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RESEARCH MEMORANDUM

AN ACTIVE PARTICLE DIFFUSION THEORY OF FLAME QUENCHING
FOR LAMINAR FLAMES

By Dorothy M. Simon and Frank E. Belles

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FOR REFERENCE

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**NATIONAL ADVISORY COMMITTEE
FOR AERONAUTICS**

WASHINGTON

March 4, 1952



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NACA RM E51118

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SUMMARY

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An approximate equation is derived for quenching distance based on the effect of the destruction of atoms and free radicals by a surface, on the chemical reaction, and on flame propagation. The quenching distance is expressed in terms of the diffusion coefficient for the active particles, the partial pressure of the active particles, the time between effective collisions of active particles and gas phase molecules, the efficiency of the surface as a chain breaker, the total pressure of the mixture, and a constant which depends on the geometry of the quenching surface.

The general equation predicts that the quenching distance of a slit (plane, parallel plates) should be 0.61 times the critical diameter for propagation through a tube. This prediction agrees quite well with the two observed factors of 0.70 and 0.62 for the ratio of the quenching distance between parallel plates and in cylindrical tubes as reported in the literature for propane-air flames. The effect of pressure on the quenching distance was calculated from the equation by using the equilibrium partial pressures of atoms and free radicals. The quenching distance for a stoichiometric propane-air flame was predicted to be proportional to the pressure to the -0.91 power which compares favorably with the values of -0.88 determined from quenching-distance measurements and -0.97 from measured critical diameters for propane-air mixtures. A comparison of the derived quenching-distance equation with the Tanford and Pease equation for the burning velocity shows that the predicted relation between burning velocity and quenching distance is consistent with the observed relation. The fact that the experimental data agree so well with the predictions of the equation suggests that the destruction of atoms and free radicals on a surface may control the quenching process under some conditions. The derived equation is used in two ways to predict quenching distances for propane-air flames: (1) with one empirical constant derived from quenching data; and (2) with a constant which is the quotient of the lean flammability limit and a rate constant from flame velocity measurements. Both methods of calculation give quenching distances which are in satisfactory agreement with the calculated values.

INTRODUCTION

The process of quenching is important to the behavior of flames because this process may control flame stabilization, pressure limits of flammability, concentration limits of flammability, and the efficiency of combustion in the region of cold surfaces. The experimental approach to the study of quenching usually involves the measurement of a quenching distance which is considered to be (1) the minimum diameter of a tube or the distance between parallel plates through which a flame will flash back; (2) the minimum distance between parallel plates for which a flame will propagate from a spark of minimum energy; or (3) the length of the dead space between a burner rim and a stable flame. The magnitude of the quenching distance varies with fuel type, fuel-oxidant ratio, pressure, temperature, and quenching-surface geometry. The quenching distance is related to the other combustion properties of the mixture such as flame speed, minimum ignition energy, and limits of flammability. Any complete theory of the combustion wave should show the relations between all the combustible mixture properties and make possible the estimation of the magnitude of one from a knowledge of the others. Also the relation of each combustion property to the true fundamental properties of the gas mixture should be clear.

One relation has been derived by Lewis and von Elbe (reference 1, pp. 211 to 480) who consider the transport of enthalpy in the combustion wave to be governed by heat transport only. Diffusion is neglected. Use of this approximation makes it possible to relate minimum ignition energy, burning velocity, and quenching distance by one equation. From this equation, Lewis and von Elbe (references 1 and 2) have calculated quenching distances for some methane-oxygen-nitrogen mixtures and propane-air mixtures at atmospheric pressure and room temperature. The average deviation of the calculated quenching distance from the measured is 23 percent for hydrocarbon-lean mixtures and is somewhat greater for hydrocarbon-rich mixtures. Because burning-velocity measurements are uncertain at low pressures, quenching-distance calculations could be made for atmospheric pressure only.

A second type of approximate theoretical treatment of the combustion wave results from considering the diffusion of atoms and free radicals as the governing process. Such an approximate treatment has been used for the study of burning velocities (flame speeds) by Lewis and von Elbe (reference 3) and later Tanford and Pease (references 4 and 5).

As part of a flame propagation investigation at the NACA Lewis laboratory, the maximum flame velocities for hydrocarbon-air mixtures for paraffin, olefin, diolefin, and acetylene hydrocarbons have been

shown to be predicted by a Tanford and Pease equation (references 6 and 7). Although the diffusion treatment has been successful in the study of flame velocity it has not been used for other processes such as ignition and quenching.

In this report the second type of approximate treatment is extended to the quenching process. A simple active particle mechanism of quenching is examined in which active particles are considered to be generated in the gas and destroyed on the container walls. Such a mechanism is shown to predict the existence of a limiting diameter for flame propagation. An equation is derived which relates the limiting diameter to the concentration of active particles, the diffusion coefficients for these active particles, the time between effective collisions of an active particle and a gas phase molecule, the efficiency of the wall to destroy chain carriers; the pressure, and a constant depending on the shape of the duct through which the flame is propagating. The predicted pressure effect is compared with the experimentally observed effect of pressure reported in the literature for two types of quenching-distance data. The derived equation is compared with the Tanford and Pease equation for flame velocity, and the relation of flame velocity to quenching distance is predicted.

