AD-751 494

FLAME PROPAGATION IN A VORTEX RING

Percival D. McCormack

University College

Prepared for:

Air Force Office of Scientific Research

October 1972

AFOSR - TR - 72 - 2144

AD751494

A F O S R INTERIM OCTOBER, 1972

SCIENTIFIC REPORT

FLAME PROPAGATION IN A VORTEX RING

P. D. McCormack, Ph.D., Sc.D.

Department of Mathematical Physics

This Research is supported by the Air Force Office of Scientific Research under Grant No. AFOSR - 72 - 2222

Approved for public release;
distribution unlimited.

Faculty of Science, University College, Cork, Ireland.

30 R

UNCLASSIFIED

Security Classification

DOCUMENT CONTROL DATA - R & D

(Security classification of title, body of abstract and indexing annotation must be entered when the overall report is classified)

1. ORIGINATING ACTIVITY (Corporate author) UNIVERSITY COLLEGE DEPARTMENT OF MATHEMATICAL PHYSICS CORK, IRELAND	2a. REPORT SECURITY CLASSIFICATION UNCLASSIFIED 2b. GROUP

3. REPORT TITLE

FLAME PROPAGATION IN A VORTEX RING

4. DESCRIPTIVE NOTES (Type of report and inclusive dates)

Scientific Interim

5. AUTHOR(S) (First name, middle initial, last name)

PERCIVAL D MCCORMACK

6. REPORT DATE	7a. TOTAL NO. OF PAGES	7b. NO. OF REFS
Oct 1972	~~22~~ 30	10

8a. CONTRACT OR GRANT NO. AFOSR-72-2222 b. PROJECT NO. 9711-02 c. 61102F d. 681308	9a. ORIGINATOR'S REPORT NUMBER(S) 9b. OTHER REPORT NO(S) (Any other numbers that may be assigned this report) AFOSR - TR - 72 - 2144

10. DISTRIBUTION STATEMENT

Approved for public release; distribution unlimited.

11. SUPPLEMENTARY NOTES	12. SPONSORING MILITARY ACTIVITY
TECH, OTHER	AF Office of Scientific Research (NAE) 1400 Wilson Boulevard Arlington, Virginia 22209

13. ABSTRACT

Enhanced flame propagation speeds in vortex rings formed of premixed combustible gases has been reported. Constant volume combustion with a rotating heat source (which the ignited vortex core is) can produce a propagating pressure wave. But this mechanism apparently fails as the propagation criterion cannot be met. Stability considerations indicate that the molecules in a vortex core are rotationally excited. Three consequences of this are examined: (a) the transport properties of the gas in the core; (b) the effect on reaction rate; (c) the possibility of heat conduction by an internal convection mechanism.

DD FORM 1 NOV 65 1473

UNCLASSIFIED

Security Classification

14. KEY WORDS	LINK A		LINK B		LINK C	
	ROLE	WT	ROLE	WT	ROLE	WT
COMBUSTION						
VORTEX RING COMBUSTION						
MOLECULAR ROTATION						

Interim Scientific Report

Flame Propagation in a Vortex Ring

Dr. P. D. McCormack,
Department of Mathematical Physics,
University College,
Cork,
IRELAND.

This research is supported by the Air Force Office of Scientific Research under Grant No. AFOSR - 72-2222.

Contents:

1. Introduction

Observations and measurements on the combustion of vortex rin· formed of an approximately stoichiometric mixture of propane and air have been carried out and reported on [1,2,3]. The vortex rings were formed conventionally by applying a pressure pulse upstream of a circular orifice. From 3 cm. to 7 cm. diameter orifices were used and the initial vortex rings would have roughly the same diameters (2R).

Ideally the vortex rings have a finite core of rotational fluid, surrounded by an irrotational vortex flow field in which the tangential velocity falls off as $\frac{1}{r}$, where r is the radial distance from the core center. If a is the initial core radius, then $a \ll R$.

If $\tilde{I}$ is the impulse of the pressure then following von Karman, the initial vortex strength is given by

$$K = \frac{\tilde{I}}{\rho} \quad \text{------------ (1)}$$

where ρ is the fluid density. Using Lamb's non-viscous analysis, the initial forward velocity of the vortex ring (with respect to the surrounding fluid) is given by the relation

$$v = \frac{K}{4\pi R}\left\{\ln\frac{8R}{a} - \frac{1}{4}\right\} \quad \text{----- (2)}$$

A .ere is viscous action between the vortex core and the surrounding . .:

(i) a increases with time (or distance from the orifice)

(ii) K and v decrease with time.

Continuum fluid dynamics can tell us nothing about the <u>structure</u> of the vortex core, nor about its size. A basic kinetic theory for the fluid in a vortex core must be resorted to. Section 2 of this report will consider this aspect further. Such a theory is required before a satisfactory theory of flame propagation through a vortex core can be developed.

It is appropriate at this stage to summarize the observations and results obtained from experiments made on the combustion of pre-mixed vortex rings.

(i) the flame propagated symmetrically from the ignition region round the vortex ring (or torus) till the two flame fronts met on the far side of the ring.

