha_L = 1 - \tau_L \) in place of transmittance \( \tau_L \) for the transmittance residual because \( \alpha_L \) is more nearly proportional to the gas pressure and to the gas absorption coefficient. The residual for gas absorptance is defined as

\[ R_\alpha = (\text{c} \alpha_L - \text{m} \alpha_L)/\text{m} \alpha_L = (\text{m} \tau_L - \text{c} \tau_L)/(1 - \text{m} \tau_L) \]  

(7)

The solution. - The solution is reached by reducing the residuals to an acceptably small value by appropriately changing the two variable parameters in the equation for the temperature profile and the one variable parameter in the equation for the pressure profile. This is done iteratively using the Newton-Raphson method (ref. 8, p. 175) because the equations are nonlinear. For two wavelengths of measurement each
iterative step involves the solution of the following three simultaneous equations for the increments $\Delta y_j$ to the current value of the three variable parameters represented by $y_j$.

\[
\begin{align*}
(1) \sum_j \left( \frac{1}{m_{N\lambda_1, L}} \cdot \frac{\partial c_{N\lambda_1, L}}{\partial y_j} \right) \Delta y_j &= -R_{\lambda_1, N} \\
(2) \sum_j \left( \frac{1}{m_{N\lambda_2, L}} \cdot \frac{\partial c_{N\lambda_2, L}}{\partial y_j} \right) \Delta y_j &= -R_{\lambda_2, N} \\
(3) \sum_j \left( \frac{1}{m_{\alpha\lambda_1, L}} \cdot \frac{\partial c_{\alpha\lambda_1, L}}{\partial y_j} \right) \Delta y_j &= -R_{\lambda_1, \alpha}
\end{align*}
\]

Note that only one wavelength is needed for $R_{\lambda_1, \alpha}$ to determine one pressure parameter. The derivatives in equation (8) are obtained numerically. The final value of the residuals is zero.

There are cases where there are more measurements than there are variable parameters. For these cases, where the final values of the residuals are not necessarily zero, a damped least-squares modification of equation (8) is used to find a solution at which

\[
R_{\lambda_1, \alpha}^2 + \sum_i R_{\lambda_1, N}^2 = R^2 \approx \text{a minimum}
\]

where there are as many residuals $R_N$ as there are $i$ wavelengths, and there is only one residual $R_{\alpha}$. The damped least squares method is used in this program. Its derivation is in the second part of appendix B.
In addition to the solution for the profile parameters, an estimate is made of the error in the parameters that would be caused by stated random errors of radiometric measurements and tabulated absorption coefficients. (Typical orders of magnitude for these errors are 1 percent in radiation and 5 percent in absorption coefficient.) The error equation is derived in appendix B.

Measurement of Gas Radiance and Transmittance

The actual gas radiance $N_L$ and transmittance $\tau_L$ are derived from measurements of detector (radiometer) output voltage $V$ that is assumed to be proportional to incoming radiant power. The factor of proportionality (calibration factor) of the detector includes the effect of all optics between the radiometer element and the gas, but it need not be known explicitly if it remains constant for all measurements. The optics include, in addition to windows, lenses, and stops, a monochromator of bandwidth $\Delta \lambda$ centered on wavelength $\lambda$. The following measurements of detector output voltage $V$ are made:

(a) $V_0$, where a calibrated source of radiation $N_o$ is placed at the gas location, in place of the gas.

(b) $V_1$, due to radiation from the gas.

(c) $V_2$, where a stable comparison source radiates through the gas path, but the gas is absent.

(d) $V_3$, when the comparison source radiates through the gas path in the presence of the gas.

By chopping the radiation from the comparison source at a unique, distinctive frequency, voltages $V_1$ and $V_3$ are distinguished from each other, and voltage $V_3$ does not include gas radiation (ref. 1, p. 28).

These four measurements yield

$$N_L = N_o \frac{V_1}{V_0}; \quad \tau_L = \frac{V_3}{V_2}$$

(10)
Computation of Gas Radiance and Transmittance

The gas radiance, integrated over a narrow wavelength band $\Delta \lambda$ centered at $\lambda$ and over a path length $L$, is

$$ N_L = \int_0^L N_\lambda^* \left( \frac{d\tau}{dx} \right) dx $$

(11)

where $N_\lambda^*$ is the Planck radiation function

$$ N_\lambda^* = \frac{c_1}{\lambda^5} (e^{c_2/\lambda T} - 1)^{-1} $$

and $\tau$ is the gas transmittance over the path from 0 to $x$. The detailed justification for equation (11) is presented in reference 5.

The gas transmittance for a band $\Delta \lambda$ is described by a band-model formulation for a nonisothermal gas based on equation (5) of reference 9. This formulation has been justified and applied in reference 2, and summarized in reference 10. For profiles with a large variation in temperature, the formulation as modified in references 3 and 11 is adopted. Other band-models can be found in the literature (ref. 12).

The transmittance $\tau$ for a single gas is a function of the dimensionless optical depth $\nu$ and is given by

$$ \tau = \exp \left\{ -\frac{\nu \beta e}{1 + \left( \frac{\nu}{2} \right)^{1/2}} \right\} $$

(12)

For a mixture of $q$ absorbing gases the combined transmittance is the product

$$ \tau = \prod_{l=1}^{q} \tau_l $$

(13)
The optical depth of a path length $x$ is

$$u = \frac{1}{\beta_e} \int_0^x k\left(\frac{\beta}{\beta_e}\right)^\eta \, dx$$

where $k$ is the absorption coefficient at local temperature $T$ and partial pressure $p$ of the absorbing gas and $\eta$ is an interpolation parameter. The parameter $\beta$ is the local value of the line overlap parameter and is given by $\beta = \frac{2\pi\gamma}{d}$ where $\gamma$ is the average line width, and $d$ is the average line spacing. The definitions of $u$ and $\tau$ given here differ slightly in form from those of references 3 and 11 for reasons of computational expediency.

A modification in references 3 and 11 replaces the constant average $\beta_e$ of reference 2 ($\beta_{av}$ of ref. 4) by a cumulative average produced by weighting $\beta(x)$ with the absorption coefficient, so that

$$\beta_e(x) = \frac{\int_0^x k\beta \, dx}{\int_0^x k \, dx}$$

The interpolation parameter $\eta$ is given by one of two formulas

$$\eta = \begin{cases} \frac{u + A_1}{u + A_2} & u > A_5 \\ \frac{uA_3}{A_5 + uA_4} & u \leq A_5 \end{cases}$$

where

$$A_5 = 1 + 0.185 \left(\frac{\beta}{\beta_e}\right)$$
Values for $A_1$, $A_2$, $A_3$, $A_4$, and $A_5$ are listed in table I in terms of $(\beta/\beta_e)$.

The computation for the initially assumed profiles $T(x)$ and $p(x)$ first determines all values of $k$, $\beta$, and $\beta_e$, as functions of $x$ from the band model data and equation (15). For example, tabulations of $k_s$ and $(\gamma/d)_s$ for $\text{H}_2\text{O}$, $\text{CO}_2$, and CO may be obtained from reference 13 or, for $\text{H}_2\text{O}$, from references 14 and 15. (The subscript $s$ here denotes the value at standard temperature and pressure.) Values of $k_s$ in the tables are denormalized to the local gas temperature and partial pressure by

$$k = k_s p \frac{273}{T}$$

where $p$ is in atmospheres and $T$ is in kelvin. Similarly, the tabulated values of $(\gamma/d)_s = \beta_s/(2\pi)$ may be used to obtain the local value as it is affected by the line-broadening effect of all gas components in accordance with the formula

$$\beta = \beta_s \left( \sum_k \alpha_k^* p_k + \sum_j \alpha_j^* p_j \right)$$

where $p_j$, $p_k$ are the partial pressures, and $\alpha_j^*$, $\alpha_k^*$ are the broadening coefficients for the $k$ absorbing gases and $j$ nonabsorbing gases.

For the absorbing gas, values of $\alpha^*$ are given in reference 16 and are listed in table II.

The path length $0 \leq x \leq L$ is divided into increments $\Delta x_i = x_i - x_{i-1}$ ($i = 2, \ldots$) and the values of $k$, $\beta/\beta_e$, $\beta_e$ are determined at each station. Then, starting with the values $\eta_1 = 0$, $u_1 = 0$, and $\tau_1 = 1$ at $x = 0$, the following sequence of computations is made for each successive increment of path:

1. Find $u_i = u_{i-1} + \Delta u_1$ with equation (14), using $k_i$, $(\beta/\beta_e)_i$, $(\beta_e)_i$, and $\eta_{i-1}$. 


(2) Find $\eta_i$ with equations (10) and (11), using $u_i$. Linear interpolation in table I is used to find $A_1$ to $A_4$, since the computation is relatively insensitive to these quantities. Equation (11) is used to find $A_5$.

(3) Find $\tau_i$ with equation (12) using $u_i$ and $(\beta_e)_i$.

For the numerical computation, equations (14) and (15) are written

\[
u_i = \frac{1}{(\beta_e)_i} \sum_{\ell=2}^{i} k_\ell \left( \frac{\beta}{\beta_e} \right)_\ell \eta_{\ell-1} \Delta x_\ell \quad (14a)
\]

\[
(\beta_e)_i = \frac{\sum_{\ell=2}^{i} k_\ell \left( \frac{\beta}{\beta_e} \right)_\ell \eta_{\ell-1} \Delta x_\ell}{\sum_{\ell=2}^{i} k_\ell \Delta x_\ell} \quad (15a)
\]

Accuracy of the Solution

There are several sources of error that affect the accuracy of the solution. First there is the basic limitation of the functional forms assumed for the temperature and pressure profiles. Obviously not all situations encountered in practice can be accommodated by these functions with acceptable accuracy. For those cases other functional forms must be used. This basic limitation is demonstrated in the section "Application of the Program to an Experiment" where an example is worked out for a temperature profile that cannot be matched exactly by the assumed functional form for the temperature.

Another source of error is generated by the nature of the set of iteration equations for the parameters, equation (8). On the left side,
the matrix of derivatives may be poorly conditioned. The conditioning of the matrix is affected by the selection of the wavelengths of measurement. Proper selection of the wavelengths is treated in the next section.

The residuals on the right side of equation (8) are not exact quantities due to errors in their components $c_{N_L}$, $c_{\tau_L}$, $m_{N_L}$, and $m_{\tau_L}$. The measured quantities $m_{N_L}$ and $m_{\tau_L}$ contain an experimental random measurement error and the computed quantities $c_{N_L}$ and $c_{\tau_L}$ are in error because of uncertainties in the tabulated gas parameters $\beta_s$ and $k_s$. There are also errors due to deficiencies in the band model used in the gas transmittance calculation. These deficiencies in the model are covered in the references cited in the previous section and will not be covered further here. Thus, even if the computer program succeeds in finding a solution that reduces the residual values to zero, the computed parameters are still in error due to the residual errors. By using equations (6) and (7) it can easily be shown that the residual errors at the solution, $\delta R_N$ and $\delta R_\alpha$ are given by

\[
\delta R_N = \frac{\delta c_{N_L}}{c_{N_L}} - \frac{\delta m_{N_L}}{m_{N_L}} \tag{20a}
\]

\[
\delta R_\alpha = \frac{m_{\tau_L}}{1 - m_{\tau_L}} \left( \frac{\delta m_{\tau_L}}{m_{\tau_L}} - \frac{\delta c_{\tau_L}}{c_{\tau_L}} \right) \tag{20b}
\]

where $\delta c_{N_L}$, $\delta m_{N_L}$, $\delta c_{\tau_L}$, and $\delta m_{\tau_L}$ are the errors in $c_{N_L}$, $m_{N_L}$, $c_{\tau_L}$, and $m_{\tau_L}$, respectively.

