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HEAT TRANSFER DURING LAMINAR FLOW FLAME QUENCHING: EFFECT OF FUELS

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ABSTRACT

Wall heat fluxes were obtained in a constant volume combustion chamber for methane-air, ethylene-air and propane-air mixtures. The experiments were performed at pressure near atmospheric over a range of equivalence ratios from 0.8 to 1.2. The unsteady heat fluxes for the three fuels were all correlated by using the heat release rates of the flames prior to quenching and the thermal diffusivity and the flame speed.

The calculations were made using a finite difference method and an integral method. Two step chemical kinetics was used in the finite difference calculations and a simplified ignition temperature approach was employed in the integral method. The results from the finite difference calculation were in good agreement with the experimental data. In the integral method, choosing a single value for the dimensionless ignition temperature for all three fuels also yielded good agreement with the experimental data.

The maximum wall heat flux accounts for one third of the steady laminar flame heat release rate for three fuels.

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INTRODUCTION

There are many factors which influence quenching and previous studies have examined; for example, one dimensional turbulent flames quenching on walls [1], two dimensional laminar flames quenching on walls [2], one dimensional flames propagating through stratified mixtures [3], flames in which radiation is important [4] and two dimensional laminar reacting boundary layers with a reaction at the surface [5]. Results from these investigations have elucidated the importance of such parameters as the Peclet number for determining a length scale and the steady state heat release rate for determining the heat transfer.

In an earlier study [6], it was shown that the unsteady heat transfer from laminar methane air flames follows the same scaling rules as in steady flames; namely, that the heat transfer was proportional to the laminar flame heat release rate prior to quenching. It was also shown that the time scale for quenching was related to the time scale of the thermal propagation of the flame prior to quenching. In the present work, measurements are reported and correlated for the heat flux for three fuels over a broad range of test conditions. In addition, results for the heat transfer were obtained from solutions of the governing equations when formulated in a finite difference form and in an integral form.
EXPERIMENTAL SYSTEM

The experimental apparatus consisted of a constant volume combustion chamber, a mixture preparation unit, a power supply and an optical system. During a test, measurements were made of the chamber pressure, the surface temperature at one location and the motion of the flame using schlieren or shadowgraph photography.

The shape of the combustion chamber was that of two cylinders intersecting at right angles. Both cylinders have a 3.50 inch inside diameter and are 7 inches long. Two quartz windows were located in the ports comprising one axis of the cylinder. In the other cylinder, tungsten spark electrodes pass through one port and a thin film resistance thermometer was mounted on the other port. Along the third axis (vertical), instrumentation ports were also available. A piezoelectric pressure transducer was located on the bottom port to measure the chamber pressure. The air and fuel were metered to produce the desired mixture ratio and the mixture was ignited with a 8 kilovolt, 200 millijoule spark. A more detailed description of the experimental procedure and the apparatus is given in Ref. 6.

CALCULATION METHODS

Finite Difference Method

The experiment was modeled as the interaction of a steady laminar flame with an impervious wall of very large heat capacity. The conservation equations for mass, momentum, energy and the mass fraction of each chemical species are written for one-dimensional unsteady conditions [7]. The chemical reaction rate constants are tabulated in Arrhenius forms. Two step chemical kinetics reaction were used and are shown in Table 1. These give good agreement with the experimental values of the flame speed and the flame temperature [8].
The governing equations were formulated in finite difference form. The resulting coupled equations were solved implicitly in time using a block tridiagonal matrix inversion method. An adaptive algorithm was used which generated a large number of nodes in the region where there are large temperature gradients. The calculations were carried out using the HCT code [9].

We assume for simplicity that the pressure was constant and equal to the value at the time of quenching, $p_q$. The wall temperature, being much less than the flame temperature, was taken to be constant at the value of the unburned gas temperature, $T_u$. The unburned gas temperature $T_u$ was calculated by assuming an isentropic compression from the initial conditions [10]. Radiative heat transfer was neglected in this calculation.