THEORY

Basis for Existence of a Critical Diameter for Flame Propagation

In the previous investigation of the process of flame propagation based on an active particle diffusion mechanism, the effect of the destruction of active particles on the container walls was considered negligible (reference 5). In order to extend the mechanism to the study of flames propagating in narrow ducts, the effect of active particle destruction on the walls must be evaluated. In the following paragraphs the potential ability of the wall to limit flame propagation is semiquantitatively discussed on the basis of a simple mechanism in which active particles are considered to be generated uniformly in the gas and destroyed on the walls only.

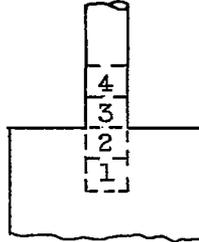
Suppose that a number of active particles N are introduced into a unit volume of combustible mixture. Assume that whenever these particles collide with a molecule of any type in the gas phase (fuel, oxygen, or nitrogen) the active particle is either regenerated or does not react. The particle is then free to react on the next collision. But when a carrier collides with the wall, it is destroyed and a combustion chain is terminated. After a time interval sufficient for each active particle to make one collision there will be less than the original number of active particles N in the unit volume of gas. In other words, the active particles do not reproduce themselves in the

"first generation" and there will be only NE active particles, where E is the efficiency of reproduction. In n generations, the total number of collisions between active particles and gas phase molecules in a unit volume may be represented by the series:

$$NE + NE^2 + \dots + NE^n$$

Since $E < 1$, the series converges to the value $NE/1-E$. This value is then the maximum number of collisions per unit volume between active particles and molecules of gas. The convergence of the series means that there is a limit to the possible number of collisions between active particles and gas phase molecules.

Now consider a propagating flame entering a tube of small diameter. In the following sketch, the unit gas volumes represented by areas 1, 2, 3, and 4 are the same size:



The volume of gas represented by area 2 is identical with that volume represented by area 1; that is, the efficiency of reproduction of active particles is the same and the gas composition is the same. Therefore the number of active particles which diffuse out of volume 2 is the same as diffused into it from volume 1. Unit gas volume 3, however, differs from 2 because the efficiency of reproduction of active particles is decreased by the effect of the walls. The maximum number of collisions between active particles and gas molecules is therefore less than in volume 2. If this total number of collisions is not sufficient to bring about complete reaction, then fewer active particles will diffuse out of volume 3 than diffused into it. In volume 4, then, the maximum number of collisions between active particles and gas phase molecules is again reduced. In this case, the efficiency of reproduction is the same in unit 4 as in 3, but the number of active particles entering 4 is less than the number which entered 3. Successive volume units would show the same effect until the flame is quenched. On the other hand, if the total number of collisions in unit volume 3 is sufficient for complete reaction, the number of chain carriers entering volume 4 is essentially the same as the number which entered volume 3. The efficiency of reaction is the same; so that reaction is complete again. The efficiency of reproduction and the number of carriers entering the unit are the same for every successive unit volume; therefore the flame continues to propagate.

The next step is to consider how important the destruction of a small fraction of the active particles could be in the quenching process. A simplified example is used for this purpose. Suppose that a unit volume of gas contains 9×10^{17} molecules and that 10^{15} active particles are introduced into it. If reaction occurs at every collision of an active particle and a molecule, and if all molecules must react for a flame to propagate, the effect of the destruction of some of the active particles may be calculated from the expression for the sum of the series. If one active particle in 100 were destroyed ($E = 0.99$), only 9.9×10^{16} collisions between active particles and molecules could occur and the flame would be extinguished. If, however, one in 1000 were destroyed ($E = 0.999$), 9.99×10^{17} collisions would occur and the flame would continue to propagate. These simple considerations suggest that the potential power of the destruction of a small fraction of chain carriers to limit flame propagation is strong.

Derivation of General Equation for Quenching Distance and Critical Diameter

It is assumed that chain carriers are introduced into the gas ahead of the flame by diffusion from the burning zone, and that they are regenerated uniformly by chemical reaction in some thin cross section of the duct. Chain branching is considered to be negligible, and the most important process of destruction of active particles is collision with the walls.

Consider a homogeneous volume element located at the mouth of a small duct. The criterion for flame propagation in this element is expressed by equation (1) in which the total number of effective collisions per unit volume before the chain carriers are destroyed at the wall is set equal to the total number of effective collisions per unit volume necessary for the flame to continue to propagate. (An effective collision is defined as one in which a step in the oxidation chain is completed.)

$$\sum_i \frac{\nu_i N_i}{\epsilon_i} = AN_T \quad (1)$$

where

ν_i average number of effective collisions of an active particle of one kind with gas phase molecules before the particle collides with the wall

N_i number of active particles of one kind per unit volume

ϵ_i efficiency of wall to prevent active particles which collide with it from returning to gas phase as chain carriers

A fraction of molecules present in gas phase which must react for flame to continue to propagate

N_T total number of molecules per unit volume

(All symbols are defined in the appendix.)

The average number of effective collisions made by an active particle generated in the gas phase while it diffuses to the wall of the cylindrical vessel is approximated by the equation of Semenov (reference 8):

$$v_i = \frac{d_1^2}{32D_i\tau_i} \quad (2)$$

where

d_1 diameter of cylinder

D_i diffusion coefficient of active particles of one kind into gas

τ_i time between effective collisions for active particles of one kind

This equation was derived for the diffusion of chain carriers to the wall in nonbranching chain reactions in which carriers are being generated uniformly per unit time and volume. The concentration of active particles may be expressed in terms of the total concentration as follows:

$$N_i = \frac{p_i}{P} N_T \quad (3)$$

where

p_i partial pressure of one kind of active particles

P total pressure

Substituting from equations (2) and (3) into equation (1) and solving for d_1 gives

$$d_1 = \left(\frac{32AP}{\sum_i \frac{p_i}{D_i\tau_i\epsilon_i}} \right)^{\frac{1}{2}} \quad (4)$$

Equation (4) is the general expression for the tube diameter which is the quenching distance for propagating flame in a cylindrical duct.

