

Monte Carlo Solution of Radiant Heat Transfer in a Nongrey Nonisothermal Gas with Temperature Dependent Properties

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The problem of radiative heat transfer in a gas filled enclosure is of considerable interest. The grey-gas assumption commonly used can be in error for several reasons. The total absorptivity of a real gas generally does not follow the exponential absorption law. In addition there is difficulty in choosing the appropriate mean absorption coefficient for a specific case. If there are large temperature variations in the gas or between the gas and a wall, significant errors can occur because of the changing distribution of energy with wave length. A grey-gas assumption with total absorptivity taken equal to total emissivity in the gas, cannot account for these effects. Ignoring the variation of absorption coefficient with temperature can also lead to considerable error.

The problem of radiative transfer to real gases has been treated previously by Hottel and Cohen (1), who have presented a method based on separating a gas volume into finite isothermal elements and solving the resulting set of transfer equations. The real gas properties are approximated by fitting a summation of exponential terms.

Another treatment of the problem is given by Bevans and Dunkle (2). The band approximation is used for the properties, and finite isothermal elements are assumed. The solution is obtained by the network method.

Deissler (3) extended the diffusion approximation with jump boundary conditions for the case of real gases to a higher order but as in (1) and (2), did not fully account for the effect of temperature on the gas properties.

Some recent papers (4, 5) have applied the Monte Carlo method used previously in the fields of rarefied gas dynamics and neutron transport to heat radiation problems involving grey gases with temperature independent properties. Monte Carlo is applied herein to a nonisothermal gas radiative transfer problem where the absorption coefficient is allowed to vary with both wave length and temperature. A comparison is made with the modified diffusion approximation including temperature effects on the absorption coefficient, with the temperature dependent grey-gas solution, with the temperature independent nongrey gas solution, and with the transparent approximation.

The procedure consists of following a bundle* of energy through a probable path until final absorption in the system. Enough such bundles are followed to give statistically meaningful results.

ANALYSIS

The radiant energy transfer and the temperature distribution are found for a nongrey nonisothermal gas between infinite parallel walls. Only the case of black walls will be treated, but extension to nongrey walls is straightforward. The refractive index of the gas is assumed to be

1. Two solutions are obtained, one for the walls at unequal temperatures and with no heat sources in the gas and the other for both walls at the same temperature and a parabolic distribution of heat sources in the gas. The geometry studied is shown in Figure 1.

No Energy Source in the Gas

The computer flow chart for this case is shown in Figure 2. In the program the random number R must be selected each time it is used, as opposed to R_1 , R_2 , and R_3 which are reassigned only at given points.

As derived in the Appendix [Equation (A4)] when a bundle is emitted from wall 0 $<1>^*$, its wave length is determined from

$$R = \frac{\int_0^\lambda \epsilon_{\lambda 0} e_{b\lambda 0} d\lambda}{\int_0^\infty \epsilon_{\lambda 0} e_{b\lambda 0} d\lambda} \quad (1)$$

where R is a random number in the range 0 to 1, $\epsilon_{\lambda 0}$ is the emissivity, and $e_{b\lambda 0}$ the black emissive power distribution of surface 0. By integration of (1) a relation $\lambda = F_0(R)$ is obtained for a given surface temperature.

If the surface is assumed to emit diffusely, the direction of the emitted bundle is shown in reference 4 to be

$$\cos \eta = \sqrt{R_1} \quad (2)$$

The distance the bundle travels before absorption in the gas is given in the appendix by Equation (A9) as

$$\ln R = - \int_0^l \tau_\lambda dl' \quad (3)$$

where $\tau_\lambda = D\kappa_\lambda$ is the monochromatic gas optical thickness. If it is assumed that the gas is divided into $1/\Delta x$ increments, each with an absorption coefficient $\kappa_{\lambda,i}$, the increment i in which absorption occurs can be found by writing (3) as

$$\ln R + \frac{\Delta x}{\sqrt{R_1}} \sum_{z=1}^i \tau_{\lambda,z} > 0 \quad (4)$$

and carrying out the summation until the inequality is satisfied $<2>$. Since the absorption coefficient is temperature dependent, solution of (4) requires a priori knowledge of the temperature distribution across the channel. This necessitates an iterative procedure.