**Integral Method**

An integral method, similar to that employed to solve the steady state boundary layer equations, was used to solve the conservation equations for unsteady reacting gases as applied to flame quenching. The following simplifications were made:

1) viscous terms were neglected,
2) the total derivative of the pressure, $\Delta p/\Delta t$, was taken to be zero,
3) radiative heat transfer was neglected, and
4) specie diffusion was assumed to be caused by Fickian diffusion only.

The gas properties were simplified by assuming:

1) equal mass diffusivities, $D$, and
2) constant specific heats $c_p$.

The reaction terms were simplified by assuming:

1) a one step unimolecular reaction,
2) a reaction rate of the form \( \omega_r = -A \rho r \mathcal{F}(T) \), and

3) an ignition temperature specification for the reaction; i.e. \( \mathcal{F}(T) = 0 \) for \( T < T_{ig} \), \( \mathcal{F}(T) = 1 \) for \( T > T_{ig} \)

The equation of continuity is satisfied by introducing a stream function \( \psi \), defined by

\[
\frac{\partial \psi}{\partial x} = \frac{\rho}{\rho_w}, \quad \frac{\partial \psi}{\partial t} = -\frac{\rho u}{\rho_w}
\]  

(1)

where \( \rho_w \) is the gas density at the wall. The governing equations in \( \psi, t \) coordinates become:

Conservation of Energy:

\[
\frac{\partial T}{\partial t} = \frac{\partial}{\partial \psi} \left[ \frac{k_p}{c_p \rho_w} \frac{\partial}{\partial \psi} \right] + \frac{A Y_r \Delta h}{c_p} \mathcal{F}(T)
\]

(2)

Conservation of Reacting Specie:

\[
\frac{\partial Y_r}{\partial t} = \frac{\partial}{\partial \psi} \left[ \frac{2 D}{\rho_w} \frac{\partial Y_r}{\partial \psi} \right] - A Y_r \mathcal{F}(T)
\]

(3)

The boundary conditions are that the wall temperature is fixed at the unburnt gas temperature, that no specie penetrates into the wall, and that the conditions far from the wall are uniform.

Defining \( \tau = t S_u z / \alpha_w \), \( z = \psi S_u / \alpha_w \), \( \theta = (T_b - T)/(T_b - T_u) \) and \( y = Y_r / Y_{ri} \), and using the conditions across the flame prior to quenching \( c_p(T_b - T_w) = Y_{ri} \Delta h \) yields

\[
\frac{\partial \theta}{\partial \tau} = \frac{\partial}{\partial z} \left[ \frac{k_p}{k_w \rho_w} \frac{\partial \theta}{\partial z} \right] - \frac{A \alpha_w}{S_u^2} y \mathcal{F}(\theta)
\]

(4)
The two parameters in this analysis, \( A \) and \( \theta_{ig} \), result from simplifications to the chemistry and were introduced in the definition of \( \omega_r \). From the solution for a steady adiabatic flame, \( A \) may be expressed as a function of \( \theta_{ig} \) and the flame speed \( S_u \). In analyzing the results from this model, the flame speed was taken as the experimentally accepted value, and the temperature \( \theta_{ig} \) was taken as an adjustable parameter.

The Integral Equations

It is now assumed, for simplicity, that the Lewis number is equal to one, although it is emphasized that the analysis could be readily extended to Lewis number not equal to unity. To apply the integral method, four regions were defined:

I) uniform gas temperature, \( \theta = 1 \), and composition \( y = 1 \), in front of the flame \((0 < z < z_p)\)

II) a preheat region where \( 1 < \theta < \theta_{ig} \) \((z_p < z < z_f)\)

III) a reaction region where \( \theta_{ig} < \theta < 0 \) \((z_f < z < z_b)\) and

IV) a product region of uniform gas temperature \( \theta = 0 \), and composition \( y = 0 \) \((z_b < z < \infty)\).

These regions are shown in Figure 1, along with the reaction rate \( \omega_r \). If non-unity Lewis number were used, then the specie and temperature profiles in front of the flame would have different length scales, and this would be included by the addition of another region, analogous to the preheat region.