(ii) although some expansion had occurred, visual observation showed that the ring was still intact when the flame fronts met.

Fig. 1 shows a photograph of a burning vortex ring.

(iii) High speed movie Schlieren photographs confirmed the ordinary photographic evidence (Schlieren is sensitive to heat output) that the ring was still intact when the two flame fronts met. There is an indication that the advancing leading edges of the 'heat fronts' are pointed rather than flat. This would support the concept of a central highly heat conductive core.

(iv) a mean flame propagation speed was arrived at by measuring the time taken for the flame fronts to traverse (half) the ring. Knowing the approximate circumference of the ring, the mean speed was computed.

Fig. 2 shows a graph of flame speed versus vortex strength for the 7 cm. orifice. Speeds of up to 1350 cm/sec. for the propane/air mixture and up to about 1550 cm/sec. for the propane/oxygen, were measured.

For a propane/air mixture the flame termperature is about 2260°K and for a constant pressure spherically expanding flame the measured velocity of flame propagation in a quiescent mixture would be about 30. $(\frac{2260}{300}) \approx$ 220 cm/sec. The turbulent flame speed is at most about twice this[4] - that is, about 400 cm/sec.

The fluid flow in a vortex core is well-ordered - at least in a macroscopic sense - and there is no axial convection round the torus under normal conditions.

It therefore appears that flame speeds in a vortex core are enhanced with respect to that in a quiescent mixture by a factor of about five.

The remainder of this report will deal with preliminary considerations of mechanisms which could be responsible for enhanced flame speeds in vortex cores.

The structure of the vortex core - in so far as molecular kinetics will determine reaction kinetics and transport processes - is a matter of basic concern with respect to flame propagation therein. The next section will deal with a new postulate which the principal investigator has formulated. This will require experimental verification and so must be regarded as tentative at present.

2. Structure of the Vortex Core

It has been generally assumed that the velocity profile in the vortex core is linear - characteristic of solid - body rotation. The core is thus a shear free region. But this leads to a velocity discontinuity between the core and the surrounding irrotational region. There must be a shear layer (or boundary layer) between the two regions. Thus on a macroscopic scale the core structure is as shown in Fig. 3.

The inner rotational core is formed initially at the orifice by the pressure pulse. Through viscous interactions with the surrounding gas the shear, or boundary layer is formed, and increases in extent with time.

It is thus pertinent to consider the inner rotational core. If it rotates with an angular velocity $\vec{\omega}$ then this is called the vortex angular velocity and

$$\vec{\omega} = \frac{1}{2} \operatorname{curl} \vec{v} \qquad (3)$$

where $\vec{v}$ is the macroscopic translational velocity.

The internal thermodynamic energy, E, of the vortex core is a good physical variable. But $\frac{1}{2}$ curl $\vec{v}$ corresponds to a uniform rotation of the molecular mass centers (for polyatomic molecules) and E is not invariant with respect to such a rotation. If $\vec{\Omega}$ is the molecular spin angular velocity, it is only when $\vec{\omega} = \vec{\Omega}$ that E is independent of curl $\vec{v}$ and so can be good physical variable. In fact unless this is so, the core could not be in equilibrium and torque must be present in the system. If the z-components of $\vec{\omega}$ and Ω are different say, then the torque would have a moment proportional to $\omega_z - \Omega_z$.

It is interesting to note that Fetter has shown that a planar lattice array of point vortexes each of strength K , confined to a circular region, must have a definite angular velocity for self-consistency. In the continuum limit of number density n, this angular velocity is given by the relation

$$\vec{\omega} = \frac{1}{2} K n \qquad (4)$$

where κ is the point vortex strength. If these are identified as molecules, each with effective radius r and spin angular velocity Ω then

$$\omega = (\pi r^2 n)\Omega \quad ------- (5)$$

$\pi r^2 n$ represents an effective molecular cross-sectional area per unit area (for a planar system). This is probably a more realistic condition for a stable vortex core than that arrived at by thermodynamic considerations alone ($\omega = \Omega$). Thus, if a vortex core is to be inherently stable, the molecules of which it is formed must be in states of non-zero angular momentum.

It is postulated that this rotational excitation occurs in wall collisions (non-specular) as gas molecules pass through the orifice. It has been shown theoretically[5] that a finite percentage of diatomic molecules in a beam colliding with a solid surface, are excited into the second, or third, rotational energy states. The pressure pulse used to form the vortex could possibly

(a) increase this percentage greatly by supplying the extra energy required

(b) cause the excited molecules to form a 'clump', or rotational core in space.

The major objection to this postulate is that rotational relaxation times are of the order of 10^{-8} second. And vortex life-times are of the order of at least 10^{-2} second. But in a volume element of a gas containing <u>only</u> rotating molecules - all in the same excited state - the relaxation time would be effectively infinite. Only the peripheral gas molecules would experience rapid attenuation of their rotational energy through interaction with the surrounding 'irrotational gas' molecules.

The gas in the vortex core would have bulk viscosity and so energy dissipation <u>within</u> the core would only occur in the presence of pressure fluctuations.