If the increment number i is greater than the number of increments available $<3>$, then the bundle must be absorbed by black surface 1. If the bundle is absorbed in the gas, then the normal distance from surface 0 at which absorption occurs is found $<5>$. The bundle is tallied as being absorbed in increment i $<6>$. Since the gas is at the steady state, a new bundle must be emitted from x . Its wave

* These bundles cannot be considered photons since the energy per bundle does not depend on wave length. They rather represent a group or bundle of photons at a given wave length such that all bundles have equal energy.

* The numbers in brackets $< >$ correspond to those in Figure 2.

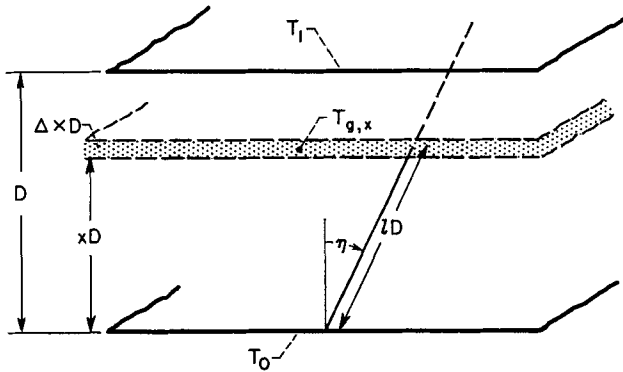


Fig. 1. Geometry for nongrey nonisothermal gas between infinite parallel black plates.

length is determined from $\lambda = F_{g,x}(R) <7>$ as calculated from Equation (A5) in the appendix. The direction of isotropic emission from any point x in the gas is shown in reference 4 to be given by

$$\cos \eta = 1 - 2R_2 \quad (5)$$

This direction is examined to determine whether it is toward surface 0 or surface 1 <8>. A check is made to determine whether the bundle is reabsorbed in the same increment i <9>. If so, the new point of absorption x is found <10, 11>, and the bundle is again tallied and re-emitted <6>, etc. If not, the increment I in which it is absorbed is calculated <12>, again by modifying Equation (3). A check is made of the increment number <13> to see whether the bundle reached the wall. If so it is tallied at that wall <14>. If not, the point of absorption x is calculated <11>, and the bundle is tallied <6> and re-emitted as before. The procedure is followed until absorption at a wall. Enough such paths are traced to give statistically meaningful results.

A similar procedure is then followed by those bundles emitted from surface 1.

The net energy transferred to surface 1 is

$$(q_{0-1})_{\text{net}} = c_0 S_{0-1} - c_1 S_{1-0} \quad (6)$$

where S_{A-B} is defined as the number of bundles emitted at surface A per unit area that are absorbed at surface B . The term c_A is the energy per bundle emitted from surface A and is defined by

$$c_A N_A = \int_0^\infty \epsilon_{\lambda A} e_{b\lambda A} d\lambda \quad (7)$$

where N_A is the total number of bundles emitted per unit area from A . For the case of black walls substitution of Equation (7) into Equation (6) gives

$$\left[\frac{(q_{0-1})_{\text{net}}}{e_{b0} - e_{b1}} \right]_{G(x)=0} = \frac{1}{1 - \left(\frac{e_{b1}}{e_{b0}} \right)} \times \left[\frac{S_{0-1}}{N_0} - \left(\frac{e_{b1}}{e_{b0}} \right) \frac{S_{1-0}}{N_1} \right] \quad (8)$$

The emissive power of a gas volume of width Δx is obtained from the number of bundles emitted in the gas volume:

$$4 \Delta x \int_0^\infty e_{g,\lambda,i} \tau_{\lambda,i} d\lambda = \left(\frac{S_{0-\Delta x,i}}{N_0} \right) e_{b0} + \left(\frac{S_{1-\Delta x,i}}{N_1} \right) e_{b1} = 4 \Delta x \tau_{P,i} e_{g,i} \quad (9)$$

where $S_{A-\Delta x,i}$ is the number of bundles absorbed and therefore re-emitted in the volume element i of width Δx that originated at surface A , and $\tau_{P,i}$ is the Planck mean optical thickness in increment i and is defined as

$$\tau_{P,i} = \left[\frac{\int_0^\infty \tau_\lambda e_{g,\lambda} d\lambda}{e_g} \right]_i \quad (10)$$

The emissive power distribution in the gas is then

$$\left(\frac{e_{g,i} - e_{b0}}{e_{b1} - e_{b0}} \right)_{G(x)=0} = \frac{1}{\left(1 - \frac{e_{b1}}{e_{b0}} \right)} \times \left\{ 1 - \frac{1}{4 \tau_{P,i} \Delta x} \left[\frac{S_{0-\Delta x,i}}{N_0} + \left(\frac{S_{1-\Delta x,i}}{N_1} \right) \frac{e_{b1}}{e_{b0}} \right] \right\} \quad (11)$$

Gas with Parabolic Source Distribution Between Plates at Equal Temperatures

The flow chart for this case is also shown in Figure 2. A parabolic distribution of heat sources of the form

$$G(x) = 4G_{\text{max}} x(1-x) \quad (12)$$

is assumed, where G is the heat generation rate per unit volume. The problem is to find the emissive power distribution in the gas.