Equations (4) and (5) are integrated over each of the four zones. The equations for regions I and IV are trivial, leaving:

\[
\frac{\partial y}{\partial t} = \frac{1}{Le} \frac{\partial}{\partial z} \left[ \frac{k_p}{k_w p_w} \frac{\partial y}{\partial z} \right] - \frac{A a_w}{S^2_u} yF(\theta) \tag{5}
\]
\[ \frac{dI_{\theta}}{d\tau} - \theta I g \frac{dz_f}{d\tau} + \frac{dz_p}{d\tau} = q_f - q_w \] (6)

\[ \frac{dI_y}{d\tau} - y(z_f(\tau), \tau) \frac{dz_f}{d\tau} + y(z_p(\tau), \tau) \frac{dz_p}{d\tau} = j_f \] (7)

\[ \frac{dI_{\theta}}{d\tau} + \theta I g \frac{dz_f}{d\tau} = -q_f - \omega I_y \] (8)

\[ \frac{dI_y}{d\tau} + y(z_f(\tau), \tau) \frac{dz_f}{d\tau} = -j_f - \omega I_y \] (9)

where

\[ I_{\theta II} = \int_{z_p}^{z_f} \theta dz, \quad I_y II = \int_{z_p}^{z_f} ydz, \quad I_{\theta III} = \int_{z_f}^{z_b} \theta dz, \quad I_y III = \int_{z_f}^{z_b} ydz \] (10)

\[ q_w = \frac{\partial \theta}{\partial z} |_{z = z_p}, \quad q_f = \frac{k_f \rho_f \theta}{k_w \rho_w \frac{\partial \theta}{\partial z}} |_{z = z_f}, \]

\[ j_f = \frac{k_f \rho_f \theta y}{k_w \rho_w \frac{\partial \theta}{\partial z}} |_{z = z_f}, \quad \omega = \frac{A \alpha_w}{S_u} \]

Prior to quenching the propagation is steady \((dz_p/d\tau = dz_f/d\tau = dz_b/d\tau = -1,\)

\(dI_{\theta}/d\tau = dI_y/d\tau = 0, \quad q_w = 0, \quad y(z_p(\tau), \tau) = 1)\) and solving the equations yields

\[ q_f = j_f = -1 + \theta I g, \quad y(z_f(\tau), \tau) = \theta I g, \quad A = \frac{S_u^2}{\alpha_w} \frac{1}{I_y III} \]

When quenching occurs, \(z_p = 0,\) and the profiles change with time. The beginning of quenching is defined to occur at \(\tau = 0.\)
Solution of the Integral Equations

Polynomial temperature and specie profiles were chosen for the four regions with the profiles satisfying continuity of the variable and its slope at the interface between the regions. Specifically, quadratic profiles were chosen for $\theta$ in regions II and III, while a quadratic profile was chosen for $y$ in region II and a cubic profile in region III. The profiles were then used to evaluate Equations (6)-(10) which gave four equations for the variables $y_w, y_f, z_f$, and $z_b$. The initial values were obtained from the steady state conditions:

$$z_f(0) = \frac{2k_f\rho_f}{k_w\rho_w}, z_b(0) = \frac{2k_f\rho_f}{k_w\rho_w} \frac{1}{1 - \theta_{ig}}, y_w(0) = 1, y_f(0) = \theta_{ig}$$

The equations were solved by matrix inversion and a Runge-Kutta fourth order integration scheme. The results for the profiles for $\theta_{ig} = 0.7$ are shown in Figs. 2a and 2b. Note that $\theta$ and $y$ are identical when $\tau = 0$ (steady state).