Molecular Orientation due to Rotation-induced Dipole Moments

Molecular rotation can endow a non-polar molecule with

(a) an electric dipole moment due to centrifugal distortion of the molecule.

(b) a magnetic dipole moment due to asymmetry in the electronic change distribution in the molecule.

In both cases, if the dipoles are aligned and each of strength μ then the interaction potential is given by

$$\Phi_{ab} = \pm \frac{\mu^2}{r_{ab}^3} \qquad (6)$$

Even for a polyatomic molecule such as propane, unless the rotational quantum number (J) is quite high, the distortion of the molecule is small and so μ is small.

If L is the rotational angular momentum, then the magnetic dipole moment is

$$\hat{\mu} = \gamma_{nr} \hat{L} \qquad (7)$$

where γ_{nr} is the nuclear rotational gyromagnetic ratio.

This can be written classically as

$$\mu^{RN} = \frac{1}{2c} \sum_s e_s (r_s \times v_s)$$

where e_s is the charge on the s^{th} nucleus
r_s " " position vector of "
v_s " " instantaneous velocity "

For example, if there were N nuclei of the same mass m and charge e then

$$\mu^{RN} = \frac{e}{2c} \sum_s (r_s \times v_s)$$

$$= \frac{e}{2mc} L \qquad (8)$$

where L is the rotational angular momentum of the molecule. Even for the maximum possible L values, μ value of less than 1 Bohr magneton are predicted.

Thus dipole-dipole interactions in a gas of rotating molecules will be weak, but they are long range and

(a) can reduce, or even eliminate, hard core interaction so that the soft-potential contribution to the transport properties predominate. In fact one would expect anomalously low shear viscosity and thermal conductivity.

(b) can cause the molecules to orient due to alignment of the axes of rotation. This should result in the gas in a vortex core being optically anisotropic and it should be possible to design an experiment to verify this. The molecular motion in a gaseous vortex core would be correlated in this sense - that is, angular correlation.

<u>Core Size</u>

An estimate of the lowest value feasible for the core diameter can be arrived at by the following arguement. To cause an overall enhanced burning velocity the core region should have a lateral extent which is at least of the order of magnitude of the flame preheat zone thickness. And for propane/air, this is about 0.1 cm. The observed initial core diameter (for the 7 cm. orifice) was about 0.5 cms., and so the shear-region must be the larger in size, even close to the orifice.

It is interesting to note that the smallest energy containing centered eddies in turbulent flows have a reciprocal wave number (size) of about .07 cms.

One must be careful to differentiate between a turbulent flame, in which a flame propagates through a system containing a random assembly of eddies, and the vortex ring flame in which flame propagation through a single "[illegible]y" in effect, is being observed.

To establish the stability and properties of a vortex core (thermodynamic and transport) which would follow from the core structure proposed here, will require extensive theoretical analysis. Detailed and critical experimentation will be required to substantiate these predictions. In the meantime, the question of flame propagation in such a vortex core has been considered. Some possible mechanisms of propagation will be outlined in the following sections.

3. Constant Volume Pressure Wave

If combustion occurred at constant volume, then as the burning vortex core is effectively a rotating heat source, a propagating pressure wave could arise at the flame front and would result in an increase in flame speed.

Following the analysis of the pressure waves generated by such a source[6], it turns out that a wave can only propagate if the core rotational frequency (ω_o, say) is larger than the natural frequency of transverse vibration of the column of gas of radius a (the initial vortex core radius in this case). The latter frequency was deduced to be given by the relation

$$\omega_T = \frac{\lambda_{mn} c_o}{a} \qquad \text{-----------(4)}$$

where c_o is the speed of sound in the burned gas.

λ_{mn} is the nth smallest root of the equation, $J_m'(\lambda)=0$

For the gas column of radius 0.1 cm. (the initial core radius), $\omega_T \sim 10^6$ radians/sec. Using an average vortex strength of 3,000 cm^2/sec. sec leads to a value for ω_o of about 10^5 radians/sec. It appears that this criterion for pressure propagation could be met only by postulating,

(i) unrealistically high vortex strength and/or

(ii) a much smaller core size (and then the problem of ignition would arise).

The analysis also predicts that the amplitude ratio of the wave $\delta p/p$ is proportional to the value of ω_o and so would increase linearly with vortex strength. The flame speed ratio, $\frac{\Delta u}{u}$ will be proportional to $\delta p/p$ and so should increase linearly with vortex strength - as indeed has been established (see Fig.[illegible])

To achieve speed increases by a factor of between 3 and 5 would require large pressure changes and the vortex ring would disintegrate.

Finally, there is no real reason to drop the constant pressure combustion condition.

In view of these various adverse factors, it is doubtful if this mechanism can be taken as operative in vortex core combustion.

4. Internal Convection Mechanism

Daniell[7] in 1930 demonstrated that essentially the laminar burning velocity was proportional to

(i) the square root of the reaction rate.