The emissive power is related to the number of emissions in the gas by

$$4 \tau_{P,i} \Delta x e_{g,i} = c_g (S_{g,\Delta x,i} + c_0 (S_{0-\Delta x,i} + c_1 (S_{1-\Delta x,i}))) \quad (13)$$

where $(S_{g,\Delta x,i})$ is the total number of bundles emitted in a volume element Δx around point i which originate in the gas owing to the gas heat sources. This includes original emissions in the gas element and re-emissions after absorption of bundles originating in other gas elements. The last two terms give the energy absorbed from the walls directly and by re-emission from the gas.

The energy per bundle originally emitted in the gas c_g is defined as

$$c_g = \frac{D \int_0^1 G(x') dx'}{N_g} = \frac{2G_{\text{max}} D}{3N_g} \quad (14)$$

where N_g is the total number of bundles originally emitted in the gas owing to the heat sources.

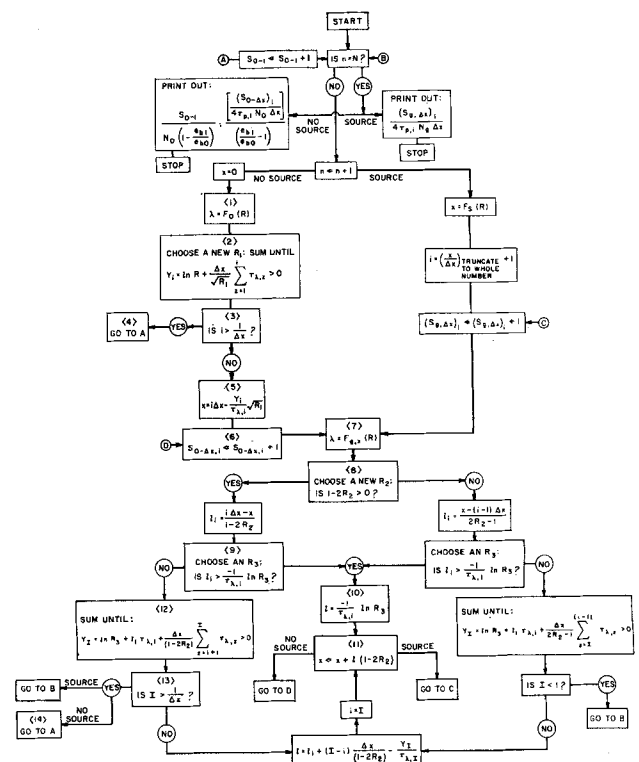


Fig. 2. Computer flow chart.

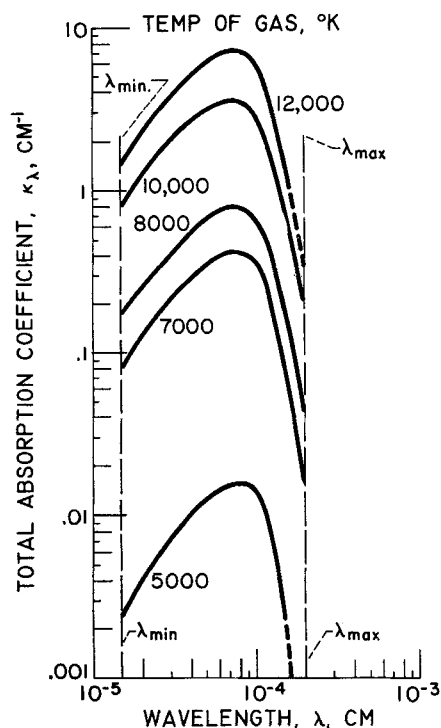


Fig. 3a. Properties of hydrogen gas. Total absorption coefficient of hydrogen gas at $P = 1,000$ atm. (from reference 6).