RESULTS AND DISCUSSION

Experimental Results

The experimental results from this study are the unsteady wall heat fluxes during the quenching of a planar, laminar flame. The wall heat flux was determined from the solution of the unsteady conduction problem in the solid using the transient surface temperature recorded from a thin film resistance thermometer [11,12]. The results for the heat flux were averaged over 3 to 10 runs. In all cases the run to run variation in the data produced an error in the heat

\* $y_w \equiv y(0,\tau), y_f \equiv y(z_f(\tau),\tau)$
flux that was only 5% of the value of the maximum heat flux. It is noted that the thickness of the thin film was measured and determined to be of the order of 5 microns [13]. The schlieren system was used to confirm the one-dimensional geometry of flame quenching near the resistance thermometer. Data were obtained for premixed ethylene-air and propane-air mixtures at pressures near atmospheric for equivalence ratios varying from $\phi = 0.80$ to $\phi = 1.20$ (cf. Table 2).

The data (and calculations) were rendered dimensionless by utilizing the heat flux, $q_c$ (cf. Table 2):

$$q_c = \left(\frac{\rho S_u}{\rho_q T_u}\right) \int_{T_u}^{T_b} c_p T \, dt = \rho_u S_u c_p \Delta T_f .$$

(11)

and the characteristic time, $t_c$ (cf. Table 2):

$$t_c = \left(\frac{a}{S_u^2}\right) \frac{p_{q} T_u}{\rho_q T_u} .$$

(12)

Values for the flame speeds for propane-air and ethylene air mixtures were obtained from [14,15,16]. Values of the thermal properties were obtained from [17,18].

The variations of the dimensionless heat flux are presented in Figs. 3 and 4 where $t=0$ corresponds to the maximum flux. It is seen that the data are successfully correlated using the characteristic time, $t_c$, and heat flux, $q_c$, over the range $0.80 < \phi < 1.20$. Note the large variation of the maximum flux $q_{wmax}$ in contrast to the small variation of $q_{wmax}/q_c$ (cf. Table 2). It is important to point out that $q_{wmax}/q_c = \text{const.} = 1/3$ for three mixtures; namely, ethylene-air, propane-air and from [6] for methane air. This is valid over the equivalence ratio range from about 0.80 to 1.20 at pressures near atmospheric.
The experimental results for the heat flux, \( q_w/q_c \), as a function of time, \( t/t_c \), have also been brought together for three mixtures; ethylene-air, propane-air and from [6] for methane-air. The range of the experimental data is contained between the solid curves of Fig. 5. To characterize the shape of the curves, the interval of time, \( t_q \), required for the heat flux to increased from 50% of the maximum value to the maximum is used. The values, \( t_q/t_c \), are tabulated in Table 2.

A length scale for quenching, \( \delta_T \), may be defined as in [6] according to

\[
\delta_T = \Delta T_f k_w/q_{w\text{max}} \tag{13}
\]

where it was shown to be proportional to the conventional measurement of the quenching distance. Values are reported in Table 2.

Finite Difference Calculations

The numerical results for \( q_{w\text{max}}/q_c \), \( t_q/t_c \) and \( \delta_T \) are presented in Table 2 and are in good agreement with the experimental data. The numerical results for the temporal variation of the heat flux for ethylene-air and propane-air mixtures, are contained within the dashed lines of Fig. 5 and are in good agreement with the experimental data. It is noted that in a previous study with methane-air mixtures both detailed kinetics and single step kinetics, were used and both gave good agreement with the experimental data [6].

Integral Method

The results from the integral method are obtained from the solution to the matrix equation, Eq. (6)-(9). A constant value for the specific heat was evaluated at the temperature of the unburned gas. The calculated heat fluxes for
the three fuels are virtually the same* and a single curve is obtained for a given value of $\theta_{ig}$. Four curves are presented in Fig. 6 for values of $\theta_{ig} =$ 0.5, 0.6, 0.7 and 0.8. A value of $\theta_{ig} =$ 0.7 gives good agreement with the experimental data. Note that $t/t_c = \tau$.

That the results of this method agree so well with both the experimental data and the more detailed finite difference calculations may seem a bit surprising in view of the rather drastic assumptions concerning the kinetics (although the assumptions for gas composition and properties are more reasonable). This simple model seems to indicate that for flame quenching at a cold wall the heat transfer is dominated by the diffusion of heat to the wall through a preheated gas layer. The parameters introduced are chosen to give the correct flame speed and temperature, and hence the correct driving force for heat transfer.