Effect of Geometry on Quenching Distance

If quenching occurs on plane parallel plates instead of on the walls of a cylinder, the constant in the expression for the average number of effective collisions of an active particle of one kind with gas phase molecules before the particle collides with the walls changes (reference 8) to

$$v_i = \frac{d_2^2}{12D_i\tau_i} \quad (5)$$

where

d_2 distance between parallel plates

The general equation for the distance between parallel plates, which is the quenching distance, becomes

$$d_2 = \left(\frac{12AP}{\sum_i \frac{P_i}{D_i\tau_i\epsilon_i}} \right)^{\frac{1}{2}} \quad (6)$$

Then the ratio of quenching distance between parallel plates to quenching diameter of a cylinder may be calculated from equations (4) and (6):

$$\frac{d_2}{d_1} = \left(\frac{12}{32} \right)^{\frac{1}{2}} = 0.61 \quad (7)$$

Pressure Dependence of Quenching Distance

The pressure dependence of the quenching distance may be determined from the general equation (equation (4)). All of the terms except A and ϵ_i are considered pressure dependent: $D_i \propto \frac{1}{P}$; $\tau_i \propto \frac{1}{P}$; and $p_i \propto P^m$. (Only one type of active particle is considered to be present.) The pressure dependence of the quenching distance is shown by the following equation:

$$d_1 \propto \left[\frac{1}{P^{(m+1)}} \right]^{\frac{1}{2}} = P^{-r} \quad (8)$$

where $r = \frac{1+m}{2}$.

Comparison of Quenching-Distance Equation and Tanford
and Pease Flame-Velocity Equation

If it is assumed that free radicals react only on collision with fuel molecules, the following expression may be written:

$$\tau_1 = \frac{1}{k_1 N_f} \quad (9)$$

In this expression, k_1 is the specific rate constant for the reaction of the active particles of one kind and the fuel molecules, and N_f is the number of fuel molecules per cubic centimeter. Substituting equation (9) in equation (4) gives

$$d_1 = \left(\frac{32AP}{N_f \sum_1 \frac{P_i k_i}{D_i \epsilon_i}} \right)^{\frac{1}{2}} \quad (10)$$

Equation (10) may be compared with the Tanford and Pease expression (reference 4) derived for the rate of flame propagation as governed by the diffusion of active particles into the unburned gas. The modified Tanford and Pease equation (reference 6) is expressed in equation (11) in terms of the symbols used in this report:

$$U_f = \left(\frac{nN_f}{PQ} \sum_1 \frac{k_1 P_i D_i}{B_i} \right)^{\frac{1}{2}} \quad (11)$$

where

U_f velocity of flame propagation

n moles of combustion product ($CO_2 + H_2O$) per mole of fuel

Q mole fraction of potential combustion products

B_i term arising from radical recombination in gas phase

From equations (10) and (11) it may be seen that

$$U_f = \frac{1}{d_1} \left[\left(\frac{32nA}{Q} \right) \left(\frac{\sum_1 \frac{k_i p_i D_i}{B_i}}{\sum_1 \frac{k_i p_i}{D_i \epsilon_i}} \right) \right]^{\frac{1}{2}} \quad (12)$$

The term in brackets must be evaluated to determine the relation of flame velocity and quenching distance for specific cases.

APPLICATION OF THEORY

Calculation of Equilibrium Flame Temperature and Atom and Free Radical Product Concentrations

In order to evaluate the quenching distance equation, it is necessary to know the concentration of active particles. The active particle concentration was obtained from hydrogen atom, oxygen atom, and hydroxyl radical equilibrium product concentrations for the oxidation reaction at flame temperature because these values may be calculated. Equilibrium product concentrations and adiabatic flame temperatures were calculated by a matrix method (reference 9) using the tables of thermodynamic constants compiled in reference 10. The heat of formation of propane is the value listed in the National Bureau of Standards compilation (reference 11). Equilibrium flame temperatures were calculated for four or five pressures (1 atmosphere and lower) for each of the following concentrations: 2.5, 3.0, 3.5, and 4.03 (stoichiometric) percent propane by volume. The calculated values of equilibrium product composition and flame temperature are given in table I.

Effect of Geometry on Quenching Distance

The quenching distances for propane-air flames reported by Friedman and Johnston (reference 12) were measured by a rectangular slit which approached the case of quenching by plane parallel walls while the critical diameters for propane-air flames reported in reference 13 were measured in cylindrical tubes. The average value for the ratio of the quenching distances obtained by the two methods was found to be 0.70 (reference 13).

Harris, Grumer, von Elbe, and Lewis also report (reference 2) flame-quenching distances between parallel plates and in cylindrical tubes for eight mixtures of propane in air. The average value for the ratio of

these two quenching distances is 0.62. The two observed ratios compare favorably with the theoretical ratio of 0.61 obtained from equation (7).