For any variation of optical thickness $\tau_{P,i}$ if the surface temperatures are equal the gas must be isothermal at the wall temperature, and one can reduce Equation (11) to the identity

$$4\tau_{P,i} \Delta x = \frac{S_{0-\Delta x,i}}{N_0} + \frac{S_{1-\Delta x,i}}{N_1} = \frac{1}{e_b} (C_0 S_{0-\Delta x,i} + C_1 S_{1-\Delta x,i})$$

Substituting this relation into Equation (13) one gets

$$\left(\frac{e_{g,i} - e_b}{\left(\frac{2G_{max}D}{3} \right)} \right)_{T_0=T_1} = \frac{(S_{g,\Delta x})_i}{4N_g \Delta x \tau_{P,i}} \quad (15)$$

The Monte Carlo program is essentially that described in the previous section except that bundles originate within the gas as points determined by the function $x = F_s(R)$, as derived in the appendix [Equation (A11)], rather than at the surfaces.

Sample Problem

The calculations were carried out for hydrogen in the temperature range of 5,000° to 12,000°K. The absorption coefficient as a function of temperature and wave length used in the problem is shown in Figure 3a. The mean absorption coefficients calculated from this data and used in the comparison solutions are shown in Figure 3b. The data is from reference 6 and is based on analytical calculations. The absorption coefficient was assumed zero outside the range $\lambda_{min} < \lambda < \lambda_{max}$.

The Monte Carlo solution is compared with a diffusion solution with jump boundary conditions for this specific problem.* The diffusion solution follows Deissler (3) but extends his results to include the variation of absorption coefficient across the channel.

The diffusion solution uses the Rosseland mean absorption coefficient κ_R . If the absorption coefficient is very small over parts of the spectrum, the value of κ_R is

* Material has been deposited as document 7972 with the American Documentation Institute, Photoduplication Service, Library of Congress, Washington 25, D. C., and may be obtained for \$1.25 for photoprints or for 35-mm. microfilm

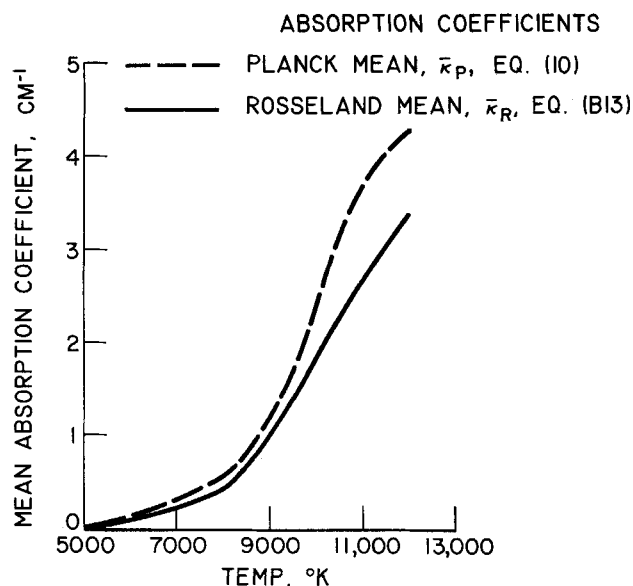


Fig. 3b. Properties of hydrogen gas. Comparison of mean absorption coefficients for data of Figure 3a. Wave length range $1.5 \times 10^{-5} < \lambda < 2.0 \times 10^{-4}$ cm.

weighted excessively by this portion of the spectrum. Because of this the problem must be solved in two parts. Over the spectrum range with appreciable absorption coefficient the diffusion solution is used, and over the remainder the gas is considered transparent.

The results for the example are also compared with the Monte Carlo temperature dependent solution based on the Planck mean absorption coefficient of the gas in each increment as defined by Equation (10) and with the Monte Carlo solution which uses the wave length dependent absorption coefficient evaluated at an average temperature. Limiting exact solutions for optically thick and transparent gases are also given.*

RESULTS

No Gas Heat Sources

The net heat transferred between the heated infinite black plates enclosing hydrogen is shown in Figure 4. The temperature of plate 0 was taken as 9,500°K. and of plate 1 as 4,500°K. The results are shown for different values of plate spacing D . The gas was assumed transparent at wave lengths less than 0.15×10^{-4} or greater than 2×10^{-4} cm.