To proceed further it is necessary to specify the errors in the measured and computed quantities. It will be assumed that all measurements have the same probable error given by $|\delta m_V/m_V|$ and that the computed values for $N_L$ and $\tau_L$ have random errors due to the uncertainty $|\delta k_s/k_s|$ in published $k_s$ values.
The uncertainty in the value of $\beta_S$ will be neglected. Thus, only two random errors will be considered, $|\delta m_V/m_V|$ and $|\delta k_S/k_S|$.

Using equations (10) and the definition $m_{\alpha_L} = 1 - m_{\tau_L}$ it can be easily shown that

\begin{align*}
\left(\frac{\delta m_{NL}}{m_{NL}}\right)^2 &= \left(\frac{\delta m_V}{m_V}\right)^2 \\
\left(\frac{\delta m_{\tau_L}}{m_{\tau_L}}\right)^2 &= 2 \left(\frac{\delta m_V}{m_V}\right)^2 \\
\left(\frac{\delta m_{\alpha_L}}{m_{\alpha_L}}\right)^2 &= 2 \left(\frac{\tau_L}{1 - \tau_L}\right)^2 \left(\frac{\delta m_V}{m_V}\right)^2
\end{align*}
\hspace{1cm} (21a, 21b, 21c)

To estimate the random errors in the computed quantities, assume a simplified transmittance equation given by $c_{\tau_L} = \exp(-kpL)$. It can then be shown that

\begin{align*}
\left(\frac{\delta c_{NL}}{c_{NL}}\right)^2 &= \left(\frac{\delta c_{\alpha_L}}{c_{\alpha_L}}\right)^2 = \left(\frac{\tau_L \ln \tau_L}{1 - \tau_L}\right)^2 \left(\frac{\delta k}{k}\right)^2 \\
\hspace{1cm} (21d)
\end{align*}

The above quantities when substituted into equations (20a) and (20b) give for the squares of the random residual errors

\begin{align*}
\delta R_N^2 &= \left(\frac{\delta m_V}{m_V}\right)^2 + \left(\frac{\tau_L \ln \tau_L}{1 - \tau_L}\right)^2 \left(\frac{\delta k}{k}\right)^2 \\
\hspace{1cm} (22a)
\end{align*}
\[ \delta R^2_{\alpha} = \left( \frac{\tau_L}{1 - \tau_L} \right)^2 \left[ 2 \left( \frac{\delta m V}{m V} \right)^2 + (\ln \tau_L)^2 \left( \frac{\delta k}{k} \right)^2 \right] \]  

(22b)

The random residual error \( \delta R^2_N \) (eq. (22a)) depends on the error \( \delta k/k \). An alternative form that eliminates this dependence is to substitute for equation (6) the expression

\[ \overline{R}_N = (\frac{c N_L}{m N_L})/m N_L \]

(23)

where \( N_L \) is an apparent radiance defined by

\[ N_L = N_L/\alpha_L \]

(24)

By repeating the previous procedure it can be shown that

\[ \delta R^2_N = \left[ 1 + 2 \left( \frac{\tau_L}{1 - \tau_L} \right)^2 \right] \left( \frac{\delta m V}{m V} \right)^2 \]

(25)

The quantity \( \delta R^2_N \) is less than \( \delta R^2_N \) whenever

\[ (\ln \tau_L)^2 > \frac{2(\delta m V/m V)^2}{(\delta k/k)^2} \]

(26)

Because experience has shown that \( \delta R^2_N \) is less than \( \delta R^2_N \) in most practical situations, the computer program presented herein uses \( \overline{R}_N \) given by equation (23) instead of \( R_N \) given by equation (6) for the residuals in equations (8) or (9).

Equations (25) and (22b) give a measure of the uncertainties in the zero values for the residuals at the solution. These expressions are used in the computer program following the procedure outlined in appendix B to compute the random errors in the temperature and pressure profile parameters.
Selection of Wavelengths of Measurement

The wavelengths differ principally in their associated gas absorption coefficients. Figure 2 shows the absorption coefficient $k$ for the 2.7 $\mu$m band of $H_2O$. At wavenumbers near the center of the band (3704 cm$^{-1}$), $k$ decreases with temperature; at the wings, $k$ increases with temperature. Substantial differences in $k$ exist, especially at a low temperature. Another difference due to wavelength is caused by a greater increase of the Planck-function radiance with temperature at the shorter wavelengths. Since the variation of $k$ with wavelength is the phenomenon that enables the profile to be determined, large differences would be expected to be favorable.

The wavelengths are selected to maximize accuracy of the solution, and equally important, to avoid an incorrect second solution that can exist. This preliminary selection is performed through an auxiliary computer program WAVES. The selection procedure will be illustrated with both modes of the temperature profile function, equations (1) and (2).

Avoiding an incorrect solution. - The WAVES program uses the following procedure: For assumed values of the two variable temperature parameters in equations (1) or (2), as applicable, and one variable pressure parameter in equation (3), the quantities $cN_L$ and $c\tau_L$ are computed for each wavelength. These computed quantities are substituted for presumed error-free measurements $mN_L$ and $m\tau_L$ of the assumed profiles. Then, taking one wavelength at a time, one parameter $w$ of the temperature profile is assigned a value different from that assumed. The quantities $cN_L$ and $c\tau_L$ change. Then, new values of the other temperature parameter and the pressure parameter are found by iteration that restore the equalities $cN_L = mN_L$ and $c\tau_L = m\tau_L$. This procedure is repeated for a number of assigned values of the temperature profile parameter $w$, and the results are tabulated by the program.
For each wavelength, the tabulation can be plotted as a curve with the independently varied parameter \( w \) as abscissa and the dependent temperature parameter as ordinate. The intersection of any two curves is a two-wavelength solution for a temperature profile.

As an example, assume a path length of 100 cm, hydrogen-air combustion at 1 atm total pressure having \( \text{H}_2\text{O} \) pressure parameters \( p_c = 0.35 \text{ atm}, \ p_w = 0.30 \text{ atm}, \) and \( n_p = 0.5 \). Computations are made for wavelengths in the 2.7 \( \mu \text{m} \) band of \( \text{H}_2\text{O} \). Results are plotted in figure 3 for the profile of figure 1(a) with \( \xi_T \) as the independent parameter and \( T_c \) as dependent, and in figure 4 for the profile of figure 1(b) with \( T_w^* \) as the independent parameter and \( T_c \) as dependent, with no wall boundary layer \( (x_1 = 0) \). To facilitate plotting and to emphasize differences in the curves, the ordinate \( Y \) of the graph is tabulated by the program as a function

\[
Y = Z + \zeta(w - w_o)
\]

where \( Z \) is the dependent parameter, \( w \) is the independent parameter, \( w_o \) is the originally-assumed value, and \( \zeta \) is chosen by the program as described in appendix C. All curves intersect at the true solution. Some pairs of curves intersect at a second point that is an incorrect solution. For example, in figure 4, wavenumbers 3500 and 3100 \( \text{cm}^{-1} \) intersect at approximately \( T_w^* = 2200 \text{ K} \) and \( T_c = 1840 \text{ K} \). A solution by the computer program converged to \( T_w^* = 2223 \text{ K} \) and \( T_c = 1873 \text{ K} \) from a starting point \( T_w^* = 2300 \text{ K} \) and \( T_c = 1800 \text{ K} \). To assure convergence to the true solution, a pair of curves should have increasing separation with distance from the true solution. Accuracy is greatest when there is a large difference of slope between a pair of curves. Where two curves become parallel, accuracy approaches zero.

Inspection of figures 3 and 4 show that no single pair of wavelengths is satisfactory for all profiles. Acceptable pairs of wavenumbers in figure 3 are (3100, 3550 \( \text{cm}^{-1} \)) and (3100, 3775 \( \text{cm}^{-1} \)). The 2000 \text{ K} almost-isothermal profile that led to figure 4 shows an acceptable pair
(3500, 3100 cm\(^{-1}\)) for \(T^*_w\) below 2000 K, and an acceptable pair
(4100, 3400 cm\(^{-1}\)) for \(T^*_w\) above 2000 K.

Tests of the pressure profile when the two pressure parameters
\(p_w\) and \(p_c\) were assumed to be variables, and only \(T_c\) was vari-
able, gave curves nearly alike for all wavelengths. Thus, poor ac-
curacy of the computed pressure profile makes this technique unac-
ceptable; it is therefore necessary to limit oneself to only one variable
pressure parameter. The reasons for this poor accuracy are (1) that
radiance and absorption coefficient usually vary more strongly with
temperature than they do with pressure and (2) that the measurement
of \(\tau_L\), equation (10) which is the principal source of information about
the pressure, is sensitive only to the integral of pressure over the
path and not to local values of pressure, whereas \(N_L\) (which is the
principal source of information about temperature) is sensitive to local
temperature.

Maximizing accuracy of the solution. - The program that led to
figures 3 and 4 does not provide an estimate of the error for pairs of
wavelengths. This estimate is provided by the main program PROFIL
(MODE=1). The error estimate is made by pairing one principal
wavelength with each of all the other wavelengths to be tested. For
each dependent profile parameter, the program tabulates the error in
the parameter due to assigned errors of the radiation-measurement
voltages \(V\) and the tabulated absorption coefficient \(k_s\).

As an example, such tabulated values are plotted in figure 5 for the
parameter \(T_c\) with the profiles and some of the wavelengths of figure 3.
The assumed errors were 1 percent in \(V\) and 5 percent in \(k_s\). Another
example with the same assumed error is plotted in figure 6 for \(T_c\)
with the profiles and some of the wavelengths of figure 4. These errors
are for profiles with \(T_c = 2000\) K, and the range of values covered by
the abscissa parameter. The errors are consistent with the slope-
difference of curve pairs in figures 3 and 4. The error is minimized
in figure 6 with wavenumber pairs (4100, 3400 cm\(^{-1}\)) above 1950 K,
and (3500, 3100 cm\(^{-1}\)) below 1850 K.
All four of these wavenumbers have been used simultaneously in a least squares solution by the program PROFIL (MODE=3). The resulting error also plotted in figure 6(b), shows improvement at all values of $T_w^*$. The effect of path length on the error at $T_w^* = 1200$ and $2000$ K is listed in table III, for this four-wavelength combination. The error varies approximately as the inverse square root of the path length, in this example.