Comparison of Predicted and Experimental Pressure Effect
on Quenching Distance

The equation for quenching distance which includes the three active particles and diffusion coefficients at room temperature and atmospheric pressure may be derived from equation (4) by substituting the diffusion coefficients for room temperature and atmospheric pressure (reference 4). For example, for the hydrogen atom,

$$d_i = \frac{D_H T_F^2}{P(298)^2} \quad (13)$$

where D_H is the diffusion coefficient of hydrogen atoms at 25° C and atmospheric pressure. Equation (13) includes the assumption of some mean temperature for the reaction zone as expressed by T_F .

In addition, if it is assumed that

$$\tau_i = \tau_H = \tau_O = \tau_{OH} \quad (14)$$

and

$$\epsilon_i = \epsilon_H = \epsilon_O = \epsilon_{OH}$$

the equation becomes

$$d_1 = \left[\left(\frac{32 T_F^2 A \tau_i \epsilon_i}{(298)^2} \right) \left(\frac{1}{\frac{P_H}{D_H} + \frac{P_O}{D_O} + \frac{P_{OH}}{D_{OH}}} \right) \right]^{\frac{1}{2}} \quad (15)$$

The pressure dependence of the first factor is P^{-1} , and the pressure dependence of the denominator of the second factor was determined as the slope of the least square lines through the logarithm of the pressures plotted against the logarithm of the relative atom concentrations

$\frac{P_H}{D_H} + \frac{P_O}{D_O} + \frac{P_{OH}}{D_{OH}}$. The diffusion coefficients previously calculated in reference 7 were used ($D_H = 1.8 \text{ cm}^2/\text{sec}$; $D_O = 0.40$; $D_{OH} = 0.28$). The

pressure dependence of the relative atom and free radical concentrations was evaluated for four propane concentrations in air (fig. 1).

The quenching distance was calculated to be proportional to the pressure to the -0.91 power at stoichiometric which may be compared with the value of -0.88 from the experimental data of Friedman and Johnston (reference 12) and -0.97 from the data of reference 13. The values of the pressure exponent for four different concentrations are listed in table II. It may be seen that the theoretical values decrease slowly with the propane concentration in air, whereas experimental values decrease more rapidly. The agreement between the theoretical and the experimental pressure effect on the quenching distance is surprisingly good.

Relation of Quenching Distance and Flame Velocity

Previously (reference 13) flame velocities at atmospheric pressure for propane-air mixtures of different hydrocarbon concentrations were reported to vary as the reciprocal of the quenching distance. In order for this observation to be consistent with equation (12), the term in brackets must be practically constant. The curve showing the relation of flame speed and critical diameter for propane-air mixtures of various hydrocarbon concentrations at atmospheric pressure and 25° C is reproduced as figure 2. For these data, the term in brackets in equation (12) was found to be roughly constant. (A, B₁, and ε₁ were assumed to be constant.) The observed correlation between flame velocity and quenching distance is then consistent with the active particle diffusion mechanism. It should be noted that the equation does not predict the flame speed to be proportional to the reciprocal of the quenching distance except when the term in brackets in equation (12) is constant. Also, the data used for the linear relation are very limited in range since flame speeds at low pressure are uncertain.

Calculation of Quenching Distance

An equation for the quenching distance between parallel plates which contains one empirical factor (Aε₁/k₁) may be obtained from equation (15) by substituting the value for τ₁ from equation (9) and the proper constant from equation (6):

$$d_2 = \left[\left(\frac{A\epsilon_1}{k_1} \right) \left(\frac{12T_F^2}{(298)^2 N_F} \right) \left(\frac{1}{\frac{P_H}{D_H} + \frac{P_O}{D_O} + \frac{P_{OH}}{D_{OH}}} \right) \right]^{\frac{1}{2}} \quad (16)$$

This equation was used with the quenching distances of Friedman and Johnston (reference 12) for propane-air flames at different pressures and three concentrations to determine the value of the empirical factor ($A\epsilon_1/k_1$).

Figure 3 shows how well the quenching data correlate with equation (15). The quenching distance squared is plotted against the factor

$\frac{12T_F^2}{(298)^2 N_F \sum_i \frac{P_i}{D_i}}$. The equation predicts that this curve should be a

straight line with a slope of $A\epsilon_1/k_1$. The data do define a straight line with a slope of 8.65×10^{10} molecules cubic centimeter⁻¹ second. This value of $A\epsilon_1/k_1$ was used to calculate quenching distances which are compared with the measured values in table III. The average deviation of the calculated values from the experimental values is ± 2.7 percent.

By using the value of the average specific rate constant calculated from the flame velocity equation (reference 1) of 2.38×10^{-13} cubic centimeters molecules⁻¹ second⁻¹, the value of $A\epsilon_1$ may be calculated to be 0.0206; A is defined as the fraction of the total molecules which must react for the flame to propagate. It was assumed that the initial reaction is between active particles and fuel molecules; therefore all the reacting molecules must be propane. The efficiency of the wall to destroy chain carriers ϵ_1 is a value between 0 and 1. The calculated value of $A\epsilon_1$ is found to be close to the value of the low inflammability limit for propane-air mixtures measured at atmospheric pressure and room temperature in a 2-inch glass tube. The value reported by Lewis and von Elbe (reference 1, p. 749) as mole fraction of propane is 0.0212. Although the correspondence between $A\epsilon_1$ and the low inflammability limit is probably fortuitous, it is consistent with the observation that the value of the low limit depends on the apparatus used for measurement.

The empirical constant from equation (15) ($A\epsilon_1/k_1$) may be well approximated by the quotient of the low inflammability limit (expressed as mole fraction of hydrocarbon) and the rate constant from the flame velocity work; this fact may be used to advantage to predict quenching distances from the equation without any factors derived from the quenching data. The quenching distances so calculated for propane are shown in table III. These values deviate from the experimental values by an average of ± 3 percent.