(ii) the square root of the ratio of the thermal conductivity to the specific heat at constant pressure. In fact,

$$u \doteq \left(\frac{1}{\rho_0}\right)\sqrt{\left(\frac{\lambda}{C_p}\right) w} \qquad (10)$$

where w is the reaction rate

λ is the thermal conductivity of the combustible mixture

C_p is the specific heat of the mixture

ρ_0 is the density " " " "

Now,

$$\lambda / C_p = \frac{4}{3}\mu + \mu_B \qquad (11)$$

where μ is the shear viscostty of the gas

μ_B is the bulk viscosity of the gas

Thus (λ/C_p) represents the effective viscosity of the gas, or the molecular interaction. As postulated in Section 2, there is no shear viscosity in the core gas and so

$$\frac{\lambda}{C_p} = \mu_B$$

in the core. If C_p is reasonably constant, then this implies that the coefficient of heat conduction for core gas is very low. A reduction in flame speed would therefore be expected from this. It is possible, however, that heat transport in a vortex core could be effected by a mechanism known as Internal Convection. The high heat conduction in liquid helium has been attributed to this mechanism[8].

Derivation of Spin-Wave Equation

A wave motion in a gas (apart from the normal pressure, or sound, wave) becomes possible if the molecules are endowed with magnetic moments associated with internal angular momentum or spin. Spin 'signals' can then be propagated through the gas from one part to another. The relevant wave equation will now be derived.

The molecules will orient or line-up in the presence of dipole-dipole interactions and if $\vec{\mu}$ is the molecular magnetic moment and n the number density the macroscopic magnetizition is given by

$$\vec{M} = n \langle \vec{\mu} \rangle \quad \text{------------ (12)}$$

and

$$\vec{\mu} = \gamma \vec{L} \quad \text{------------ (13)}$$

where γ is the gyromagnetic ratio
L is the rotational momentum
$\langle \ \rangle$ implies the ensemble average.

A disturbance, such as a sudden rise in temperature (as in ignition) will destroy this magnetization and lead to a diffusion of spins.

If $\vec{J}_M = n[\vec{c}\,\vec{\mu}]$ is the flux of magnetization ($\vec{c}$ is the mean molecular speed) then $\vec{M}$ and $\vec{J}_M$ satisfy the following equations of change.[9]

$$\partial_t M + \nabla\cdot[\vec{u}\vec{M} + \vec{J}_M] = n\,\partial_c \langle\vec{\mu}\rangle \quad \text{----- (14)}$$

$$\partial_t \vec{J} + \nabla\cdot[\vec{u}\,\vec{J}_M + n\langle\vec{c}\,\vec{c}\,\vec{\mu}\rangle] + (\nabla\vec{u})^{t}\cdot\vec{J}_M - \rho^{-1}(\nabla\cdot P)\vec{M} = n\,\partial_c\langle\vec{c}\,\vec{\mu}\rangle \quad \text{--------- (15)}$$

It can be shown[10] that if the distribution function is taken in the form

$$f = f^{0}[1+\phi]$$

that to this first order of approximation the collision, or source, terms in equations (14) and (15) are given by

$$n\,\partial_c\langle\vec{\mu}\rangle = -\frac{\mathcal{M}}{\tau_\mu} \qquad (16)$$

$$n\,\partial_c\langle\vec{c}\,\vec{\mu}\rangle = -\frac{\vec{J}_\mu}{\tau'_\mu} \qquad (17)$$

where $\mathcal{M} = \vec{M} - \vec{M}_0$ is the deviation of the magnetization from its stationary value.

$$\vec{M}_0 = n^\circ\langle\vec{\mu}\rangle$$

and

$$\tau_\mu = \langle\vec{\mu}^2\rangle \Big/ \left(n\left[\vec{\mu};\vec{\mu}\right]\right) \qquad (18)$$

$$\tau_{\mu'} = \langle\vec{\mu}^2\rangle \Big/ \left\{2n\left[\vec{\mu}\times\vec{W};\vec{\mu}\times\vec{W}\right]\right\} \qquad (19)$$

where $\tau_\mu, \tau_{\mu'}$ are relaxation times

$$\vec{W} = \left(\frac{m}{2kT}\right)^{1/2}\vec{c}$$

$[\;\;]$ implies a square-bracket integral. If γ is independent of L then τ_μ reduces to the spin relaxation time τ_{sp} defined as

$$\tau_{sp} = \left(\frac{r}{2n}\right)\left[\vec{\Omega};\vec{\Omega}\right]$$

where $\vec{\Omega} = (2\Gamma kT)^{-1/2}\vec{L}$ is the dimensionless angular momentum

Γ is the moment of inertia of the molecule.

r is the number of degrees of rotational freedom.