PROGRAM DESCRIPTION

The accuracy of the temperature profile found with measured data is dependent on the pressure and temperature profiles, path length, and wavelengths selected for measurement. It is desirable as a preliminary step to assume realistic values for the path length and pressure and temperature profiles for the absorbing gas, and then to select wavelengths and estimate the accuracy of the temperature profile parameters as was illustrated in the Selection of Wavelengths of Measurement section.

A separate main program WAVES (described in "Avoiding an incorrect solution") is designed for the selection of wavelengths. Using these wavelengths, a principal main program PROFIL gives results in three modes of operation:

MODE=1: This program computes the error in the dependent profile parameters that would be caused by assigned random errors of radiometric measurements and tabulated absorption coefficients. For given values of all profile parameters, gas radiance and transmittance are calculated and the parameter errors are computed as in appendix B. Actual radiometric measurements are not required. The estimate may be made for any pair of wavelengths consisting of one "principal" wavelength and any one of up to seven others.

MODE=2: This program computes values for the dependent profile parameters using the iterative procedure described previously. Limits are assigned to the dependent parameters by the user; if a limit is
reached during the iteration, that parameter becomes fixed, and the iteration proceeds for the remaining dependent parameters. When a least-squares solution is used, the magnitude of the final root-mean-square residual $R$ (eq. (9)) is also provided. In addition, using the same procedure as in MODE=1, the error in the dependent parameters that would be caused by assigned random errors in the radiometric measurements and tabulated absorption coefficients is computed.

**MODE=3**: This program is used to find the change of temperature profile that would be caused by a change in one of the independent profile parameters. A second set of data cards is required that incorporate the change. Starting with an assumed profile and gas-property data, the resulting radiance and transmittance that would be measured are calculated. The second set of data cards is then introduced to change one of the independent profile parameters, and the computation in MODE=2 is performed using the previous radiance and transmittance values to yield a revised profile. This process is useful in identifying independent profile parameters to which the temperature profile is unusually sensitive.

The flowchart for program PROFIL is figure 7. After reading input data and calculating some initial conditions, the main program calls subroutines TEMP that calculates profiles, and TRANS that calculates gas transmittance and radiated flux. The subroutines are principally a computation using equations presented in the text. The equation numbers appear on comment cards in the listings.

The test result DONE=1 is obtained when (1) the number of iterations reaches a preset number, or (2) when the root-mean-square sum of all residuals is less than $10^{-4}$, or (3) when the fractional change of the variable parameters per iterative step has become less than $10^{-4}$ for $T_W$ and $T_C$, and less than $10^{-3}$ for $p_C$ and $n_T$. Criterion (3) is needed when there are more residuals than variable parameters, because the residuals then reach a nonzero minimum.

A subsidiary loop of moderate complexity determines the variable parameter increments and tests the parameters for exceeding their
limits. The loop contains a control index number \( \text{KEY} \) that manipulates the index of FORTRAN DO statements as follows. The variable profile parameters in equation (1) are \( n_T, T_c, p_c, T_w^{*} \). They are represented by a FORTRAN subscripted variable \( \text{PA}(K) \) that is controlled by a DO index \( K=K1, K2, K3 \). An index initially \( K=1, 3, 1 \) selects parameters \( n_T, T_c, p_c \) for the profiles of figure 1(a) and \( K=2, 4, 1 \) selects parameters \( T_c, p_c, T_w^{*} \) for the profiles of figure 1(b).

Any parameter in either profile can be fixed when it reaches an assigned limit by changing the index parameters \( K1, K2, K3 \). This is done by setting \( K1, K2, K3 \) equal to the subscripted quantities \( \text{KEY1(\text{KEY})}, \text{KEY2(\text{KEY})}, \text{KEY3(\text{KEY})} \) that can be manipulated. The subscript \( \text{KEY} \) can select any combination of numbers for \( K1, K2, K3 \) as shown in table IV. The variable parameters for each \( \text{KEY} \) are also listed. By designating the profiles of figure 1(a) as \( \text{PROF}=1 \) and the profiles of figure 1(b) as \( \text{PROF}=2 \) the table is valid for \( \text{PROF}=1 \) and \( \text{PROF}=2 \) when subsequent additions are made, \( K1=K1-1+\text{PROF}, \) and \( K2=K2-1+\text{PROF}. \) The initial profile with no limits reached is \( \text{KEY}=1. \)

Before entering the loop, \( \text{KEY}=1, \) and \( K1, K2, K3, \) are set as in the table. This frees the currently fixed parameters to return inside their limits during every iterative step. Thus, on first entering the loop, all three parameters (corresponding to \( \text{KEY}=1 \)) are incremented and compared with their limits. If the \( K'th \) parameter is within its limit, a limit-indicating variable \( \text{LIM}(K4)=0 \) where \( K4=K-\text{PROF}+1 \) (to be valid for \( \text{PROF}=1 \) and \( \text{PROF}=2 \)). If the \( K'th \) parameter is outside the limit, \( \text{LIM}(K4)=1. \) The value of \( \text{KEY} \) is a number from 1 to 8 given by

\[
\text{KEY}=1+4*\text{LIM}(1)+2*\text{LIM}(2)+\text{LIM}(3)
\]

If this new value of \( \text{KEY} \) is not 1 or 8 the preceding procedure of this paragraph is repeated only once from the start of the loop with the new value of \( \text{KEY}, \) and the corresponding \( K1, K2, K3 \) to find new parameter increments and tentative new parameter values. The loop is then exited, the tentative new parameter values are then accepted,
and the iteration proceeds. At the solution the error of the profile parameters is estimated. The program listing with a FORTRAN symbol list is appendix D. The subroutine listings are appendixes E and F.

The flow chart for program WAVES is figure 8. After reading the input data, the program (following the procedure described in Selection of Wavelengths of Measurement) first sets $mN_L = cN_L$ and $m\tau_L = c\tau_L$ for the initial profile. Then follow three nested loops. An outer DO loop for selecting each given wavelength, a DO loop for assigning given values to one independent variable profile parameter; and an iteration loop like PROFIL that finds the other two dependent variable parameters. If a variable parameter reaches a limit during iteration, the iteration is ended. After completion of the two DO loops the results are tabulated. The program listing, with FORTRAN symbols not used in program PROFIL, is appendix G.

Successive problems in the same run may omit input data that is not changed. (Both PROFIL and WAVES programs.) The READ data is omitted by not putting IREAD=1 in the NAMELIST data. In the NAMELIST, the data-input parameters of temperature, $T_w$, $T_c$, and $n_T$, and pressure, $p_w$, $p_c$, and $n_p$ are given starting values that are not changed by the program because they are replaced by different internal symbols for computation. After computation the values of the internal symbols are printed, but with the corresponding symbols of the initial data-input parameters.

PROFIL PROGRAM USE

Input

The input consists of four types of data: (1) computer program control constants (2) measurements of gas radiance and transmittance at selected wavelengths (3) tabulations from the literature of gas transmission parameters at selected wavelengths and (4) independently determined or estimated profiles of partial pressures of the gas reaction products.
The collected input data are read in with a FORTRAN NAMELIST for single-subscript quantities, followed by a FORTRAN READ STATEMENT for multiple-subscript quantities. An example in appendix H shows this input data in the same format as punched on cards, for MODE=1, five wavenumbers, and two gases, H₂O and N₂. The data conform to the following specifications.

**NAMELIST DATA.** - The following list gives the FORTRAN symbol with its subscripted maximum dimension and equivalent algebraic symbol, in the `NAMELIST' sequence.

<table>
<thead>
<tr>
<th>FORTRAN symbol</th>
<th>Algebraic symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>MODE</td>
<td></td>
<td>MODE=1 finds error estimate of pairs of wavenumbers consisting of the first wavenumber paired with each succeeding wavenumber. MODE=2 finds solution to given measurements, with error estimate. MODE=3 finds gas radiance and transmittance for given input, then requires NAMELIST repeated that may have changes from the first NAMELIST, and finds solution the same as MODE=2.</td>
</tr>
<tr>
<td>PROF</td>
<td></td>
<td>PROF=1 profile figure 1(a), variable parameters TC, PC, NT. PROF=2 profile figure 1(b), variable parameters TW, TC, PC, with given boundary layer wall temperature TWB, thickness X(JB).</td>
</tr>
<tr>
<td>FORTRAN symbol</td>
<td>Algebraic symbol</td>
<td>Description</td>
</tr>
<tr>
<td>----------------</td>
<td>-----------------</td>
<td>-------------</td>
</tr>
<tr>
<td>IREAD</td>
<td></td>
<td>IREAD=1 requires READ data for GAS, ALPH, KTAB, BTAB. With IREAD=1 omitted, READ data must be omitted</td>
</tr>
<tr>
<td>PATH</td>
<td>L</td>
<td>Test section path length, cm</td>
</tr>
<tr>
<td>I1 (8 maximum)</td>
<td></td>
<td>Number of wavenumbers for computation (when IREAD=1, I1 must equal number of data cards for KTAB and BTAB)</td>
</tr>
<tr>
<td>WAVE(8)</td>
<td>( \lambda )</td>
<td>Wavenumber cm(^{-1})</td>
</tr>
<tr>
<td>MRL(8)</td>
<td>( m_{NL} )</td>
<td>Measured radiance ( W ), cm(^{-1}) cm(^{-2}) ster(^{-1}) (eq. (10))</td>
</tr>
<tr>
<td>MTAUL(8)</td>
<td>( m_{rL} )</td>
<td>Measured transmittance (eq. (10))</td>
</tr>
<tr>
<td>ERRV</td>
<td></td>
<td>Percent error of radiation measurement</td>
</tr>
<tr>
<td>ERRK</td>
<td></td>
<td>Percent error of tabulated absorption coefficient</td>
</tr>
<tr>
<td>TW</td>
<td>( T_w, T^* )</td>
<td>Gas temperature, K, at wall. For PROF=2 with boundary layer, ( T^* ) approximates free stream temperature near the wall</td>
</tr>
<tr>
<td>TC</td>
<td>( T_c )</td>
<td>Gas temperature, K, on axis</td>
</tr>
<tr>
<td>NT</td>
<td>( n_T )</td>
<td>Gas temperature profile equation exponent</td>
</tr>
<tr>
<td>TWB</td>
<td>( T_w )</td>
<td>Gas temperature, K, at wall for PROF=2 with boundary layer</td>
</tr>
<tr>
<td>FORTRAN symbol</td>
<td>Algebraic symbol</td>
<td>Description</td>
</tr>
<tr>
<td>----------------</td>
<td>------------------</td>
<td>-------------</td>
</tr>
<tr>
<td>JB (minimum is 1 at wall)</td>
<td>$X(JB)$</td>
<td>Index for $X(JB)$ giving distance $x$ from wall where boundary layer ends, for PROF=2</td>
</tr>
<tr>
<td>UPLIM(4)</td>
<td></td>
<td>Upper limit of profile parameters TW, TC, PC, NT</td>
</tr>
<tr>
<td>BOTLIM(4)</td>
<td></td>
<td>Lower limit of profile parameters TW, TC, PC, NT</td>
</tr>
<tr>
<td>L1 (3 maximum)</td>
<td>$L_1$</td>
<td>Number of absorbing gases</td>
</tr>
<tr>
<td>L2 (6 maximum)</td>
<td>$L_2$</td>
<td>Number of absorbing plus non-absorbing gases</td>
</tr>
<tr>
<td>PS</td>
<td>$P_S$</td>
<td>Gas static pressure, constant along optical path</td>
</tr>
<tr>
<td>PC(6)</td>
<td>$P_C$</td>
<td>Partial pressure of each gas, on axis</td>
</tr>
<tr>
<td>NP(6)</td>
<td>$n_p$</td>
<td>Pressure profile equation exponent of each gas</td>
</tr>
<tr>
<td>PW(6)</td>
<td>$P_w$</td>
<td>Partial pressure of each gas, at wall</td>
</tr>
<tr>
<td>NK (8 maximum)</td>
<td>$N_K$</td>
<td>Number of tabulated values of KTAB read in for data</td>
</tr>
<tr>
<td>TKTAB(8)</td>
<td></td>
<td>Temperatures at which values of KTAB are tabulated in READ data</td>
</tr>
<tr>
<td>NB (8) maximum)</td>
<td>$N_B$</td>
<td>Number of tabulated values of BTAB read in for data</td>
</tr>
<tr>
<td>TBTAB(8)</td>
<td></td>
<td>Temperatures at which values of BTAB are tabulated in READ data</td>
</tr>
</tbody>
</table>
FORTRAN symbol | Algebraic symbol | Description
--- | --- | ---
J1 (41 maximum) | Number of stations along optical path. Must be odd. Omit if J1=21 in DATA-statement of program is acceptable.
Z(J) | Station distance ratio, from wall to center, as fractional value 0 to 1. Omit if list in DATA-statement of program is acceptable. Maximum J=(J1+1)/2
ITER | Maximum number of iterations