DISCUSSION

This simplified treatment of the process of flame quenching does not give the complete picture of conditions existing in the flame,

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but it suggests that the destruction of active particles on a surface could account for flame quenching by a cold surface. These considerations also give a better understanding of the possible relation between the chemical oxidation process and the fundamental combustion property called quenching distance by showing that a flame might be extinguished by the loss of a few chain carriers. On the basis of an active particle diffusion process, the relation between two fundamental combustion properties, flame velocity and quenching distance, is clarified. The rate of flame propagation may be accounted for by the diffusion of active particles into the unburned gas ahead of the flame, while flame quenching may be governed by the diffusion of active particles to the walls. The process of flame propagation appears to be closely related to the chemical reaction between active particles and the molecules of the combustible mixture, whereas flame quenching is more closely related to the chain termination step in the oxidation process.

This mechanism of quenching indicates that the nature of the surface should be important. The results of experiments to determine the effect of the nature of the surface on the quenching distance are conflicting. In general, either no surface effect or only a slight surface effect has been observed. It may be that the surfaces used were not really very different. All surfaces may have appeared to be similar because each was covered with an adsorbed water layer, or the efficiency of removal of chain carriers from the gas phase by any surface at flame temperature may be the same.

The equation developed in this report has been shown to predict quenching distances both at atmospheric and low pressure. The average deviation of the calculated values from the experimental values was 3 percent. The equation based on heat transport which was previously discussed (references 1 and 2) was found to be limited to the prediction of quenching distances at atmospheric pressure until reliable burning velocities are measured for low-pressure flames. Quenching distances were predicted by the second equation for propane-air mixtures with an average deviation of 23 percent from experimental values. The new equation appears to be more useful for the calculation of quenching distances because low pressure values may be predicted and the agreement with experimental values is good.

The correspondence between quenching distances calculated by either equation and experimental quenching distances is so close and the assumptions in the derivations are so broad that a choice between the two mechanisms is not justified. Undoubtedly, both processes occur. The fact that the new equation based on the diffusion of chain carriers fits so well suggests that the destruction of chain carriers on a surface may control the quenching process under some conditions.

SUMMARY OF RESULTS

The results of this investigation of quenching distance may be summarized as follows:

1. An equation for the quenching distance in a cylinder was derived:

$$d_1 = \left(\frac{32AP}{\sum_i \frac{p_i}{D_i \tau_i \epsilon_i}} \right)^{\frac{1}{2}}$$

where

d_1 diameter of cylinder

A fraction of molecules present in gas phase which must react for flame to continue to propagate

P total pressure

p_i partial pressure of one kind of active particles

D_i diffusion coefficient of active particles of one kind into gas

τ_i time between effective collisions for active particles of one kind

ϵ_i efficiency of wall to prevent active particles which collide with it from returning to gas phase as chain carriers

2. The ratio of the quenching distance between plane parallel plates and the critical diameter for flame propagation in a cylinder was calculated to be 0.61. This value compared favorably with two experimental values of 0.70 and 0.62.

3. The effect of pressure on quenching distance was satisfactorily predicted by the derived equation.

4. The predicted relation between quenching distance and flame velocity was consistent with the observed relation.

5. The derived equation for quenching distance was used with either an empirical constant or a constant which was the quotient of the lean-limit fuel concentration and a rate constant from flame-speed calculations to predict quenching distances satisfactorily.

CONCLUSIONS

From the results of this study it may be concluded that:

1. The quenching-distance data for propane-air flames are consistent with a mechanism of the process based on wall destruction of chain carriers.

2. Quenching distances for propane-air (hydrocarbon lean) flames can be estimated from the derived equation using the lean inflammability limit and the flame-speed rate constant.

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APPENDIX - SYMBOLS

The following symbols are used in this report:

| | |
|----------|--|
| A | fraction of molecules present in gas phase which must react for flame to continue to propagate |
| B_1 | term arising from radical recombination |
| D_H | diffusion coefficient for hydrogen atoms into air at 25° C and atmospheric pressure |
| D_i | diffusion coefficient of active particles of one kind into gas at reaction-zone temperature and pressure |
| D_O | diffusion coefficient for oxygen atoms into air at 25° C and atmospheric pressure |
| D_{OH} | diffusion coefficient for hydroxyl radicals into air at 25° C and atmospheric pressure |
| d_1 | diameter of tube |
| d_2 | distance between parallel plates |
| E | efficiency of reproduction of active particles |
| k_i | specific rate constant for reaction of active particles of one kind with fuel molecules |
| N | number of active particles per unit volume |
| N_f | number of molecules of fuel per unit volume |
| N_i | number of active particles of one kind per unit volume |
| N_T | total number of molecules per unit volume |
| n | number of generations and moles of combustion product ($CO_2 + H_2O$) per mole of fuel |
| P | total pressure |
| P_H | partial pressure of hydrogen atoms |
| p_i | partial pressure of active particles of one kind |
| p_O | partial pressure of oxygen atoms |

| | |
|--------------|--|
| p_{OH} | partial pressure of hydroxyl radicals |
| Q | mole fraction of combustion products |
| T_F | flame temperature |
| U_F | velocity of flame propagation |
| ϵ_i | efficiency of wall to prevent active particles which collide with it from returning to gas phase as chain carriers with gas phase molecules before particle collides with wall |
| ν_i | average number of effective collisions of an active particle of one kind with gas phase molecules before particle collides with wall |
| τ_H | time between effective collisions for hydrogen atoms |
| τ_i | time between effective collisions for active particles of one kind |
| τ_O | time between effective collisions for oxygen atoms |
| τ_{OH} | time between effective collisions for hydroxyl radicals |