Comparison with Steady State Heat Transfer Data

It is instructive to compare the maximum heat flux during unsteady quenching with the maximum value for a steady flame, as determined from a porous plug burner [19,20]. For the three fuels considered in this study, the maximum heat flux is approximately $q_{wmax}/q_c = 1/3$. For steady state flame quenching, the results are $q_{wmax}/q_c = 0.084$ for propane [19] and $q_{wmax}/q_c = 0.07$ for butane [20]. Thus $q_{wmax}/q_c$ for porous plug flames is approximately 1/4th of the value which results during unsteady quenching.

*Note that most fuels have approximately the same value (0.9) for the parameter $k_{f\rho_f}/k_{w\rho_w}$.
SUMMARY AND CONCLUSIONS

Measurements have been made to determine the heat transfer to a wall from a propagating laminar flame. The geometry of the interaction of the flame and the wall was essentially one dimensional and the pressure was nearly atmospheric. The experiments were performed with three different fuel-air mixtures (methane-air, ethylene-air and propane-air) over a range of equivalence ratios from 0.8 to 1.2. The experimental data for all three mixtures are correlated over the range of the test conditions.

The experimental data satisfy the relation $q_{\text{wmax}}/q_c \sim 1/3$ so that the maximum wall heat flux accounts for one third of the steady laminar flame heat release rate.

The finite difference calculations are in good agreement with the experimental data for all three fuels. The integral method yields results that are in good agreement with the data for a value of $\theta_{\text{ig}}$ equal to 0.7.

ACKNOWLEDGEMENTS

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REFERENCES

CAPTIONS

Fig. 1. Definition of the four regions in the integral method

Fig. 2a. Dimensionless temperature profiles as functions of dimensionless distance and time

Fig. 2b. Dimensionless specie mass fraction profiles as functions of dimensionless distance and time

Fig. 3. Experimental results for ethylene-air mixture: wall heat flux versus time for five equivalence ratios. The values of $t_c$ and $q_c$ are in Table II.

Fig. 4. Experimental results for propane-air mixture: wall heat flux versus time for four equivalence ratios. The values of $t_c$ and $q_c$ are in Table II.

Fig. 5. Experimental and finite difference method results for wall heat flux

Fig. 6. Experimental and integral method results for wall heat flux

Table I. Two step chemical reaction rates for ethylene and propane

Table II. Experimental and finite difference method results
Figure 1.
Figure 2a.
range of finite difference method results