If there is no streaming motion then $|\vec{\mu}| = 0$ and from the above equations result the following coupled differential equations

$$\partial_t \mathcal{M} + \vec{j} + \tau_{\mathcal{M}}^{-1}\mathcal{M} = 0 \quad \text{-------(21)}$$

$$\partial_t \vec{j} + \omega_{sp}\mathcal{D}_{sp}\Delta\mathcal{M} + \omega_{sp}\vec{j} = 0 \quad \text{----(22)}$$

where

$$\omega_{sp} = (\tau_{\mathcal{M}'})^{-1}, \quad \mathcal{D}_{sp} = kT/m\omega_{sp}$$

$$\vec{j} = \nabla\cdot\vec{J}_{\mathcal{M}}$$

If the inertial term is ignored in eq.(21) then one gets the constitutive relation

$$\vec{j} = -\mathcal{D}_{sp}\Delta\mathcal{M} \quad \text{-----------(23)}$$

or

$$\vec{J}_{\mathcal{M}} = -\mathcal{D}_{sp}\nabla\mathcal{M} \quad \text{---------(24)}$$

Equation (24) relates the spin flux to the gradient of spin, or magnetization, deviation. Using this in equation (21) gives the equation

$$\partial_t\mathcal{M} - \mathcal{D}_{sp}\Delta\mathcal{M} + \frac{\mathcal{M}}{\tau_{\mathcal{M}}} = 0 \quad \text{-----(25)}$$

Thus $\mathcal{D}_{sp}$ is identified as the coefficient of spin diffusion . . $\tau_{\mathcal{M}}$ is the spin relaxation time. But this is a parabolic equation which describes a 'collective' motion of the medium which tends to 'smooth out' irregularities of the spin deviations. This equation would imply that a deficit of magnetization in one region stimulates an <u>immediate</u> response through the system.

One can obtain uncoupled partial differential equations for $\vec{\mathcal{M}}$ and $\vec{j}$ from equations (21) and (22) by differentiating (21) with respect to time and eliminating $\vec{j}$ and $\partial_t\vec{j}$ from the resulting equations by the use of equations (21) and (22). This results in the telegrapher's equation

$$\ddot{\mathcal{M}} + (\omega_{sp} + \tau_{\mathcal{M}}^{-1})\dot{\mathcal{M}} - \omega_{sp}\mathcal{D}_{sp}\Delta\mathcal{M} = 0 \quad \text{--------(26)}$$

which implies that the spin deviations propagate in a wave-like way with a finite velocity of propagation and are confined to a characteristic signal cone.

The coefficient $\omega_{sp} \mathcal{D}_{sp}$ has the dimensions of velocity squared. This the wave-velocity, c where

$$c^2 = \omega_{sp} \mathcal{D}_{sp} = \frac{kT}{m} \quad \text{--------(27)}$$

For normal temperatures this predicts a value for c in the region of 10^5 cm/sec. Normally $\omega_{sp} \sim \tau_M^{-1}$ and so the damping coefficient in equation (26) is just $2\omega_{sp}$ or $2\tau_M^{-1}$. As ω_{sp} is about 10^8 sec^{-1} the damping would be far too great to allow propagation of the wave. But accepting that the spin relaxation time (decay time would be more accurate) in a vortex core is much larger than in normal gas, the damping becomes negligible and to a first approximation can be ignored. Equation (26) then becomes a pure wave equation. The boundary, or initial conditions are:

$$M = M_0 \text{ at } x > 0, \ t = 0$$
$$M = 0 \text{ at } x = 0, \ t \geq 0$$

The step change M_0 in the spin at the ignition point will propagate at about 10^5 cms/sec through the core.

In effect there are two kinds of fluid present in the vortex core:

(i) the rotational, or gyroscopic fluid, which has low velocity and molecules with extra spin. It could be called a superfluid.

(ii) the normal fluid - which is created when the temperature rises. It has normal viscosity and normal spin.

There is no net mass flux and so

$$\rho_s v_s + \rho_n v_n = 0 \quad \text{--------(28)}$$

The heat current is carried by the normal fluid and for a one dimensional system the heat flux is given by

$$q = \rho S T v_n$$

where S is the entropy per unit mass. It has been shown[8] that

$$\dot{v}_n + \left(\frac{\rho_s}{\rho_n}\right) S \nabla T = 0 \quad \text{--------(29)}$$

and as

$$v_n - v_s = v_n \frac{\rho}{\rho_s}$$

$$\therefore \dot{v}_n - \dot{v}_s = -\left(\frac{\rho}{\rho_n}\right)_s \nabla T \qquad (30)$$

It is this concept of 2 fluid components which is the basis for the internal convection of heat. The differential equation for internal convection is as follows:

$$\rho_n \frac{\partial (v_n - v_s)}{\partial t} = \rho S \nabla T + \frac{\eta_n}{\rho S T}\left(\nabla \times \nabla \times q - \frac{4}{3}\nabla \nabla \cdot q\right) \qquad (31)$$

where η_n is the viscosity of the normal fluid. For stationary heat transfer,

$$\Lambda \nabla T = -\nabla \times \nabla \times q \qquad (32)$$

where $\Lambda = (\rho S)^2 T / \eta_n$

is a coefficient characteristic of heat transfer by internal convection. It is analogous to the normal coefficient of heat conductivity.

Using typical values of

S = 1.0 cal/ °K·gm.
ρ = 10^{-3} gms./c.c
η_n = 1 micropoise
T = 300°K

gives a value of

$\Lambda \doteq$ 3 cal/°K·cm.sec.