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TABLE I - CALCULATED PARTIAL PRESSURES OF FREE RADICALS AND EQUILIBRIUM

FLAME TEMPERATURES FOR PROPANE-AIR MIXTURES AT VARIOUS PRESSURES



| Propane in air (percent by volume) | Total pressure (atm) | Partial pressure of H atom (atm) | Partial pressure of O atom (atm) | Partial pressure of OH radical (atm) | Equilibrium flame temp- erature (°K) |
|--|----------------------------|--|--|--|---|
| 2.50 | 1.00 | 0.05×10^5 | 1.69×10^5 | 26.12×10^5 | 1719 |
| 2.50 | .50 | .04 | 1.19 | 15.51 | 1719 |
| 2.50 | .066 | .03 | .42 | 3.36 | 1717 |
| 2.50 | .013 | .02 | .18 | .97 | 1715 |
| 3.00 | 1.00 | 1.04 | 10.34 | 96.41 | 1941 |
| 3.00 | .50 | .85 | 7.19 | 56.68 | 1939 |
| 3.00 | .066 | .46 | 2.41 | 11.74 | 1929 |
| 3.00 | .013 | .25 | .94 | 3.19 | 1913 |
| 3.50 | 1.00 | 9.55 | 30.58 | 221.16 | 2134 |
| 3.50 | .50 | 7.37 | 20.54 | 126.79 | 2125 |
| 3.50 | .066 | 3.07 | 6.00 | 23.79 | 2089 |
| 3.50 | .013 | 1.33 | 2.04 | 5.84 | 2048 |
| 4.03 | .659 | 37.18 | 27.29 | 201.19 | 2255 |
| 4.03 | .222 | 20.22 | 14.51 | 82.12 | 2223 |
| 4.03 | .065 | 9.73 | 6.75 | 28.89 | 2182 |
| 4.03 | .033 | 6.37 | 4.34 | 16.04 | 2157 |
| 4.03 | .016 | 3.99 | 2.65 | 8.43 | 2130 |

TABLE II - COMPARISON OF THE CALCULATED AND EXPERIMENTAL
PRESSURE EFFECTS ON THE QUENCHING DISTANCE

| Volume percent propane in air | Pressure exponent | | |
|--|-------------------|------------------------------|------------------------------|
| | Theoretical | From data of reference 12 | From data of reference 13 |
| 4.03 | -0.91 | -0.88 | -0.97 |
| 3.50 | -.90 | -.85 | -.92 |
| 3.00 | -.88 | -.83 | -.85 |
| 2.50 | -.87 | ---- | -.76 |



TABLE III - COMPARISON OF CALCULATED AND EXPERIMENTAL
QUENCHING DISTANCES



| Volume percent propane | Pressure (atm) | Quenching distances (cm) | | |
|------------------------|----------------|--------------------------|--------------------|------------|
| | | Experimental | Calculated | |
| | | | Empirical constant | Lean limit |
| 4.03 | 0.0832 | 1.80 | 1.81 | 1.79 |
| 4.03 | .133 | 1.16 | 1.19 | 1.17 |
| 4.03 | .216 | .73 | .76 | .75 |
| 4.03 | .359 | .48 | .50 | .49 |
| 4.03 | .600 | .31 | .32 | .32 |
| 4.03 | 1.000 | .20 | .20 | .20 |
| 3.50 | .0832 | 2.06 | 2.04 | 2.02 |
| 3.50 | .133 | 1.33 | 1.34 | 1.32 |
| 3.50 | .216 | .84 | .86 | .85 |
| 3.50 | .359 | .57 | .57 | .56 |
| 3.50 | .600 | .36 | .35 | .35 |
| 3.50 | 1.000 | .25 | .24 | .24 |
| 3.00 | .0832 | 2.84 | 2.83 | 2.79 |
| 3.00 | .133 | 1.87 | 1.87 | 1.84 |
| 3.00 | .216 | 1.16 | 1.23 | 1.21 |
| 3.00 | .359 | .78 | .78 | .77 |
| 3.00 | .600 | .52 | .50 | .49 |
| 3.00 | 1.000 | .37 | .32 | .32 |