READ statement data. - The following list gives the FORTRAN symbol with its subscripted maximum dimension, the format of each card, and the equivalent algebraic symbol.

<table>
<thead>
<tr>
<th>FORTRAN symbol</th>
<th>Format</th>
<th>Algebraic symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>GAS(6)</td>
<td>6A6</td>
<td></td>
<td>Names of all gases</td>
</tr>
<tr>
<td>ALPH(3, 6)</td>
<td>(12F6.0)</td>
<td>α*</td>
<td>Broadening factor for up to 3 absorbing gases by up to 6 total number of gases. Card sequence is one card for each L1 absorbing gases. Each card lists the broadening factor for each of L2 gases.</td>
</tr>
</tbody>
</table>
The two gas transmittance parameters KTAB and BTAB depend on temperature. For $\text{H}_2\text{O}$ and $\text{CO}_2$, they are tabulated in references 10 to 12 with KTAB and BTAB normalized to S. T. P. The program interpolates between tabulated values to find a tabulated value at local temperature, then denormalizes to obtain $KK$ and $BB$ at local temperature and pressure in accordance with equations (18) and (19). Linear interpolation is used. If the profile temperature is outside the temperature range of the tabulation, $KK$ and $BB$ are limited to the extreme tabulated value. It is thus desirable to prepare the tabulation with a temperature range running from the lower to upper limits appearing on other input cards for the profile temperatures $TC$, $TW$, and $TWB$. 

<table>
<thead>
<tr>
<th>FORTRAN symbol</th>
<th>Format</th>
<th>Algebraic symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>KTAB(8, 3, 8)</td>
<td>(12F6.0)</td>
<td>$k_o$</td>
<td>Absorption coefficient at S. T. P. for up to $I_1=8$ wavenumbers, $L_1=3$ gases, $NK=8$ tabulated points. Card sequence is one set of cards for each of $L_1$ absorbing gases. Each set has $I_1$ cards corresponding to the wavenumbers in NAMELIST. Each card lists absorption coefficients corresponding to temperatures $TTAB$ in NAMELIST.</td>
</tr>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>BTAB(8, 3, 8)</td>
<td>(12F6.0)</td>
<td>$\beta_o$</td>
<td>Line-broadening coefficient at S. T. P. for up to $I_1=8$ wavenumbers, $L_1=3$ gases, $NB=8$ tabulated points. Card sequence same as for KTAB above. Each card lists broadening coefficients corresponding to temperature $TBTAB$ in NAMELIST.</td>
</tr>
</tbody>
</table>
Output

An example of the output shown in appendix H for MODE = 1 and PROF = 2 consists of four parts:

1. The input NAMELIST and READ data.
2. Estimated error of the profile parameters caused by the residuals, equations (20) and (25), due to the errors of measurement ERRV and of absorption coefficient ERRK. The example has ERRV = 1 percent and ERRK = 5 percent. The example shows four wavenumbers 3100, 3400, 4100, and 3000 cm$^{-1}$ successively paired with the first wavenumber 3500 cm$^{-1}$. The first pair have residuals $R_N = 2.0$ and 3.2 percent at 3500 and 3100 cm$^{-1}$, and $R_\alpha = 4.4$ percent at 3500 cm$^{-1}$. These residuals cause the listed three errors for each parameter, and their rms total.

3. Transmittance at each wavenumber.
4. Temperature and pressure profiles.

An example shown in appendix I for MODE = 3 was in the same run and followed the preceding example. The READ statement data and most items in the NAMELIST were not changed. Thus, only two data cards were required. The first four wavenumbers were used in a least squares solution. Appendix I shows the input data in the same format as punched on cards. The first NAMELIST has MODE = 3 and II = 4. The required second NAMELIST has a change in the nonvariable pressure parameter, $p_w = 0.36$ replacing $p_w = 0.30$. The output consists of four parts.

1. The first input NAMELIST and the second NAMELIST that differs by the new $p_w = 0.36$ and an internal change to MODE = 2. Because IREAD = 1 was omitted, the READ data were not required or printed out.

2. Each iteration step lists the parameters, the residuals $R_N$ for each wavenumber, the residual $R_\alpha$ for the first wavenumber, the rms total residual, and a step size that is the total fractional change of the variable parameters. In this example the 20 percent change of $p_w$ from 0.30 to 0.36 caused errors $\delta T_c = 1.2$ K or 0.06 percent, $\delta P_c = -0.019$ atm or 5.4 percent, and $\delta T_w = 14$ K or 0.5 percent. Because
four wavenumbers were used (I1=4) the iteration was terminated by the small step size, as the residuals became stationary and remained nonzero.

3. Estimated error of the profile parameters caused by the residuals $\delta R_N$ and $\delta R_\alpha$. The percent errors are $\delta T_c = 3.5$ percent, $\delta p_c = 7.1$ percent and $\delta T_w = 6.6$ percent. These errors are much larger than those listed in (2) above caused by the change of $p_w$.

4. Temperature and pressure profiles.
The output in MODE=2 is the same as MODE=3 without the first NAMELIST.

WAVES PROGRAM USE

Input

The input includes all quantities listed for PROFIL. Three additional quantities in the NAMELIST select the independent temperature parameter and assign values to it that differ from the initial value. The independent parameter is determined by index K4 of PA(K4), where K4=1 for $n_T$, K4=2 for $T_c$, and K4=4 for $T_w$. The program selects the dependent parameter in accordance with the profile, either PROF=1 or PROF=2.

<table>
<thead>
<tr>
<th>FORTRAN symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>K4</td>
<td>Index of independent variable temperature parameter PA(K4)</td>
</tr>
<tr>
<td>NPA</td>
<td>Number of values of PA1 to be used, up to ten.</td>
</tr>
<tr>
<td>PA1(10)</td>
<td>Values that may be assigned to PA(K4).</td>
</tr>
</tbody>
</table>

Output

An example in appendix J shows the input data in the same format as punched on cards for four wavenumbers and two gases, $H_2O$ and $N_2$. The output has four parts:
1. The NAMELIST and READ data
2. Temperature and pressure profiles
3. At each solution found by iteration, the four variable profile parameters, wavenumbers, number of iterations, final rms residual
4. Tabulations of dependent parameter against independent parameter for each solution in (2), with the dependent parameter modified for plotting by equation (27) with the constant \( \xi \)

Examples of plotted tabulation are figures 3 and 4.

DIAGNOSTICS

A warning is printed each time:
1. The pressure of all absorbing gases exceeds the static pressure at any point on the pressure profile.
2. During iteration when a variable parameter reaches the assigned upper or lower limit.

APPLICATION OF THE PROGRAMS TO AN EXPERIMENT

Three steps are used to determine whether this method will be sufficiently accurate for an application. These steps will be summarized in this section, and an example of an application will be given. The steps are:
1. Estimates of the temperature and pressure profiles are made, and the profile equations are selected.
2. Some wavenumbers for measurement are selected, and then compared using graphs of the output of the WAVES program. This was demonstrated in figures 3 and 4.
3. Accuracy of the dependent profile parameters is determined for the best pairs of wavenumbers selected from graphs in step (2). This was demonstrated in figures 5 and 6. Tests with the PROFIL program in MODE=3 may be run with a perturbation of an independent profile parameter. The resulting change of all dependent profile parameters
may be judged acceptable or excessive. This is demonstrated in appendix I.

Based on the results of steps (2) and (3), it can then be determined if there exists a pair of wavenumbers that lead an acceptably low level of random error in the computed parameters. The experimental measurements are then made at the wavenumbers chosen and the results serve as inputs to the PROFIL program in MODE=2 for determining the temperature and pressure profiles.

An example of the PROFIL program is given to illustrate the limitation of the assumed functional form of the temperature profile as described by two variable parameters. An assumed profile with a high temperature core is shown in figure 9. This profile cannot be matched exactly by equations (1a) or (1b). The pressure profile is the same as used in other examples; hydrogen-air combustion at 1 atm, parameters $p_w = 0.30$ atm, $p_c = 0.35$ atm, and $n_p = 0.50$.

By following steps (1) to (3) given at the beginning of this section it was found that wavenumbers of 3100 cm$^{-1}$ and 3500 cm$^{-1}$ were suitable for use. The radiance and transmittance of the assumed profile were calculated at these wavenumbers to represent error-free measurements. With these measurements as input data, the PROFIL program in MODE=2 found the profiles with equations (1a) and (1b) that are plotted in figure 9. The profiles in figure 9(a) and (c) use an independently determined wall temperature $T_w = 1100$ K that was made 100 K lower than the assumed profile $T_w = 1200$ K. This represents an error of $T_w$. The difference between the assumed and computed profiles is an error of approximation due to limitations in the ability of the profile functions to assume an arbitrary shape. This may be compared with the error band that is due to an assumed radiance measurement error of one percent and a tabulated absorption coefficient error of five percent.