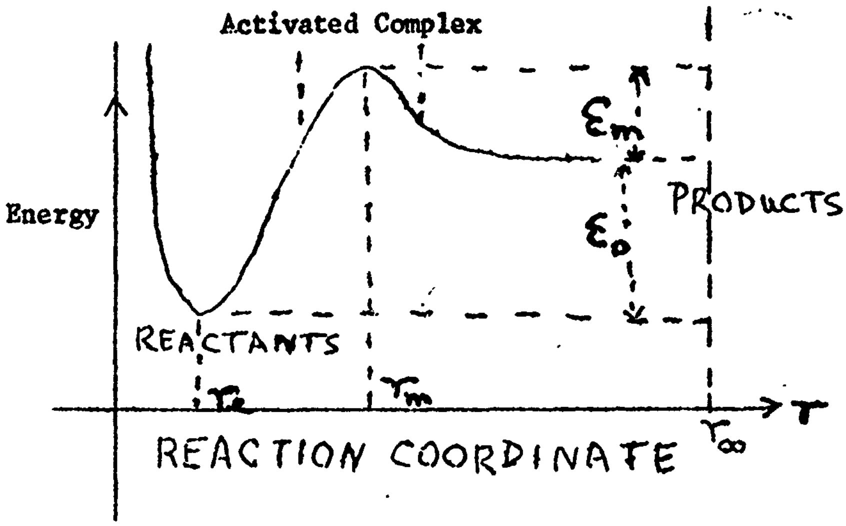
This compares with a thermal conductivity of about 10^{-4} for a normal gas, and so an enormous increase in the capacity to conduct heat is indicated.

This estimate is probably excessively high due to the ideal fluid model used. But it does indicate that the process of internal convection in vortex cores could easily produce thermal conductivities such that flame speeds as high as those observed would be feasible (a 25-fold increase in heat conduction would be quite sufficient).

5. Effect of Molecular Rotation on the Chemical Reaction Rate.

The collision of reactant molecules can produce products only if the energy of the reactants (that is, their relative kinetic energy) exceeds a certain minimum value known as the activation energy, E.

The situation is illustrated schematically below for a one-dimensional potential energy surface.



The Boltzman energy distribution law states that the probability that a molecule possesses energy $E\ (= \varepsilon_D + \varepsilon_m)$ is proportional to $\mathrm{EXP}(-E/RT)$. This factor actually represents the fraction of collisions between reactant molecules in which reaction products can be formed. That is, to form products the colliding molecules must reach the top of the potential energy barrier.

Absolute reaction rate theory assumes that the reacting system at the top of the barrier is a molecule - or activated complex - which is in equilibrium with the reactants. The rate at which the activated complex decays to products is then equal to the reaction rate.

The rate of dissociation of a diatomic complex formed of 1 atom of A and 1 atom of B will be studied here.

Suppose the number of combined pairs is N_{AB}, then the rate constant for dissociation is

$$k_D = \frac{kT}{h(P.f.)_{vib}} \operatorname{Exp}\left\{-\frac{\varepsilon_D + \varepsilon_m}{kT}\right\} \text{------} (33)$$

where h is Planck's constant

$(P.f.)_{vib.}$ is the vibrational partition function

k_D is the number of dissociations per unit time per unit complex.

Effect of Rotation on k

In deriving eq.(33) it is assumed that the molecule is in its lowest rotational state. If this is not so, then the effect on dissociation can be accounted for by adding the rotational potential to the potential-energy curve.

For the rotational state with quantum number j the rotational potential is given by,

$$\frac{j(j+1)h^2}{8\pi^2 m r^2}$$

The addition of this potential to the potential energy curve

(a) shifts the positions of the maximum and minimum slightly

(b) raises the minimum by

$$j(j+1)h^2/8\pi^2 m r_e^2$$

(c) raises the maximum by

$$j(j+1)h^2/8\pi^2 m r_m^2$$

Thus $\varepsilon_D + \varepsilon_m$ is changed by the difference between these quantities and so

$$k_{D,j} = \frac{kT}{h(P.f)_{VIB}} \text{EXP}\left\{-\frac{\varepsilon_D + \varepsilon_m + j(j+1)K^2(r_m^{-2} + r_e^{-2})}{kT}\right\} \quad (34)$$

where K^2 =

For a rotational state j, then, the factor by which the rate constant will change will be

$$k_{D,j}/k_D = \text{EXP}\left\{\frac{j(j+1)K^2(r_m^{-2} - r_e^{-2})}{kT}\right\} \quad (35)$$

Now at large distances the attractive force between atoms is predominantly van der Waal's, whose potential varies as r^{-6}

Hence, the effective potential energy at $r > r_m$ is

$$\varepsilon_P = j(j+1)K^2/r^2 - C/r^6 \quad (36)$$

For an atom with radius 2A°,

$$C \sim 1.4 \times 10^{-58}$$

and it can be shown that

$$r_m^2 = 1.728\left(\frac{3C}{kT}\right) \quad (37)$$

For j = 3(say), this leads to

$$k_{D,3}/k_D \sim 1.03$$

A 3% increase in reaction rate is forecast. Even if a j = 10 value was used, the factor only rises to 1.35 - a 35% increase.