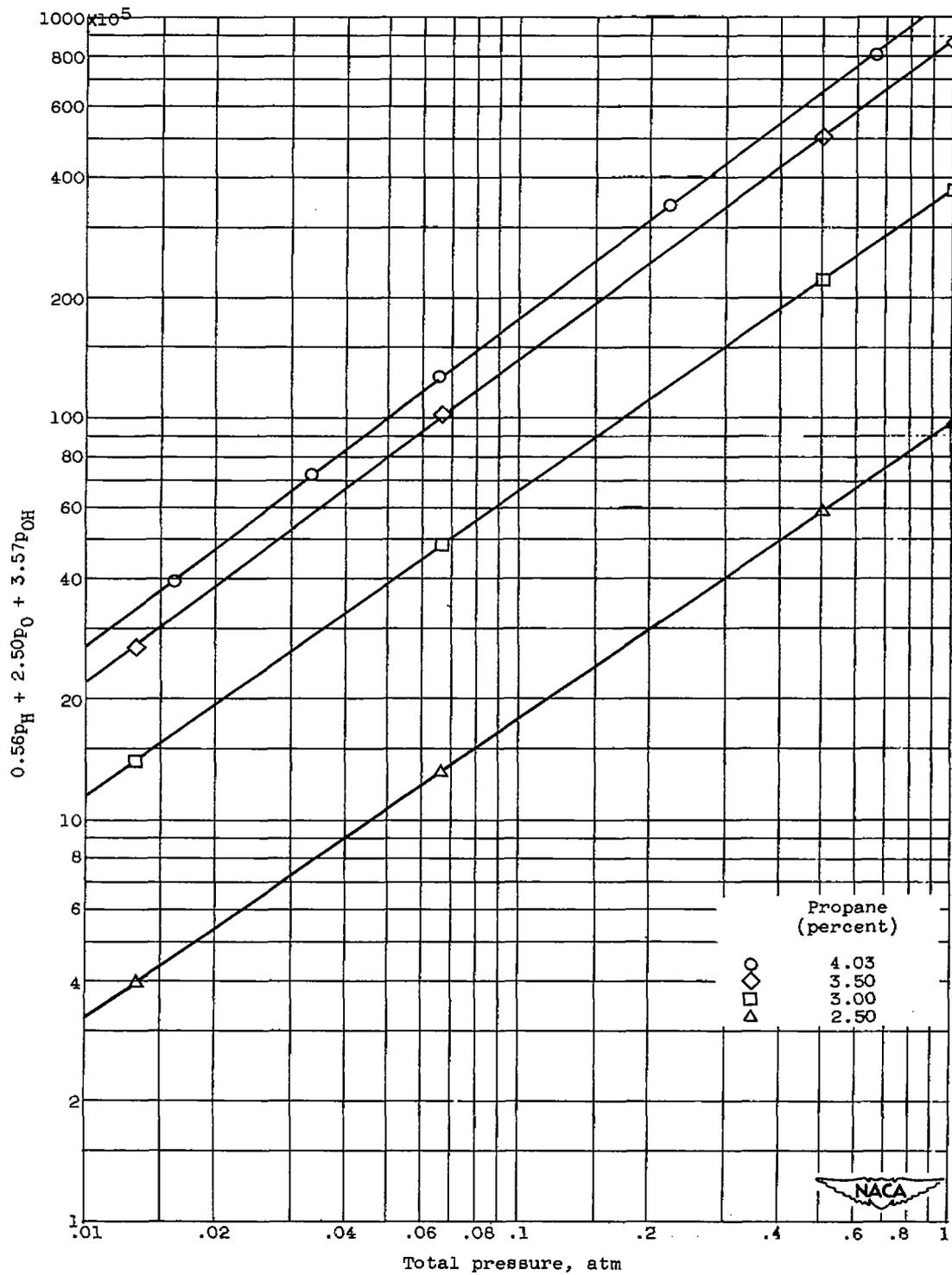


Figure 1. - Variation of relative active particle concentration with total pressure.

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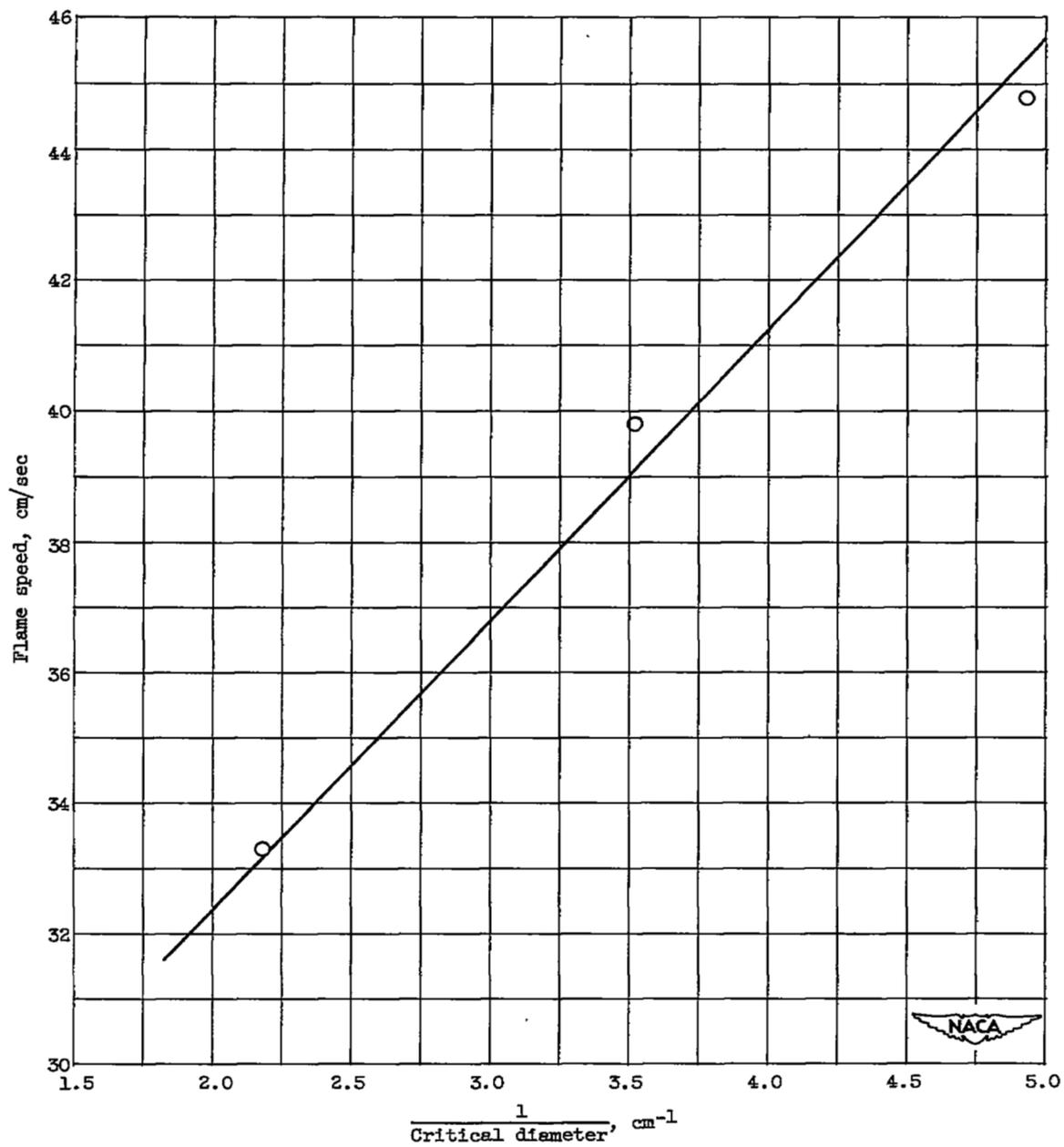