Comparison of the exact Monte Carlo solution to the wave length dependent, temperature independent absorption coefficient $\kappa(\lambda, T_c)$ solution shows a lower heat transfer rate for the exact solution. This is because the wave length dependent gas absorption coefficient is evaluated at 7,000°K., the average of the wall temperatures. However the larger slope of the curve of gas absorption coefficient with temperature (Figure 3b) near the higher wall temperature indicates that a higher mean gas temperature should be used to evaluate $\kappa(\lambda, T_c)$ for this case.

Also shown is the Monte Carlo solution with a temperature dependent Planck mean absorption coefficient $\kappa_P(T)$ which gives lower heat transfer than the exact solution because the mean absorption coefficients are weighted according to the Planck energy distribution based on the local gas temperature [Equation (10)]. This gives most weight to the absorption coefficient in the wave lengths where the local Planck energy distribution is a maximum. The energy absorbed locally however will have a wave length distribution based on its source energy spectrum. In the present case this gives an exaggerated absorption

* See footnote in column 1.

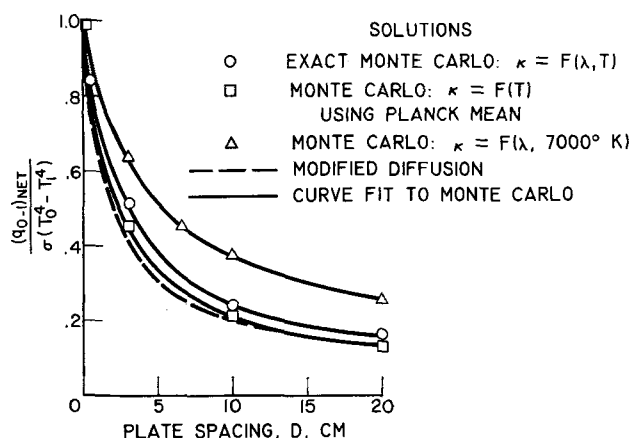


Fig. 4. Heat transfer through hydrogen between black plates. No gas heat source. Plate temperatures $T_0 = 9,500^\circ\text{K}$, $T_1 = 4,500^\circ\text{K}$.

coefficient for calculating the energy absorbed from the hot wall and a consequently smaller heat transfer than the exact solution.

The modified diffusion solution is in close agreement with the Monte Carlo solution with the Planck mean absorption coefficient. This agreement might be expected, since both solutions are based on a temperature dependent mean absorption coefficient. The diffusion solution is in better agreement with the exact solution as the plate spacing is increased. The approximation of the temperature dependence of the absorption coefficient as a parabolic form and the neglect of variation of absorption coefficient over a mean free path still introduce some error.

The gas emissive power distributions for various plate spacings are shown in Figure 5. The local gas emissive power is dependent on the temperature surroundings viewed and the absorption coefficient. For the example shown elements near the hot wall attain equilibrium temperatures close to the hot wall temperature. Elements near the cold wall are less readily influenced by the hot wall, especially for large plate spacing, because the large absorption coefficient in the hotter portion of the gas masks the hot wall. This leads to the large emissive power gradient near the hot wall for cases with temperature dependent absorption coefficient.

In Figure 5a the exact solutions for various plate spacings are shown. As the plate spacings get larger, the jump between the emissive powers of the wall and the gas at the wall become smaller and approach zero as the plate spacing becomes very large. As the plate spacing ap-

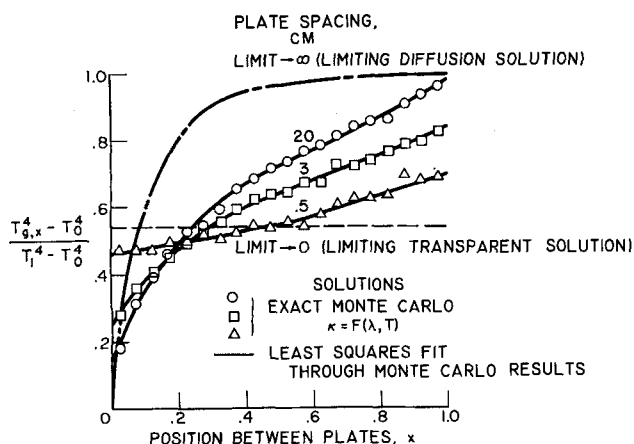


Fig. 5a. Emissive power distribution in hydrogen between parallel plates. No gas heat source. Plate temperatures $T_0 = 9,500^\circ\text{K}$, $T_1 = 4,500^\circ\text{K}$. Exact solutions, various spacings.