The PROFIL program data cards and output for figure 9(a) are shown in appendix K. The output format is the same as shown and described for MODE=3, appendix I, without the first namelist.
CONCLUDING REMARKS

All of the examples presented in this report were for hydrogen-air combustion at a pressure of 1 atmosphere with a path length of 100 cm. These reactants produce $\text{H}_2\text{O}$ as the absorbing gas. It was shown in Table III that the random error in the computed profiles decreases with increasing path length. It can also be shown that the random error in the profiles will decrease with increasing pressure or by using a gas with greater absorptance such as $\text{CO}_2$. However, in applications where the path length, gas pressure, and gas type are all fixed, a user of this computer program has only the choice of the wavelengths of measurement at his disposal in order to attempt to bring the computed profile errors within acceptable bounds.
APPENDIX A

SYMBOLS

A matrix of first derivatives
A₁ to A₅ coefficients in eqs. (16) and (17)
a element of A
B matrix of second derivatives
b element of B
d average spectral line spacing
k gas absorption coefficient, cm⁻¹
L total path length of profile
nₜ exponent in equation for temperature profile
nₚ exponent in equation for pressure profile
Nₗ actual gas radiance
m temperature-gradient, eq. (2)
N* radiance by Planck function
Nₗ apparent radiance defined by eq. (24)
p partial pressure of absorbing gas
pₛ static pressure
q number of absorbing gases
R total residual, rms value; also column matrix of residuals
R (subscripted) residual, eq. (6) based on Nₗ and τₗ
δR (subscripted) residual errors, eqs. (20a) and (20b)
R (subscripted) residual, eqs. (23), based on Nₗ
δR (subscripted) residual error, eq. (25)
T  temperature
T*  temperature parameter in temperature profile, eq. (2), fig. 2(b)
u  dimensionless optical depth
V  detector output voltage
w  independently varied parameter
xL  boundary layer thickness
x  distance along profile or optical path
y  dimensionless path-length ratio, eq. (1) or variable parameter, eq. (8), (B1)
Y  graph-plotting ordinate, eq. (27)
Z  dependent parameter
z  dimensionless path-length ratio, eq. (2)
αL  absorption factor of gas
α*  spectral line-broadening coefficient
β  spectral-line overlap factor, band model parameter
γ  average spectral line width
η  interpolation parameter
λ  wavelength
ρ  gas density
τL  transmittance
ξ  graph-plotting constant, eq. (27)

Subscripts:
c  centerline of profile
s  standard conditions
w  ends of profile (wall)
p  pressure
T  temperature
N  radiance
e  effective value
L  total path length
α  absorptance
λ  wavelength
o  initial conditions

Superscripts:
c  computed
m  measured

Running indices:
i  path length; also wavelength in eq. (6)
j  absorbing gases
k  nonabsorbing gases; also dependent parameters in matrix solution
l  intermediate index for path length
APPENDIX B

PROFILE PARAMETER ERROR ESTIMATE

In order to use matrix notation and FORTRAN coding, the four variable parameter symbols $T_c$, $T_w$, $p_c$, and $n_T$ are replaced by one subscripted symbol $y_j$. Only three of these are treated as dependent variables at any one time.

Due to random errors in the measured and computed terms that form the residuals $R_N$ and $R_\alpha$, there will also be a random error $\delta y_j$ associated with each parameter $y_j$. The random errors in the residuals are denoted by $\delta R_i$ (see eqs. (20) and (22)).

When the number of equations is equal to the number $m$ of unknowns, the errors $\delta y_j/y_j$ are a solution of $m$ equations in $m$ unknowns,

$$
\sum_{j=1}^{m} \frac{\partial R_i}{\partial (\delta y_j/y_j)} \cdot \left( \frac{\delta y_j}{y_j} \right) = \delta R_i \quad i = 1, m
$$

(B1)

or, in matrix notation,

$$
A \left( \frac{\delta y}{y} \right) = \delta R
$$

(B2)

The elements of $A$ are partial derivatives in equation (B1) that are found by numerical differentiation in the computer program.

When the number $n$ of equations is greater than the number $m$ of unknowns, the least squares method is applied to give the equation

$$
A^T A \left( \frac{\delta y}{y} \right) = A^T \delta R
$$

(B3)

where $A^T$ is the transpose of $A$. This can be written as
\[
\frac{\delta y}{y} = \left[(A^T A)^{-1} A^T\right] R
\]

which is equivalent to the set of \( n \) equations, and \( m \) unknowns,

\[
\sum_{i=1}^{n} \frac{\partial (\delta y_i / y_i)}{\partial R_i} \cdot \delta R_i = \frac{\delta y_i}{y_i}
\]

Each term in equation (B5) isolates the contributions of \( \delta R_i \) to the total error of each variable parameter. Since the sign of \( \delta R_i \) is equally likely to be plus or minus, the rms total for all \( n \) terms gives the estimated error for each \( j \) parameter.

**Damped Least Squares Method**

Where an iterative method of solution is used to deduce the profile parameters from experimental measurements, the profile parameter fractional increments are \( \delta y_j / y_j \) for an iterative step. The increment size is determined by the residuals \( R_i \) which are to be minimized. These residuals are: \( \overline{R}_N \), equation (23), at each wavelength \( \lambda_i \); \( R_\alpha \), equation (7), at wavelength \( \lambda_1 \). The least squares method, equation (B3), minimizes \( R \) by reducing \( A^T R \) to zero. Near the solution where \( -A^T R \) becomes zero, damping is required to prevent oscillation of the variable parameters about the solution (refs. 17 and 18). When a damping factor is selected in accordance with equation (11) of reference 19, equation (B3) becomes

\[
\left[A^T A + (p/q)Q\right] \frac{\delta y}{y} = -A^T R
\]

The elements of matrix \( A \) are first derivatives of the residual, given by

\[
a_{ij} = y_j (\partial R_i / \partial y_j)
\]
where $R_1$ is by definition a fractional value. The transpose of $A$ is $A^T$. The damping increases the principal diagonal of $A^TA$ by a factor $1 + (p/q)$ where $Q$ is a diagonal matrix whose elements are the principal-diagonal elements of $A^TA$. The number $q$ is the length of the principal-diagonal vector of $A^TA$ whose elements are $q_{i,i}$ so that
\[
q = \left( \sum_{i} q_{i,i}^2 \right)^{1/2}
\] (B8)

The number $p$ is the length of a vector given by the matrix product $B^TR$, whose elements are $p_{i}$, so that
\[
p = \left( \sum_{i} p_{i,i}^2 \right)^{1/2}
\] (B9)

The elements of $B$ are second derivatives of the residual given by
\[
b_{ij} = y_j^2 \frac{\partial^2 R_i}{\partial y_j^2}
\] (B10)

Finite differences are used to find $a_{ij}$ and $b_{ij}$. First treat the profile parameter $y_1$ as follows for all wavelengths:

(a) Calculate current values of $N_L$ and $\tau_L$
(b) Increase $y_1$ by multiplying it by 1.01
(c) Calculate new values $N_{L,a}$ and $\tau_{L,a}$
(d) Decrease $y_1$ by a factor 0.99/1.01
(e) Calculate new values $N_{L,b}$ and $\tau_{L,b}$
(f) Restore $y_1$ to its starting value by multiplying it by $1/0.99$

The first derivatives for the $i$th wavelength, $j$th parameter are
Next, repeat the procedure (steps (b) through (f)) for the succeeding profile parameters $y_j$. 

\[ a_{ij} = \left( cN_L, b - cN_L, a / [0.02(1 - m_{N_L})] \right) \]  

\[ a_{ij} = \left( c\tau_L, b - c\tau_L, a / [0.02(1 - m\tau_L)] \right) \]  

Next, repeat the procedure (steps (b) through (f)) for the succeeding profile parameters $y_j$. 

\[ b_{ij} = \left( cN_L, a + cN_L, b - 2cN_L / [0.01^2(1 - m_{N_L})] \right) \]  

\[ b_{ij} = \left( c\tau_L, a + c\tau_L, b - 2c\tau_L / [0.01^2(1 - m\tau_L)] \right) \]
APPENDIX C

DETERMINATION OF $\xi$ IN EQUATION (27)

The WAVES program involves the determination of how wavelength $\lambda$ affects the relation between a dependent temperature profile parameter $Z$ and an independent temperature-profile parameter $w$. At the initial value $w_0$, the value of $Z(w_0)$ is invariant with wavelength. However, $Z(w, \lambda)$ changes slightly with wavelength when $w \neq w_0$. The temperature-profile determination depends on these small changes. A graph of $Z$ against $w$ on an ordinary sheet of graph paper would show curves of considerable slope, so that differences between curves for various values of $\lambda$ would not be readily apparent. To exaggerate these differences, the ordinate is changed from $Z$ to $Z + \xi(w - w_0)$.

The value of $\xi$ is determined as follows.

Let the range of the independent parameter be

$$w_n \leq w \leq w_m$$

Among the values of $Z(w)$ for all the wavelengths which are tried in the computation, there will be a maximum value $Z_{\max}(w_n)$ and a minimum value $Z_{\min}(w_n)$. Similarly, there will be a maximum value $Z_{\max}(w_m)$ and a minimum value $Z_{\min}(w_m)$. The value of $\xi$ is taken as

$$\xi = \frac{1}{2} \left[ \frac{Z_{\max}(w_n) + Z_{\min}(w_n)}{2(w_n - w_0)} + \frac{Z_{\max}(w_m) + Z_{\min}(w_m)}{2(w_m - w_0)} \right]$$

(C1)

The total span of ordinate values is thereby reduced severalfold.
APPENDIX D

PROFIL PROGRAM

Program Symbols

The following FORTRAN symbol list includes symbols in the subroutines of appendixes E and F. It does not include symbols defined for NAMELIST and READ data in the section PROFIL PROGRAM USE.