To explain the 5-fold increase in flame speed in vortex cores, the reaction rate would have to increase by a factor of 25.

So the enhancement of reaction rate in the presence of molecular rotational excitation would appear to be ruled out as being responsible for the high flame propagation speed in vortex cores.

6. Concluding Remarks

The high flame propagation speeds observed in vortex rings formed of premixed combustible gases could be explained if the heat transport capability of the gas mixture was increased sufficiently.

In a gas of molecules with spin, heat transport could occur via a spin (or entropy) wave mechanism instead of the normal diffusion process. An internal convection analysis shows that the effective coefficient of heat conductivity in this case is several orders of magnitude greater than the normal coefficient. A very high flame speed would result from this.

This mechanism depends on the vortex core being comprised of rotationally excited molecules. Thermodynamic and stability considerations suggest that this must be so. Such a core structure has several implications:

(i) the spin (or rotation) attenuation time in a gas of rotating molecules must be of the order of a second (the vortex life-time in air). The vortex core gas then must have almost zero shear viscosity, but would have bulk viscosity. Indeed it is frequently assumed that the core is a shear-free region (that it rotates as a solid-body).

This remains to be shown.

(ii) the core will have a small, but finite, magnetization.

(iii) the core gas would be optically anisotropic.

In the area of Air Force technology three complementary project require to be carried out:

(i) the combustion of vortex rings formed of gaseous oxygen and entrained atomized liquid fuel. This will increase the energy density of the flame.

(ii) the repetitive formation of vortex rings and their combustion (a frequency of 10 per second should be possible.)

Both of these projects are necessary steps to establish the feasibility of a practical combustion, or light source, based on this phenomenon.

(iii) the use of lasers to ignite the vortex ring. This could have a bearing on the use of such a configuration in fusion reaction.

REFERENCES:

(1) 'Combustible Vortex Rings' Proc. Royal Irish Academy Vol. 71 No. 6 (1971)

(2) 'Flame Propagation in Vortex Cores'. Combustion & Flame (in the press, 1972)

(3) "Vortex Ring Combustion" 8th AFOSR Combined Contractor's Meeting on Combustion Dynamics Research Chicago, 1972. AFOSR - TR - 72 - 0653

(4) Gerstein, M. and Dugger, G. L. Report 1300 NACA, Washington, D.C. (1957)

(5) "Rotational Transitions in the Scattering of a Beam of Light Diatomic Molecules from a Surface". R. Logan Molecular Physics 17 No. 2 (1969)

(6) B. T. Chu N.A.C.A., TN 3411

(7) P. G. Daniell, Proc. Royal Society London 126A, 393 (1930)

(8) Superfluids. F. London John Wiley & Sons (1954) pp. 157-164

(9) Dahler, G. Phys.Rev. 129, 1464 (1963)

(10) Dahler, G. and Hoffman, D. K. Ch.1 Transfer & Storage of Energy by Molecules. Volume 3. Wiley-Interscience (1970)