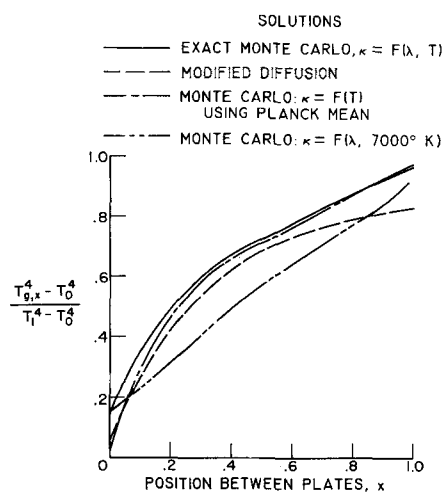


Fig 5b. Emissive power distribution in hydrogen between parallel plates, $T_0 = 9,500^\circ\text{K}$, $T_1 = 4,500^\circ\text{K}$. Plate spacing 20 cm.

proaches zero, the emissive power becomes constant since any gas element views both walls equally well. The constant is not the average of the emissive powers of the walls as would be the case for a grey gas. The reason is that the wave length dependent absorption coefficient is lower for the wave lengths of energy leaving the hot wall and is comparatively large at the wave lengths of local gas emission, which leads in turn to an equilibrium temperature nearer that of the cold wall.

Figure 5b compares the exact Monte Carlo solution with various approximate solutions at the larger plate spacing. The agreement was better at a small plate spacing, since the temperature range, and therefore the variation in absorption coefficient with temperature, is less. The wave length dependent, temperature independent absorption coefficient solution gives emissive power distributions with less slope at the hot wall than the exact solution, since there is no temperature effect on the absorption coefficient.

The temperature dependent Monte Carlo solution with a Planck mean absorption coefficient gives curves of shape similar to the exact solution but of higher values of gas temperature. This is again due to the erroneously high absorption of energy in each element because of the large mean absorption coefficient computed on the basis of the local gas temperature. This effect becomes smaller for optically thick gases.

The slope near the walls for the modified diffusion solution does not correspond to the exact solution because the effects of the wall are only included in the emissive power jump at the wall and not in the gas away from the wall. As the plate spacing becomes larger, this approximation improves. At the cold wall however the results are still poor because of the low absorption coefficient there.

Parabolic Heat Source in the Gas

For a symmetrical distribution of heat sources between the black walls at equal temperatures the heat transferred to each wall is equal to one-half the total heat generated.

The emissive power distribution in the gas is shown in Figure 6a for the exact solutions for various values of the plate spacing D . The limiting transparent solution is compared. The gas temperatures become higher at larger plate spacing because of the increasing difficulty of transferring heat to the walls from positions near the center line.

In Figure 6b, the simplified solutions are compared with the exact solution for a large plate spacing.

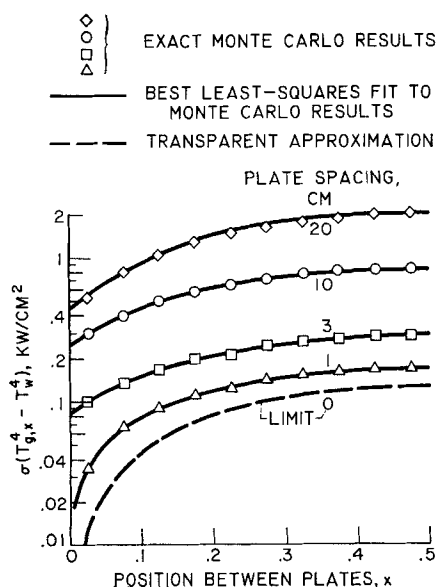


Fig. 6a. Emissive power distribution in hydrogen between parallel black plates, parabolic heat source. Plate temperatures $T_w = T_0 = T_1 = 7,000^\circ\text{K}$. $G_{\max} = 0.145 \text{ kw./cc}$. Exact solution, various plate spacings.

The various approximate Monte Carlo solutions give excellent agreement to the exact solution for smaller plate spacings because of the small temperature variations in the enclosure.

The diffusion solution gives better agreement with increasing plate spacing and higher temperatures, where the absorption coefficients are larger. In Figure 7 the difference between the gas center line and wall emissive powers is plotted for the exact Monte Carlo solution. This is compared with the two limiting solutions, the diffusion solution applicable for large plate spacing and the transparent approximation for small plate spacing. The exact solution is seen to approach the limiting solutions on a percentage difference basis.