Figure 2. - Correlation of flame speed with critical diameter for various propane-air mixtures at atmospheric pressure and 23° C (reference 9).

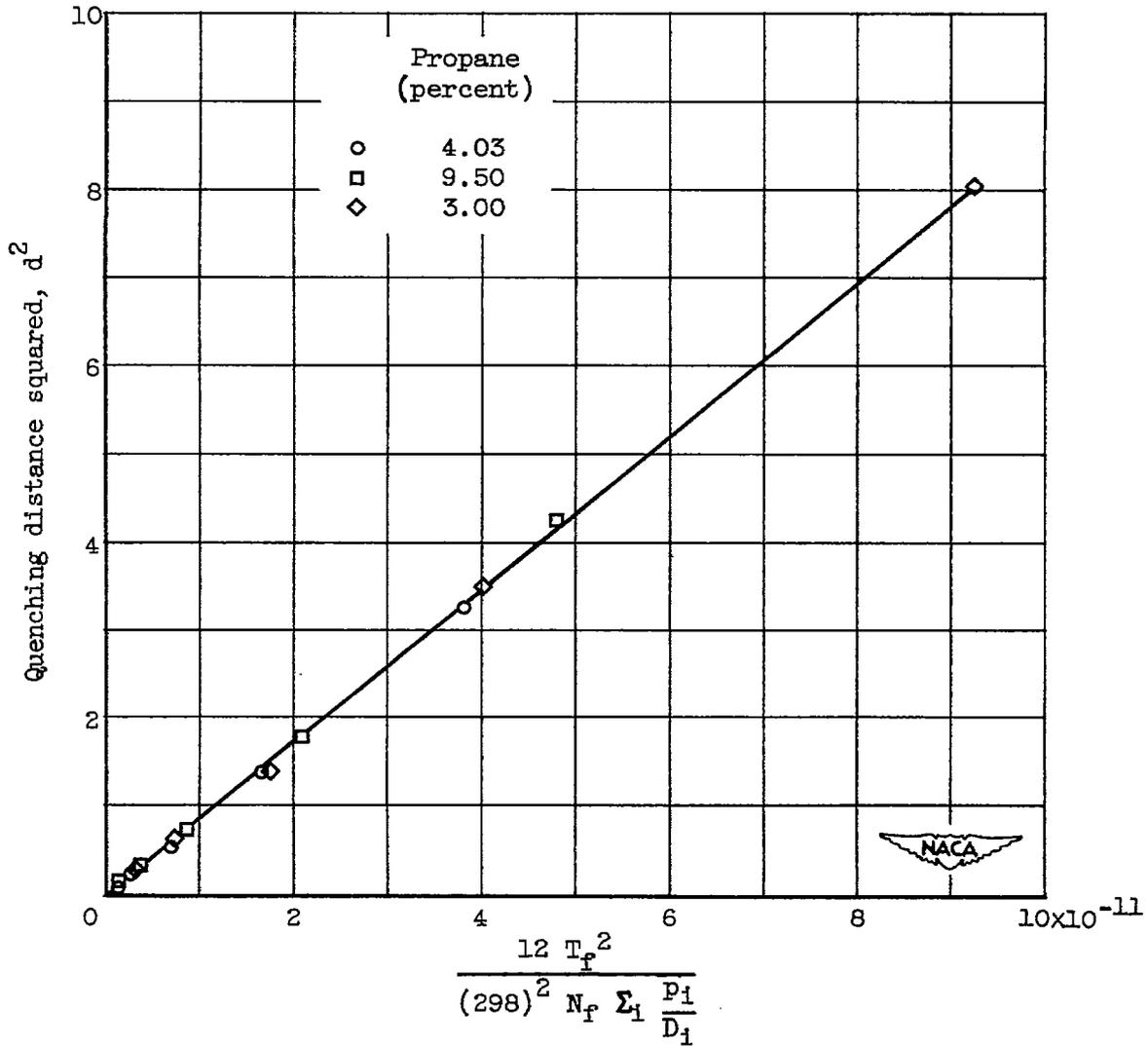


Figure 3. - Correlation of experimental data with equation for quenching distance.

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