FIG. 1 BURNING VORTEX RING

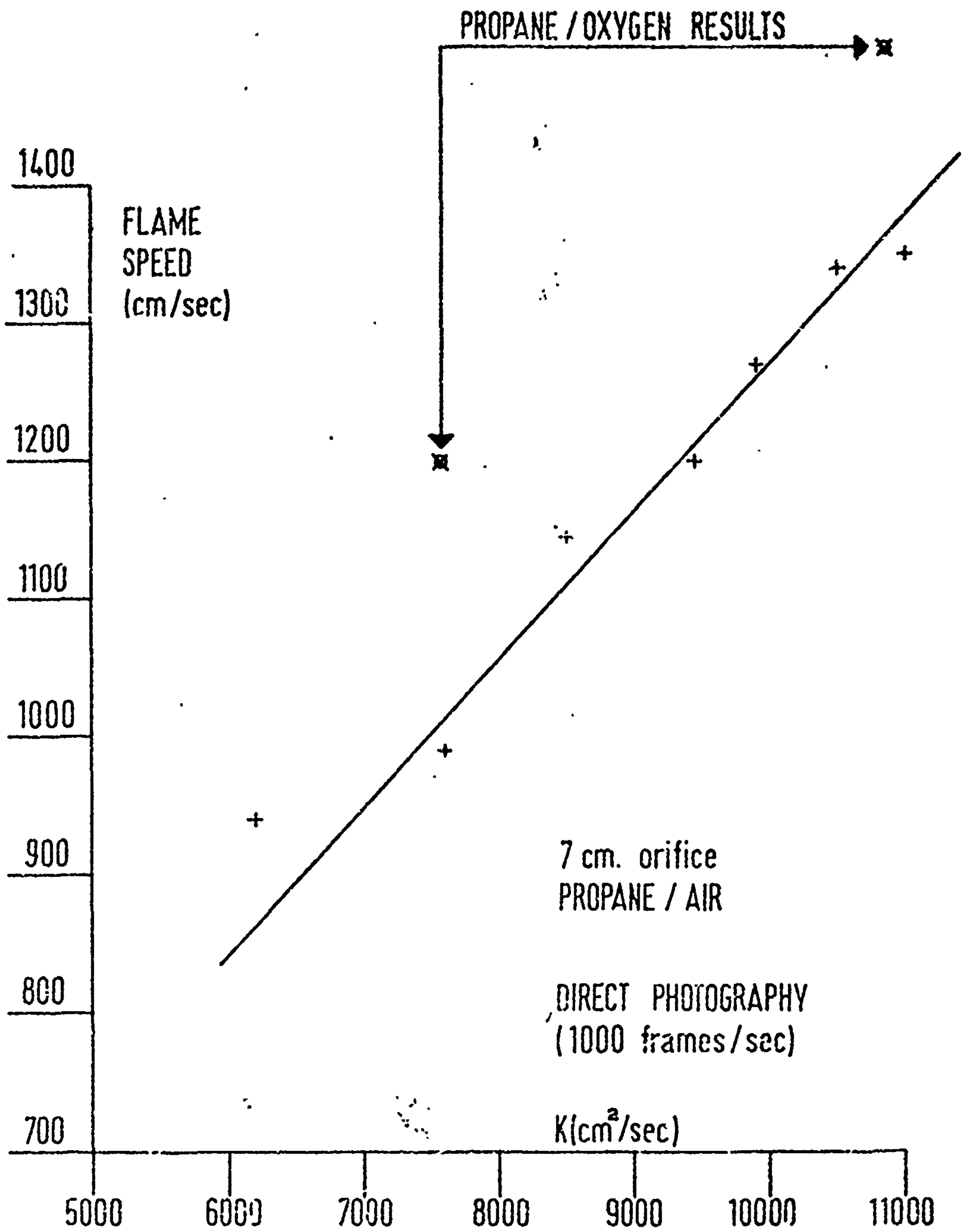


FIG. 2 FLAME SPEED VS. VORTEX STRENGTH

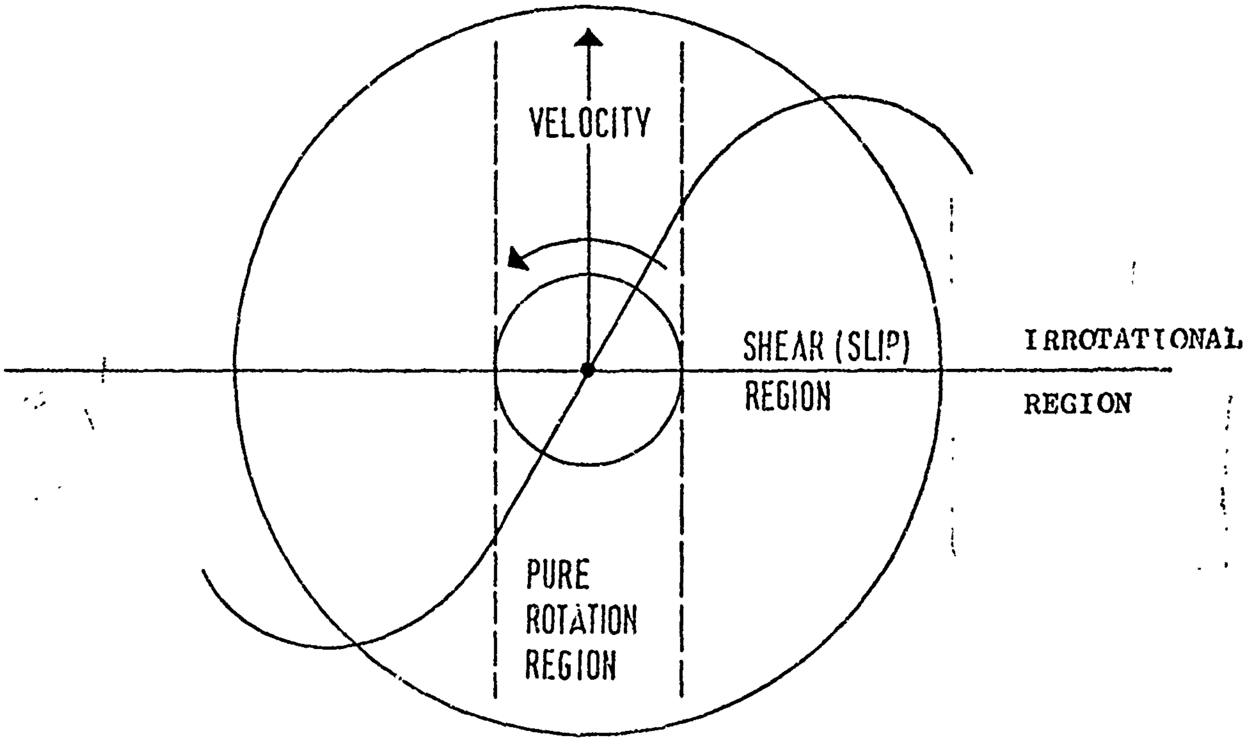


FIG. 3 VORTEX CORE