<table>
<thead>
<tr>
<th>FORTRAN symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>A(5,5)</td>
<td>Condensed matrix of first derivatives</td>
</tr>
<tr>
<td>B(4)</td>
<td>Condensed matrix of second derivatives</td>
</tr>
<tr>
<td>BB(8, 3, 41)</td>
<td>Denormalized and broadened BO</td>
</tr>
<tr>
<td>BE(8, 3, 41)</td>
<td>BB weighted by KK</td>
</tr>
<tr>
<td>BO(8, 3, 21)</td>
<td>Interpolated local value of BTAB</td>
</tr>
<tr>
<td>CP(6, 41)</td>
<td>Constant of pressure profiles; ratio of each absorbing gas pressure to first absorbing gas pressure; ratio of each nonabsorbing gas pressure to the total pressure of non-absorbing gases</td>
</tr>
<tr>
<td>Cl</td>
<td>Constant of pressure profile of first absorbing gas, PW(1)/PC(1)</td>
</tr>
<tr>
<td>DAMP</td>
<td>Damping constant for diagonal of least squares matrix</td>
</tr>
<tr>
<td>DEL(4)</td>
<td>Fractional change of variable parameter for derivatives (in data statement)</td>
</tr>
<tr>
<td>DPA(4)</td>
<td>Variable parameter increment for iteration step</td>
</tr>
<tr>
<td>DPAPA(4)</td>
<td>Fractional value of DPA</td>
</tr>
<tr>
<td><strong>FORTRAN symbol</strong></td>
<td><strong>Description</strong></td>
</tr>
<tr>
<td>---------------------</td>
<td>--------------------------------------</td>
</tr>
<tr>
<td>DPV(3)</td>
<td>DPA in condensed matrix</td>
</tr>
<tr>
<td>DTAU(8, 41)</td>
<td>Increment in transmittance</td>
</tr>
<tr>
<td>DUM</td>
<td>Dummy to prevent overflow or underflow</td>
</tr>
<tr>
<td>DUM1</td>
<td>Dummy to prevent overflow or underflow</td>
</tr>
<tr>
<td>DUM2</td>
<td>Dummy to prevent overflow or underflow</td>
</tr>
<tr>
<td>DX(41)</td>
<td>Distance between stations X along path</td>
</tr>
<tr>
<td>ERR(10)</td>
<td>Residual caused by errors ERRV and ERRK</td>
</tr>
<tr>
<td>ETA(8, 3, 41)</td>
<td>Interpolation parameter</td>
</tr>
<tr>
<td>G(10, 6)</td>
<td>First derivatives for least squares matrix</td>
</tr>
<tr>
<td>GSAV(8, 4)</td>
<td>Dummy variable equal to G</td>
</tr>
<tr>
<td>GV(9, 5)</td>
<td>Dummy variable equal to G in condensed matrix</td>
</tr>
<tr>
<td>H(9, 5)</td>
<td>Second derivatives for damping least squares matrix</td>
</tr>
<tr>
<td>HV(9, 5)</td>
<td>Dummy variable equal to H</td>
</tr>
<tr>
<td>IA</td>
<td>Index parameter equal to I</td>
</tr>
<tr>
<td>IB</td>
<td>Index parameter equal to II</td>
</tr>
<tr>
<td>ITER1</td>
<td>Iteration counter</td>
</tr>
<tr>
<td>I2</td>
<td>Wavenumber index parameter I+1</td>
</tr>
<tr>
<td>JMIR</td>
<td>Index for reflection of profile about center</td>
</tr>
<tr>
<td>J2</td>
<td>Path index parameter (J1+1)/2</td>
</tr>
<tr>
<td>J3</td>
<td>Path index parameter J1+1</td>
</tr>
<tr>
<td>KO(8, 3, 21)</td>
<td>Interpolated local value of KTAB</td>
</tr>
<tr>
<td>KEY</td>
<td>Selector for variable parameters</td>
</tr>
<tr>
<td><strong>FORTRAN symbol</strong></td>
<td><strong>Description</strong></td>
</tr>
<tr>
<td>-----------------------</td>
<td>---------------------------------------------------------------------------------</td>
</tr>
<tr>
<td>KEY1(8)</td>
<td>Index parameter (data statement)</td>
</tr>
<tr>
<td>KEY2(8)</td>
<td>Index parameter (data statement)</td>
</tr>
<tr>
<td>KEY3(8)</td>
<td>Index parameter (data statement)</td>
</tr>
<tr>
<td>KK(8, 3, 41)</td>
<td>Denormalized KO</td>
</tr>
<tr>
<td>KV</td>
<td>Index of condensed matrix</td>
</tr>
<tr>
<td>KV2</td>
<td>Index parameter KV+2</td>
</tr>
<tr>
<td>K1</td>
<td>Index parameter for variable parameters</td>
</tr>
<tr>
<td>K2</td>
<td>Index parameter for variable parameters</td>
</tr>
<tr>
<td>K3</td>
<td>Index parameter for variable parameters</td>
</tr>
<tr>
<td>LX</td>
<td>Index parameter for error array</td>
</tr>
<tr>
<td>L3</td>
<td>Index parameter for gas type</td>
</tr>
<tr>
<td>MAX</td>
<td>Largest absolute value of all DPAPA for an iteration step</td>
</tr>
<tr>
<td>NEWLIM</td>
<td>Controls number of tests for upper and low parameter limits</td>
</tr>
<tr>
<td>NP1</td>
<td>Equals pressure profile equation exponent NP(1)</td>
</tr>
<tr>
<td>NTEST</td>
<td>Diagnostic indicator of absorbing gas pressure being greater than static</td>
</tr>
<tr>
<td>P(6, 41)</td>
<td>Pressure of each gas at each station along path</td>
</tr>
<tr>
<td>PAERR(4, 10)</td>
<td>Error of variable parameter caused by a residual ERR</td>
</tr>
<tr>
<td>PA1(4)</td>
<td>Tentative value of new PA for an iterative step</td>
</tr>
<tr>
<td>PSUM</td>
<td>Sum of pressure of all absorbing gases along path</td>
</tr>
<tr>
<td><strong>FORTRAN symbol</strong></td>
<td><strong>Description</strong></td>
</tr>
<tr>
<td>------------------------</td>
<td>------------------------------------------------------</td>
</tr>
<tr>
<td>R(8, 41)</td>
<td>Gas radiance</td>
</tr>
<tr>
<td>RA(8)</td>
<td>Equals CRL during numerical differentiation</td>
</tr>
<tr>
<td>RAB(8)</td>
<td>Equals CRL before numerical differentiation</td>
</tr>
<tr>
<td>RB(8)</td>
<td>Equals CRL during numerical differentiation</td>
</tr>
<tr>
<td>R1(8)</td>
<td>Constant of Planck equation</td>
</tr>
<tr>
<td>R2(8)</td>
<td>Constant of Planck equation</td>
</tr>
<tr>
<td>STEP</td>
<td>Sum of fractional changes to variable parameters for an iteration step</td>
</tr>
<tr>
<td>T(41)</td>
<td>Temperature at each station along path</td>
</tr>
<tr>
<td>TAU(8, 4, 41)</td>
<td>Transmittance at each station along path</td>
</tr>
<tr>
<td>U(8, 3, 41)</td>
<td>Optical depth at each station along path</td>
</tr>
<tr>
<td>WAVOUT(10)</td>
<td>Wavenumbers in sequence for printout</td>
</tr>
<tr>
<td>X(41)</td>
<td>Actual path lengths Z·PATH/2</td>
</tr>
<tr>
<td>Y(21)</td>
<td>Dummy equal to Z, the normalized path length</td>
</tr>
</tbody>
</table>
APPENDIX E

TEMP SUBROUTINE LISTING

SUBROUTINE TEMPS

C TEMP AND PRINCIPAL PRESSURE PROFILE EDI(1,2,3)

C PRESSURE PROFILE OF OTHER ABSORBING GASES

C TEMPERATURE BOUNDARY LAYER, WALL TEMPERATURE TWB

C PRESSURE PROFILE FOR 1 WAVELENGTHS PLANCK FUNCTION

REAL YH,KTAB,KU,WPT

COMPO TETF,TW,, L1,J1,J2,J3,C1,PSUM,JB,R1(8),R2(8),X(141)

X PA(1),CT,UB(1),BY(1),X(111),MX,MB,PS,PATH,L2, T(21),L3,

X L2,PP2,PP1(1,1),MP2(1,1),W1,1,W2,2,MP3(1,1),LMP3(1,1),

X TP(1),J5(1,3),J7(1,3),J8(1,3),J6(1,3),J6(1,3),

X T(1,1,3),P(1,1,3),J(1,1,3),I(1,1,3),W(1,1,3),

X T(1),J(1),P(1),I(1),W(1),

L1=140,J2=140,L3=140,

L1=25,J2=25,J3=25,

C IF (KU,J1,J2,J3) .LT. 0.14 , RETURN

C IF (KU,J1,J2,J3) .LT. 0.14 , RETURN

C IF (KU,J1,J2,J3) .LT. 0.14 , RETURN

C IF (KU,J1,J2,J3) .LT. 0.14 , RETURN

END
APPENDIX F

TRANS SUBROUTINE LISTING

ORIGINAL PAGE IS OF POOR QUALITY
GO 260   720 DO 9 J=2,1
GO 273   730 B(E2R(I,L,J))/B(E1L,J)
GO 254   740 IF(B(E1L,J)>100,100,B(E1L,J))
GO 266   750 AV(AV(I,L,J))=B(E1L,J)*ETA(I,L,J-1)
GO 267   760 SI=SI+AV(I+1)AV(I)*DX(I)*.5
GO 270   770 AV=AV2
GO 271   780 J=1,...,J=51/B(E1L,J)
GO 272   790 DO 10 I=2,7
GO 275   800 IF(B(E1L,J)*B(E1L,J)>30,30,B(E1L,J))
GO 277   810 RATIO=B(E1L,L,J)/B(E1L,L,J-1)
GO 300   820 AS=41*J8*88
GO 301   830 IF(U(I,L,J)*A5>ETA(I,L,J)+ETA(I,L,J)*ETA(I,L,J)-4*ETA(I,L,J))
GO 302   840 ETA=ETA(I,L,J)+A2(I,L,J)*A3(I,L,J)*ETA(I,L,J)
GO 303   850 ETA(I,L,J)=ETA(I,L,J)+A3(I,L,J)*ETA(I,L,J)
GO 304   860 ETA(I,L,J)=ETA(I,L,J)+A4(I,L,J)*ETA(I,L,J)
GO 305   870 GO TO 11
GO 306   880 11 CONTINUE
GO 310   890 11 CONTINUE
GO 311   900 6 CONTINUE
GO 311   910 C TAU FOR L1 QASES, EQ (9), (13)
GO 315   920 DO 12 I=1,18
GO 322   930 DO 13 J=1,21
GO 323   940 TAUL(I,J)=0
GO 324   950 DO 14 L=1,21
GO 327   960 TAUL(I,J)=TAUL(I,J)+ETA(I,L,J)*ETA(I,L,J)*57000*ETA(I,L,J)
GO 330   970 14 TAUL(I,J)=TAUL(I,J)+ETA(I,L,J)*ETA(I,L,J)
GO 332   980 13 CONTINUE
GO 334   990 12 TAU(I,J)=TAUL(I,J)
GO 334   1000 C S A S R A D I A N C E C R L ( E O48)
GO 334   1010 DO 15 I=1,18
GO 334   1020 CR(I)=0
GO 334   1030 DO 15 J=1,18
GO 334   1040 CR(I)=CR(I)+CR(J)*CR(J)-10
GO 334   1050 15 CR(I)=CR(I)+CR(J)*CR(J)+CR(I,J)*5/(1-CTAU(I,J))
GO 335   1060 RETURN
GO 352   1070 END
The following FORTRAN symbol list is limited to symbols not in the PROFIL symbol list, APPENDIX D, and not in the NAMELIST data in the section WAVES PROGRAM USE.