CONCLUSIONS

The results indicate that for gases with large optical thickness the diffusion approximation modified for temperature dependent absorption coefficient is applicable. In the other extreme the transparent solutions are applicable. It may be possible in certain cases to divide the energy spectrum so that different solutions are used in different regions.

In general however the diffusion or transparent assumptions or the use of temperature and/or wave length independent absorption coefficients can give very misleading results. In addition it is very difficult to predict the magnitude or sign of the error, since it will strongly depend on the properties of the particular gas.

The Monte Carlo method is flexible enough to remove any or all of the above assumptions and can be modified to include other effects such as scattering, nongrey, and/or nondiffuse walls, etc. These would be extremely difficult to include in other methods.

Monte Carlo is relatively easy to program as compared with setting up the integral equations, and its chief drawback is the large use of computer time in complex cases.

The present results for the longest running cases of large plate spacing and absorption coefficient varying with wave length and temperature consumed on the order of $\frac{1}{2}$ hr. of computer time on the IBM-7094 computer. Convergence was checked by the usual procedure of reducing increment size and increasing the number of

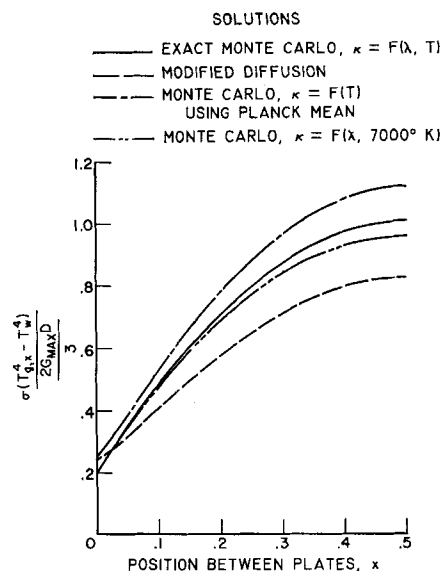


Fig. 6b. Emissive power distribution in hydrogen between parallel black plates, parabolic heat source. Plate temperatures $T_w = T_0 = T_1 = 7,000^\circ\text{K}$. $G_{\max} = 0.145 \text{ kw./cc}$.

bundles and iterations until no changes were observed. Three to four iterations were usually required.

The running time was of course strongly dependent on the particular problem, initial guesses, and accuracy required. However since this may often be the only feasible way of obtaining solutions in such cases, this use of computer time is generally justified.

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NOTATION

- C_1 = constant in Planck energy distribution, $5.9529 \times 10^{-16} \text{ (kw.) (sq.cm.)}$
 C_2 = constant in Planck energy distribution, $1.4387 \text{ (cm.) (}^\circ\text{K.)}$

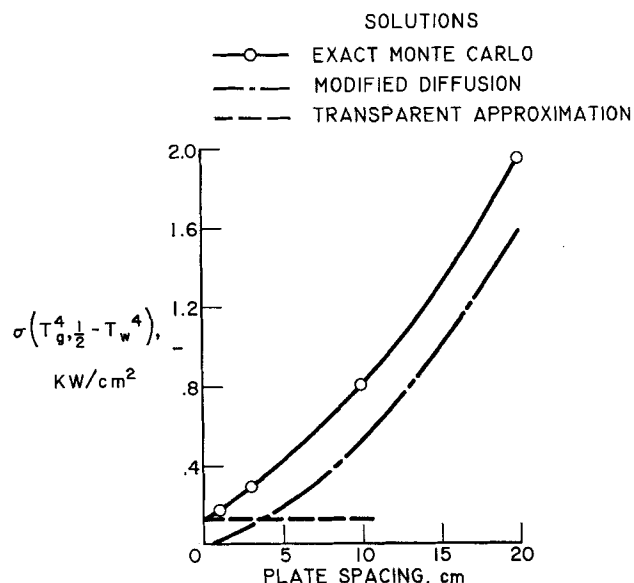


Fig. 7. Comparison of approximations for large and small plate spacing, parabolic source case. Plate temperatures $T_w = T_0 = T_1 = 7,000^\circ\text{K}$. $G_{\max} = 0.145 \text{ kw./cc}$.

c = energy per bundle, kw.
 D = distance between infinite parallel plates, cm.
 e = emissive power, kw./sq.cm.; $\int_0^\infty e_\lambda d\lambda$