range of experimental results

Figure 5.
<table>
<thead>
<tr>
<th>Fuels</th>
<th>Chemical Process</th>
<th>Reaction Rate (cm³-mole-sec-cal)</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ethylene</td>
<td>( \text{C}_2\text{H}_4 + 2\text{O}_2 \rightarrow 2\text{CO} + 2\text{H}_2\text{O} )</td>
<td>( 1.1 \times 10^{14} e^{-40000/RT} [\text{C}_2\text{H}_4]^{0.1}[\text{O}_2]^{1.65} )</td>
</tr>
<tr>
<td>(\text{C}_2\text{H}_4)</td>
<td>( 2\text{CO} + 2\text{H}_2\text{O} \rightarrow \text{C}_2\text{H}_4 + 2\text{O}_2 )</td>
<td>( 10^{14} e^{-40000/RT} [\text{CO}]^{1}[\text{H}_2\text{O}]^{1} )</td>
</tr>
<tr>
<td></td>
<td>( \text{CO} + \frac{1}{2} \text{O}_2 \rightarrow \text{CO}_2 )</td>
<td>( 2.656 \times 10^{14} e^{-40000/RT} [\text{CO}]^{1}[\text{H}_2\text{O}]^{0.5}[\text{O}_2]^{0.25} )</td>
</tr>
<tr>
<td></td>
<td>( \text{CO}_2 + \text{CO} + \frac{1}{2} \text{O}_2 \rightarrow )</td>
<td>( 10^{9} e^{-40000/RT} [\text{CO}_2]^{1} )</td>
</tr>
<tr>
<td>Propane</td>
<td>( \text{C}_3\text{H}_8 + \frac{7}{2} \text{O}_2 \rightarrow 3\text{CO} + 4\text{H}_2\text{O} )</td>
<td>( 2.4 \times 10^{12} e^{-30000/RT} [\text{C}_3\text{H}_8]^{0.1}[\text{O}_2]^{1.65} )</td>
</tr>
<tr>
<td>(\text{C}_3\text{H}_8)</td>
<td>( 3\text{CO} + 4\text{H}_2\text{O} \rightarrow \text{C}_3\text{H}_8 + \frac{7}{2} \text{O}_2 )</td>
<td>( 10^{12} e^{-30000/RT} [\text{CO}]^{1}[\text{H}_2\text{O}]^{1} )</td>
</tr>
<tr>
<td></td>
<td>( \text{CO} + \frac{1}{2} \text{O}_2 \rightarrow \text{CO}_2 )</td>
<td>( 2.656 \times 10^{14} e^{-40000/RT} [\text{CO}]^{1}[\text{H}_2\text{O}]^{0.5}[\text{O}_2]^{0.25} )</td>
</tr>
<tr>
<td></td>
<td>( \text{CO}_2 + \text{CO} + \frac{1}{2} \text{O}_2 \rightarrow )</td>
<td>( 10^{9} e^{-40000/RT} [\text{CO}_2]^{1} )</td>
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Table I.
<table>
<thead>
<tr>
<th>Fuels</th>
<th>$\phi$</th>
<th>$P_q$</th>
<th>$T_u$</th>
<th>$T_b$</th>
<th>$S_u$</th>
<th>$t_c(a)$</th>
<th>$q_c(b)$</th>
<th>$\frac{t_q}{t_c}$</th>
<th>$\frac{q_{wmax}}{q_c}$</th>
<th>$\delta(c)$</th>
<th>$\delta_T(c)$</th>
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<tbody>
<tr>
<td>Ethylene ($C_2H_4$)</td>
<td>0.8</td>
<td>1.159</td>
<td>312</td>
<td>2165</td>
<td>64.6</td>
<td>0.046</td>
<td>2.268</td>
<td>1.885</td>
<td>0.308</td>
<td>70</td>
<td>2.196</td>
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<tr>
<td></td>
<td>0.9</td>
<td>1.188</td>
<td>315</td>
<td>2300</td>
<td>73.5</td>
<td>0.035</td>
<td>2.874</td>
<td>2.086</td>
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<tr>
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<td>2380</td>
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<td>1.209</td>
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<td>2400</td>
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<td>1.2</td>
<td>1.204</td>
<td>316</td>
<td>2370</td>
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<tr>
<td>Propane ($C_3H_8$)</td>
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<td>1.073</td>
<td>306</td>
<td>2120</td>
<td>36.8</td>
<td>0.143</td>
<td>1.255</td>
<td>1.884</td>
<td>0.354</td>
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<td>1.909</td>
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<tr>
<td></td>
<td>1.0</td>
<td>1.086</td>
<td>307</td>
<td>2250</td>
<td>42.1</td>
<td>0.108</td>
<td>1.590</td>
<td>1.813</td>
<td>0.350</td>
<td>92</td>
<td>1.926</td>
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<tr>
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<td>1.1</td>
<td>1.091</td>
<td>307</td>
<td>2265</td>
<td>45.2</td>
<td>0.093</td>
<td>1.753</td>
<td>1.674</td>
<td>0.325</td>
<td>89</td>
<td>2.204</td>
</tr>
<tr>
<td></td>
<td>1.2</td>
<td>1.090</td>
<td>307</td>
<td>2240</td>
<td>41.1</td>
<td>0.111</td>
<td>1.589</td>
<td>1.725</td>
<td>0.334</td>
<td>93</td>
<td>2.036</td>
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Table II.

$^a$ From Eq. (12)

$^b$ From Eq. (11)

$^c$ From Eq. (13)
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