<table>
<thead>
<tr>
<th>FORTRAN SYMBOL</th>
<th>DESCRIPTION</th>
</tr>
</thead>
<tbody>
<tr>
<td>AMAX</td>
<td>Maximum value of dependent profile parameter to determine ZETA</td>
</tr>
<tr>
<td>AMIN</td>
<td>Minimum value of dependent profile parameter to determine ZETA</td>
</tr>
<tr>
<td>KEY</td>
<td>Selector for variable profile parameters, ( \text{KEY}=K^4+\text{PROF}-1 )</td>
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<tr>
<td>KEY4 (5)</td>
<td>Index parameter (data statement)</td>
</tr>
<tr>
<td>K5</td>
<td>Index parameter to select dependent variable profile parameter</td>
</tr>
<tr>
<td>NPB</td>
<td>Index parameter NPA-1</td>
</tr>
<tr>
<td>PAVAV (8,10)</td>
<td>Dependent variable parameter after correction by ZETA</td>
</tr>
<tr>
<td>PAVAVE (4)</td>
<td>Saves initial value of independent variable parameter</td>
</tr>
<tr>
<td>ZETA (11)</td>
<td>Graph-plotting constant (APPENDIX C)</td>
</tr>
</tbody>
</table>
I04:29 102a 30 5b L1,J1,L2
004:27 123m 56 JUM:SUM=1,(J1,J1)
004:31 104a 30 57 L1,J1,L2
004:34 105m 57 CPEL,J1=J1,DUM
004:36 166a 57 CONTINUE
004:40 107a CALL TEMP
004:41 108a CALL TRANS
004:42 109a DO 63 ISJ=1,11
004:45 110a 90L16(CKL1)
004:46 111a 62 90L16(CTAUUL1)
004:50 112a WRITE(6,90)ABSL1,L1,J1,J1,L1,J1,J1
004:54 113a WRITE(6,90)
004:56 114a WRITE(6,90)
004:56 115a C INDEPENDENT VARIABLE PARAMETER PA(I4)
004:57 116a DO 60 IP=1,11
004:60 117a IE=1
004:61 118a IE=1
004:62 119a DO 60 IE=1,11
004:63 120a PA(I4)=PA(I)
004:64 121a IE=10
004:65 122a IE=10
004:66 123a 70C CALL TEMP
004:67 124a 70C CALL TEMP
004:68 125a CALL TEMP
004:69 126a IF(I16.EQ.1) WRITE(6,77)
004:70 127a 7TESTD
004:71 128a C FIND RESIDUALS, TEST FOR SOLUTION OR MAXIMUM ITERATION NUMBER
004:72 129a TAUL:CTAUUL1
004:73 130a QB1[C1,C1]
004:74 131a EQJ[C1,J1,J1,1]
004:75 132a SIIJ=TAUL(IJ)/TAUL(JJ)
004:76 133a RESID.SQRT(1/TAUL(I1))=1.02*(1-CTAUUL1/1.+TAUL(I1))
004:77 134a R (1023)
004:78 135a IF((1+RGT0.0) .AND. [1+I16.GT.0]) GO TO 624
004:79 136a ITER1=ITER1+1
004:80 137a C DERIVATIVE EQ(11) B12
004:81 138a OEL(I1)=EI/PA(I1)
004:82 139a DO 3 K=1,K2,K3
004:83 140a PA(I1)=PA(I1)+DEL(I1)
004:84 141a CALL TEMP
004:85 142a CALL TEMP
004:86 143a CALL TEMP
004:87 144a CALL TEMP
004:88 145a CALL TEMP
004:89 146a CALL TEMP
004:90 147a CALL TEMP
004:91 148a CALL TEMP
004:92 149a CALL TEMP
004:93 B058:149a CALL TEMP
004:94 150a CALL TEMP
004:95 151a CALL TEMP
004:96 152a CALL TEMP
004:97 153a 3 CONTINUE
004:98 154a CALL TEMP
004:99 155a CALL TEMP
005:00 156a 1 CHANGE DERIVATIVE VARIABLES TO CONDENSE ARRAY K(I1,1,K2,K3 TO K1,KV
005:00 157a 4V3=
005:00 158a DO 7 K=1,K2,K3
### Profiles and Computation

<table>
<thead>
<tr>
<th>PROFILE PARAMETERS</th>
<th>TEMP</th>
<th>AXIAL</th>
<th>WALL</th>
<th>TEMP</th>
<th>PRESS</th>
<th>WALL</th>
<th>TEMP</th>
<th>PRESS</th>
<th>WAVE</th>
<th>RES.</th>
<th>PERCENT</th>
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<td>3500</td>
<td>1700.00</td>
<td>6000</td>
<td>2000.00</td>
<td>3500</td>
<td>1700.00</td>
<td>3500</td>
<td>1700.00</td>
<td>3500</td>
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<tr>
<td>PARAMETER ERROR</td>
<td>PERCENT</td>
<td>.08</td>
<td>-7.48</td>
<td>.46</td>
<td>4.96</td>
<td>3500</td>
<td>2.08</td>
<td>.09</td>
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<td>.07</td>
<td>1.2</td>
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<td>RMS TOTAL</td>
<td>.02</td>
<td>4.0</td>
<td>7.1</td>
<td>8.2</td>
<td>8.0</td>
<td></td>
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</tr>
<tr>
<td>PARAMETER ERROR</td>
<td>PERCENT</td>
<td>.08</td>
<td>-7.77</td>
<td>2.94</td>
<td>19.48</td>
<td>3500</td>
<td>2.08</td>
<td>.09</td>
<td>1.3</td>
<td>.07</td>
<td>1.2</td>
</tr>
<tr>
<td>RMS TOTAL</td>
<td>.02</td>
<td>5.2</td>
<td>7.2</td>
<td>12.3</td>
<td>7.1</td>
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<td></td>
<td></td>
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<tr>
<td>PARAMETER ERROR</td>
<td>PERCENT</td>
<td>.08</td>
<td>-7.48</td>
<td>.46</td>
<td>4.96</td>
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<td>.09</td>
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<td>.07</td>
<td>1.2</td>
</tr>
<tr>
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<td>4.9</td>
<td>7.2</td>
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</table>

### Wavenumber (1/cm) Residual Percent

| Wavenumber (1/cm) Residual Percent |
|---|---|---|---|---|---|---|---|---|---|---|---|
| 3500 | 3500 | 3500 | 3500 | 3500 | 3500 | 3500 | 3500 | 3500 | 3500 | 3500 |

### Transmittance

| Transmittance | 0.89 | 0.92 | 0.60 | 0.65 | 0.85 | 0.88 | 0.00 | 0.00 | 0.00 | 0.00 | 0.00 |

### Temperature Profile

<table>
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<th>Partial Pressure Profiles Each 0.48 at 420 NCH</th>
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<tr>
<td>0.03</td>
<td>1700.00</td>
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<tr>
<td>0.50</td>
<td>1700.97</td>
</tr>
<tr>
<td>1.00</td>
<td>1711.68</td>
</tr>
<tr>
<td>2.57</td>
<td>1729.25</td>
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<td>5.00</td>
<td>1757.78</td>
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<td>12.21</td>
<td>1836.33</td>
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<td>15.00</td>
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<td>1925.00</td>
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<td>100.00</td>
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### Appendix I

#### Data Cards Contained in Cards of Appendix II, With Data For
Four-Well Numbers (51-60), Profile PROP = 6

<table>
<thead>
<tr>
<th>Card Number</th>
<th>Data Card</th>
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<tbody>
<tr>
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</tr>
<tr>
<td>2</td>
<td>56789</td>
</tr>
<tr>
<td>3</td>
<td>98765</td>
</tr>
<tr>
<td>4</td>
<td>45678</td>
</tr>
<tr>
<td>5</td>
<td>87654</td>
</tr>
<tr>
<td>6</td>
<td>78965</td>
</tr>
<tr>
<td>7</td>
<td>65432</td>
</tr>
<tr>
<td>8</td>
<td>23456</td>
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<tr>
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<td>56789</td>
</tr>
<tr>
<td>10</td>
<td>98765</td>
</tr>
</tbody>
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Printout of Input Data

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#### Appendix II

#### Data Cards Contained in Cards of Appendix I, With Data For
Four-Well Numbers (1-50), Profile PROP = 6

<table>
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<tbody>
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Printout of Input Data
### Computation and Profiles

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<th>AREA</th>
<th>AREA</th>
<th>WALL</th>
<th>WALL</th>
<th>PRESS</th>
<th>PRESS</th>
<th>EXPOSED TEMP</th>
<th>EXPOSED TEMP</th>
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#### Incidence SPA

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#### Incidence SPA

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#### Incidence SPA

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#### Incidence SPA

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#### Incidence SPA

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#### Incidence SPA

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#### Parameter Error

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<th>WAVELENGTH/CHR</th>
<th>RESIDUAL PERCENT</th>
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<tbody>
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</tbody>
</table>

#### Temperature Profile

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<th>PARTIAL PRESSURE PROFILES EACH GALATH</th>
<th>TEMPERATURE</th>
<th>PARTIAL</th>
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<tbody>
<tr>
<td></td>
<td></td>
<td>TEMPERATURE</td>
<td>PRESSURE</td>
</tr>
<tr>
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</table>

#### Wave Number/Chr

<table>
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<th>TRANSMISSION</th>
<th>TEMPERATURE</th>
<th>PRESSURE</th>
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<tbody>
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#### Parameter Error

<table>
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<th>PERCENT</th>
<th>WAVELENGTH/CHR</th>
<th>RESIDUAL PERCENT</th>
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#### Parameter Error

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<th>WAVELENGTH/CHR</th>
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</table>
### Profiles and Computation

**Temperature Profile (K) vs Temp. °C**

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<th>Temp °F</th>
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<td>133.00</td>
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<td>0.05</td>
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<tr>
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<td>1968.94</td>
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</table>

**Potted Pressure Profiles Each Gas (atm)**

<table>
<thead>
<tr>
<th>K</th>
<th>N2</th>
<th>H2</th>
<th>O2</th>
<th>CH4</th>
<th>CO2</th>
<th>CO2</th>
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<td>17000</td>
<td>0.000</td>
<td>0.000</td>
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<td>0.000</td>
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<tr>
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<td>133.45</td>
<td>16900</td>
<td>0.000</td>
<td>0.000</td>
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<td>0.000</td>
</tr>
<tr>
<td>1.00</td>
<td>1071.63</td>
<td>6960</td>
<td>0.000</td>
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### Profile Parameters

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<th>Temp. Exponent</th>
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<th>Axial Press (atm)</th>
<th>Wall Temp. (°C)</th>
<th>Number of Iteration</th>
<th>Last Iteration</th>
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<tr>
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<td>Parameters</td>
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<tr>
<td>Parameters</td>
<td>PA</td>
<td>62000</td>
<td>2144.81</td>
<td>2443.06</td>
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DEPENDENT PARAMETER TCM WITH ZETA = -57.03

<table>
<thead>
<tr>
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<th>3100µ</th>
<th>3500µ</th>
<th>3775µ</th>
<th>4100µ</th>
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<td>0.20</td>
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<tr>
<td>0.30</td>
<td>0.35</td>
<td>0.40</td>
<td>0.45</td>
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<tr>
<td>0.60</td>
<td>0.65</td>
<td>0.70</td>
<td>0.75</td>
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<tr>
<td>0.90</td>
<td>0.95</td>
<td>1.00</td>
<td>1.05</td>
<td>1.10</td>
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</table>