$e_{b\lambda}$, $e_{g\lambda}$ = Planck black body emission distribution;
 $2\pi C_1$

$$\lambda^5 \left[\exp \left(\frac{C_2}{\lambda T} \right) - 1 \right]$$

G = heat generation rate per unit volume, kw./cc.
 i = increment index
 l = bundle path length to point of absorption nondimensionalized by D
 N = total number of bundles originally emitted per unit area
 q = energy per unit area, kw./sq.cm.
 R = randomly chosen number in range from 0 to 1
 S = number of bundles per unit area
 T = temperature, °K.
 x = normal distance from surface 0, nondimensionalized by D

Greek Letters

ϵ = emissivity
 η = angle to normal of surfaces
 κ = gas absorption coefficient, cm.⁻¹
 λ = wave length, cm.
 σ = Stefan-Boltzmann constant, 5.670×10^{-15} kw./sq.cm.) (°K.⁴)
 τ = optical thickness, κD
 τ_P = Planck mean optical thickness [Equation (10)]
 τ_R = Rosseland mean optical thickness

Subscripts

A = surface
 $A - \Delta x$ = originally emitted at A , absorbed in Δx
 b = black: wall emissivity of 1
 g = gas
 i = gas increment number
 t = total
 w = of the wall
 x = at point x
 Δx = gas increment
 λ = wave length dependent
 0 = of surface 0
 $0 - 1$ = emitted at 0, absorbed at 1
 1 = of surface 1

Superscript

$-$ = value integrated over wave length range $\Delta\lambda$

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APPENDIX

Derivation of Monte Carlo Relations

Determination of wave length of bundle emitted from a surface The total energy per unit area emitted from surface A is

$$q_A = \int_{\lambda=0}^{\infty} \epsilon_{\lambda A} e_{\lambda b, A} d\lambda \quad (A1)$$

and the frequency distribution of energy in a wave length band $d\lambda$ is

$$df_A(\lambda) = \frac{\epsilon_{\lambda A} e_{\lambda b, A} d\lambda}{\int_0^\infty \epsilon_{\lambda A} e_{\lambda b, A} d\lambda} \quad (A2)$$

Transforming to a uniform density distribution by means of the cumulative distribution function

$$R = \int_0^\xi df_A(\xi) \quad (A3)$$

one gets

$$R = \frac{\int_0^\lambda \epsilon_{\lambda A} e_{\lambda b, A} d\lambda}{\int_0^\infty \epsilon_{\lambda A} e_{\lambda b, A} d\lambda} \quad (A4)$$

If R is taken as a random number in the range of 0 to 1, then (A4) can be solved for the wave length of emission λ .

Determination of wave length of bundle emitted from a gas For emission from a gas a similar procedure yields

$$R = \left[\frac{\int_0^\lambda \kappa_{\lambda} e_{g, \lambda} d\lambda}{\int_0^\infty \kappa_{\lambda} e_{g, \lambda} d\lambda} \right]_i \quad (A5)$$

Determination of bundle path length to absorption The number of bundles dN that will be absorbed in a nondimensional distance dl divided by the number of bundle originally emitted is

$$\frac{dN}{N_0} = \frac{-\tau_{\lambda} N dl}{N_0} = df_n \quad (A6)$$

Solving for N/N_0 and substituting above one obtains

$$df_n = -\tau_{\lambda} \exp \left[- \int_0^l \tau_{\lambda} dl'' \right] dl' = d \left[\exp \left(- \int_0^l \tau_{\lambda} dl'' \right) \right] \quad (A7)$$

This can be transformed to the uniform distribution

$$R = \int_0^l df_n = 1 - \exp \left[- \int_0^l \tau_{\lambda} dl' \right] \quad (A8)$$

Since R is evenly distributed between 0 and 1, it can be replaced by $1 - R$ to give

$$\ln R = - \int_0^l \tau_{\lambda} dl' \quad (A9)$$

Point of emission of bundle in gas for gas heat source case If an energy distribution of the form given by Equation (12) is assumed, the cumulative distribution is

$$R = \frac{\int_0^x G(x') dx'}{\int_0^1 G(x') dx'} = 2x^2 [(3/2) - x] \quad (A10)$$

It can be shown by Rolle's theorem and its corollaries (7) that this equation, which must be solved for x in terms of R , has one and only one real root in the range of interest; this root is

$$x = F_S(R) = \frac{1}{2} + \cos \left(\frac{\Gamma + 4\pi}{3} \right) \quad (A11)$$

where

$$\Gamma = \cos^{-1} (1 - 2R) \quad (A12)$$