ORIGINAL PAGE IS OF POOR QUALITY
**APPENDIX K**

**EXAMPLE OF PROFILE WITH HIGH-TEMPERATURE CORE**

Data Cards With Measured Data, Two Wave Numbers, Profile PROF = 2

---

No Boundary Layer, Gases H₂O and N₂

---

**SNAM1:** nodex1, profy1, path = 10, mg1 = 1, wvl = 3520, 1013, 443,

---

**K:**

---

**example of profile:**

---

**with high-temperature core**

---

**Data Cards With Measured Data, Two Wave Numbers, Profile PROF = 2**

---

**No Boundary Layer, Gases H₂O and N₂**

---

**SNAM1:** nodex1, profy1, path = 10, mg1 = 1, wvl = 3520, 1013, 443,

---

**K:**

---

**EXAMPLE OF PROFILE:**

---

**WITH HIGH-TEMPERATURE CORE**

---

**Data Cards With Measured Data, Two Wave Numbers, Profile PROF = 2**

---

**No Boundary Layer, Gases H₂O and N₂**

---

**SNAM1:** nodex1, profy1, path = 10, mg1 = 1, wvl = 3520, 1013, 443,

---

**K:**

---

**Printout of Input Data**

---

**SNAM1:** nodex1, profy1, path = 10, mg1 = 1, wvl = 3520, 1013, 443,

---

**K:**

---

**Printout of Input Data**

---

**SNAM1:** nodex1, profy1, path = 10, mg1 = 1, wvl = 3520, 1013, 443,

---

**K:**

---

**Printout of Input Data**

---

**SNAM1:** nodex1, profy1, path = 10, mg1 = 1, wvl = 3520, 1013, 443,

---

**K:**

---

**Printout of Input Data**

---

**SNAM1:** nodex1, profy1, path = 10, mg1 = 1, wvl = 3520, 1013, 443,

---

**K:**

---

**Printout of Input Data**

---

**SNAM1:** nodex1, profy1, path = 10, mg1 = 1, wvl = 3520, 1013, 443,

---

**K:**

---

**Printout of Input Data**

---

**SNAM1:** nodex1, profy1, path = 10, mg1 = 1, wvl = 3520, 1013, 443,

---

**K:**

---

**Printout of Input Data**

---

**SNAM1:** nodex1, profy1, path = 10, mg1 = 1, wvl = 3520, 1013, 443,

---

**K:**

---

**Printout of Input Data**

---

**SNAM1:** nodex1, profy1, path = 10, mg1 = 1, wvl = 3520, 1013, 443,

---

**K:**

---

**Printout of Input Data**

---

**SNAM1:** nodex1, profy1, path = 10, mg1 = 1, wvl = 3520, 1013, 443,

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**K:**

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**SNAM1:** nodex1, profy1, path = 10, mg1 = 1, wvl = 3520, 1013, 443,

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**K:**

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**K:**

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**K:**

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**K:**

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**K:**

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**SNAM1:** nodex1, profy1, path = 10, mg1 = 1, wvl = 3520, 1013, 443,

---

**K:**

---

**Printout of Input Data**

---

**SNAM1:** nodex1, profy1, path = 10, mg1 = 1, wvl = 3520, 1013, 443,
<table>
<thead>
<tr>
<th>Temperature (°C)</th>
<th>Partial Pressure Profiles Each 25°C, atm</th>
</tr>
</thead>
<tbody>
<tr>
<td>97.50</td>
<td>1185.29</td>
</tr>
<tr>
<td>99.33</td>
<td>1262.32</td>
</tr>
<tr>
<td>99.50</td>
<td>1185.19</td>
</tr>
<tr>
<td>99.75</td>
<td>1262.32</td>
</tr>
</tbody>
</table>

**PARAMETERS**

**Temperature (°C)**

**Partial Pressure Profiles Each 25°C, atm**

**COMPONENT AND PROFILES**

**WAVENUMBER/M:CHST**

**TRANSMITTANCE**

**RESIDUAL PERCENT**

**ERROR**

**PERCENT**

**TOTAL**

**WAVENUMBER/M:CHST**

**RESIDUAL PERCENT**

**FINAL RESIDUAL**

**TOTAL RESIDUAL**

**ORIGINAL PAGE IS OF POOR QUALITY**
REFERENCES


### TABLE I. - COEFFICIENTS TO BE USED IN EQUATION (16)

<table>
<thead>
<tr>
<th>$\beta/\beta_e$</th>
<th>$A_1$</th>
<th>$A_2$</th>
<th>$A_3$</th>
<th>$A_4$</th>
<th>$A_5$</th>
</tr>
</thead>
<tbody>
<tr>
<td>0</td>
<td>-0.68</td>
<td>-0.35</td>
<td>0.55</td>
<td>0.07</td>
<td>1.00</td>
</tr>
<tr>
<td>2</td>
<td>-0.37</td>
<td>0.62</td>
<td>0.71</td>
<td>0.43</td>
<td>1.37</td>
</tr>
<tr>
<td>5</td>
<td>0.60</td>
<td>3.15</td>
<td>0.90</td>
<td>0.79</td>
<td>1.93</td>
</tr>
<tr>
<td>10</td>
<td>3.19</td>
<td>9.25</td>
<td>1.15</td>
<td>1.30</td>
<td>2.85</td>
</tr>
<tr>
<td>20</td>
<td>9.10</td>
<td>22.2</td>
<td>1.63</td>
<td>2.26</td>
<td>4.70</td>
</tr>
<tr>
<td>50</td>
<td>29.1</td>
<td>67.1</td>
<td>2.78</td>
<td>4.56</td>
<td>10.25</td>
</tr>
<tr>
<td>100</td>
<td>105</td>
<td>209</td>
<td>4.05</td>
<td>7.09</td>
<td>19.50</td>
</tr>
</tbody>
</table>

### TABLE II. - SPECTRAL LINE BROADENING COEFFICIENT, $\alpha^*$ (FROM REF. 16)

<table>
<thead>
<tr>
<th>Absorbing gas</th>
<th>Broadening gas</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>$H_2O$</td>
</tr>
<tr>
<td>$H_2O$</td>
<td>1</td>
</tr>
<tr>
<td>$CO_2$</td>
<td>1</td>
</tr>
<tr>
<td>$CO$</td>
<td></td>
</tr>
<tr>
<td>$CH_4$</td>
<td>1.25</td>
</tr>
</tbody>
</table>
TABLE III. - ESTIMATED PERCENT ERROR OF $T_c$ AND $T_w^*$ AND TRANSMITTANCE FOR VARIOUS PATH LENGTHS
FOR PROFILE OF FIGURE 1(b)

[Measurement wavenumbers 3100, 3400, 3500, and 4100 cm$^{-1}$; $T_c = 2000$ K, $n_T = 0.5$, $p_c = 0.35$ atm, $p_w = 0.30$ atm, $n_p = 0.5$. Errors caused by one percent error of radiance measurement, and five percent error of tabulated absorption coefficients.]

<table>
<thead>
<tr>
<th>Percent error in $T_c$</th>
<th>Path length, cm</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>50</td>
</tr>
<tr>
<td>$T_c^<em>$ $T_w^</em>$ $K$</td>
<td></td>
</tr>
<tr>
<td>1200</td>
<td>3.0</td>
</tr>
<tr>
<td>2000</td>
<td>11.5</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Percent error in $T_w^*$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1200</td>
</tr>
<tr>
<td>2000</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Transmittance at 3500 cm$^{-1}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1200</td>
</tr>
<tr>
<td>2000</td>
</tr>
</tbody>
</table>
TABLE IV. - PARAMETER INDEX CONTROL

<table>
<thead>
<tr>
<th>KEY</th>
<th>KEY1(KEY)</th>
<th>KEY2(KEY)</th>
<th>KEY3(KEY)</th>
<th>Variable parameters</th>
<th>Fig. 1(a), PROF=1</th>
<th>Fig. 1(b), PROF=2</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>K1</td>
<td>K2</td>
<td>K3</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>1</td>
<td>1</td>
<td>3</td>
<td>1</td>
<td>n₁ Tc p_c</td>
<td>Tc p_c Tw</td>
<td></td>
</tr>
<tr>
<td>2</td>
<td>1</td>
<td>2</td>
<td>1</td>
<td>n₁ Tc</td>
<td>Tc p_c</td>
<td></td>
</tr>
<tr>
<td>3</td>
<td>1</td>
<td>3</td>
<td>2</td>
<td>n₁ p_c</td>
<td>Tc T*</td>
<td></td>
</tr>
<tr>
<td>4</td>
<td>1</td>
<td>1</td>
<td>1</td>
<td>n₁</td>
<td>Tc</td>
<td></td>
</tr>
<tr>
<td>5</td>
<td>2</td>
<td>3</td>
<td>1</td>
<td>Tc p_c</td>
<td>p_c Tw</td>
<td></td>
</tr>
<tr>
<td>6</td>
<td>2</td>
<td>2</td>
<td>1</td>
<td>Tc</td>
<td>p_c</td>
<td></td>
</tr>
<tr>
<td>7</td>
<td>3</td>
<td>3</td>
<td>1</td>
<td>p_c</td>
<td>T*</td>
<td></td>
</tr>
<tr>
<td>8</td>
<td>0</td>
<td>0</td>
<td>0</td>
<td>None</td>
<td>None</td>
<td></td>
</tr>
</tbody>
</table>
(a) Non-isothermal temperature profiles, $T_W = \text{constant}$.

(b) Near-isothermal temperature profiles, with $T_W = \text{constant}$ and boundary layer thickness $x_1 = \text{constant}$.

(c) Partial pressure profile for each absorbing gas.

Figure 1. - Assumed profile functions.
Figure 2. - Absorption coefficient for H$_2$O.

Figure 3. - Test of wavenumbers for profile of figures 1(a) with $T_w = 1000$ K, $p_c = 0.35$ atm, $n_H = 0.35$ atm, $n_H = 0.35$, path length 100 cm, Hydrogen-air combustion at 1 atm.
Figure 4. - Test of wavenumbers for profile of figure 1(b) with $n_T = 0.5$, $p_c = 0.35$ atm, $p_w = 0.30$ atm, $n_0 = 0.50$, path length 100 cm. Hydrogen-air combustion at 1 atm.

Figure 5. - Estimated error in $T_e$ due solely to errors in radiometer and tabulated absorption coefficients. Profile of figure 1(a), with $T_e = 2000$ K, $T_{w} = 1000$ K, $p_c = 0.35$ atm, $p_w = 0.65$ atm, $n_0 = 0.50$, path length 100 cm, Hydrogen-air combustion at 1 atm. Error of radiometry 1 percent, error of tabulated absorption coefficient 5 percent.
Figure 6. - Estimated error in $T_c$ due solely to errors in radiometry and in tabulated absorption coefficients. Profile of figure 1(b) with $T_e = 2000$ K, $n_T = 0.5$, $p_e = 0.35$ atm, $p_W = 0.30$ atm, $n_p = 0.50$, path length 100 cm. Hydrogen-air combustion at 1 atm. Error of radiometry 1 percent, tabulated absorption coefficient 5 percent.
Figure 7. - Flow chart for PROFIL.
WAVES

READ

Write INPUT

Calculate ERROR-FREE measurements (subroutines TEMP, TRANS)

1

Do 100

Calculate radiance and transmittance (subroutines TEMP, TRANS)

Next parameter value or wave number

Test for solution and max. iteration if YES, DONE=1

DONE=1

Yes

Matrix of derivatives for one wavenumber (subroutines TEMP, TRANS)

Parameter increment

Parameter outside limit

$Y_{\lambda}$

100 continue

Write results

Next iteration step

2

Next problem

Figure 8. - Flow chart for WAVES.
Figure 9. Example of profile with high-temperature core. Wavenumbers of measurement 3500 and 3100 cm$^{-1}$. 

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