ASYMPTOTIC COMBUSTION OF SPHERICAL DROPS

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ABSTRACT
     An analysis is made to determine the rates of drop shirnkage and flame
     movement during the asymptotic combustion of spherical drops controlled
     by the transport of heat and mass. The effects of unsteady diffusion
     and radial convection of heat and mass are taken into account. Exact
     solutions of the equations governing spherically-symmetric transport
     phenomena are obtained from which the expressions describing the radius
     time history for the drop and flame surface are determined. The ef-
     fects of gas inertia, transient terms and radial convection resulting
     from unequal fluid densities are established and the regions of appli-
     cability of previously reported approximate solutions are determined.

Introduction

     The combustion of liquid fuel sprays is of considerable practical impor-

tance in oil burners, diesel engines, gas turbines and liquid propellant rocket

motors. A first step toward any understanding of spray combustion and its ap-

plication to the design of efficient combustion systems is knowledge of the

mechanics governing the burning of single fuel droplets. Extensive research

on this problem has been performed. Most of them emphasize the spherical-

symmetric, gas transport processes for the vaporization (with or without com-

bustion) of single-component droplets. Wise and Agoston [1] and Williams [2]

have reviewed the state of the art to the mid-fifties and the early seventies,

respectively. Recently, Sirignano and Law [3] have surveyed the progress made

on transient, convective, multicomponent droplet vaporization, with particu-

lar emphasis on the internal transport processes and their influences on the

bulk vaporization processes. Faeth [4] has reviewed the present understanding

of spray combustion including the transient evaporation, ignition and combustion processes of individual droplets. Only a brief summary of some recent works on droplet evaporation and combustion is presented here:

Two theoretical models have been formulated in order to gain physical insight on the vaporization processes of a spherically symmetric single-component drop in a quiescent atmosphere: the quasi-steady and transient diffusion models. The former, also referred to as the d^2 law model, has concluded that (i) the mass burning rate is proportional to the instantaneous droplet diameter d which varies with time t according to the square law; (ii) The flame front standoff ratio (ratio of the flame-to-droplet diameter) is constant during the course of burning. Flame extinction occurs when the droplet vanishes; and (iii) The flame temperature is constant and equal to the adiabatic flame temperature.

Although the predicted evaporation times agree well with the results of laboratory-scale tests, several observations indicate that combustion of fuel droplets is inherently a transient diffusion controlling process. Depending upon the intensity of convective transport through internal circulation, the diffusion-limit [5-8] and rapid-mixing models [9] have been developed to represent two extreme ratios (slowest and fastest, respectively) of internal heat transfer in the liquid phase. In the former model which is relevant for more viscous fuel or during the initial period, the heat in the droplet is transported by diffusion alone. However, in the latter model which is relevant for less viscous fuel, the combined internal convective-diffusive transports are so rapid that the droplet temperature is maintained spatially uniform but temporally varying. Results from these two models should provide lower and upper bounds on the evaporation behavior. Faeth [5] and recently Law et al. [8,9] have analyzed both limiting cases under the assumptions of quasi-steady gas phase processes. The predicted behavior on the temporal variations of the droplet and flame sizes were found to agree with the experimental observations under a convective-free environment [10,11]. Crespo et al [6] and Waldman [7] have independently employed the perturbation method, one using the ratio of the ambient-gas and liquid densities and the other using the ratio of the droplet radius to the diffusion field radius as the small parameter, to analyze the effects of unsteady droplet heating on combustion with the assumption that the temperature and regression rate of the droplet surface are given constants. The inner (droplet vicinity) region is in a quasi-steady state and is characterized by a balance between convection and

diffusion, while the outer region is dominated by unsteady diffusion. Both approximate solutions represent, in essence, a perturbation of the quasi-steady result.

The most complete model is developed by Kotake et al. [12] which considers the unsteady diffusion-controlled combustion of liquid droplets including liquid-phase heat conduction. Theoretical results obtained by a numerical method have later been found to be erroneous [13]. In the absence of combustion, the heat-transfer controlling shrinkage history of a droplet may be divided into three stages [14]: (i) the early (or heat-up) period where the srhinkage is controlled by drop heat capacity, (ii) the asymptotic stage where interfacial phase change is the controlling mechanism, and (iii) the intermediate stage where both effects are of comparable importance. Theoretical results for category (ii) predicts that the shrinkage rate obeys the square law [14,15]. Theory compare well with test data [14].

The present study deals with droplet evaporation accompanied by combustion. The method of similarity transformation is applied to solve a complete set of spherically-symmetric time-dependent equations of heat and mass transfer in the gas phases including the effects of heating up of the liquid phase. Exact solutions are obtained for the burning rate and the temporal motion of the flame in the asymptotic stage of droplet combustion. The results are adequate except for the initial period and are superior to the existing transient-diffusion solutions due to their simplicity.

Analysis

Consider an evaporating and burning spherical drop in a quiescent oxidizing atmosphere surrounded concentrically by a spherical flame front as shown in Fig. 1. The radius of the liquid drop is R_1. Its surface temperature and vapor concentration are T_ℓ and C_ℓ, respectively. The radial distance of the combustion surface from the center of the liquid drop is R_2 and its temperature is T_f. The oxygen-inert gas mixture at a large distance from the flame surface is at the temperature T_∞ and the oxidizer concentration C_∞. Oxidizer is delivered inward to the combustion surface by convection and diffusion. The fuel evaporates and diffuses, without chemical change, to the combustion surface. The location of the combustion surface is defined by the condition that the ratio of the mass rate of delivery of fuel vapor to oxidizer corresponds to stoichiometric proportions. It is assumed that the reactants are consumed instantaneously upon reaching the flame front, resulting in the re-

lease of the combustion heat. The physical properties of combustion products and inert gas in the oxidizer-inert gas mixture are alike and assumed independent of the distance r from the droplet center; consequently, of temperature and gas composition. The effects of variable properties on single droplet evaporation may be compensated provided the constant properties are evaluated at an appropriate reference temperature according to: (i) a simple 1/3 rule [13], (ii) an arithmatic average [16], or (iii) a logarithmic mean [17].

The equations of continuity for an incompressible fluid can be integrated to give $v_i r^2 = f(t)$ for $i = 1,2$. Here, v denotes the radial velocity and the subscripts 1 and 2 refer to the gas mixtures within and outside the flame surface, respectively. A mass balance at the drop surface gives

$$v_1 = -E_1 \dot{R}_1 R_1^2 / r^2 \tag{1-a}$$

wherein $E_1 = \rho_\ell / \rho_1 - 1$. Similarly, the radial velocity of the oxidizer-inert gas mixture is found to be

$$v_2 = E_2 \dot{R}_2 R_2^2 / r^2 \tag{1-b}$$

$\dot{R}_1$ and $\dot{R}_2$ are the front velocities of the drop and flame surfaces, respectively. E_2 is equal to unity.

The equations of temperature T_i and concentration C_i read

$$\frac{\partial T_i}{\partial t} + v_i \frac{\partial T_i}{\partial r} = \frac{a_i}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial T_i}{\partial r}) \tag{2}$$

and

$$\frac{\partial C_i}{\partial t} + v_i \frac{\partial C_i}{\partial r} = \frac{D_i}{r^2} \frac{\partial}{\partial r} (r^2 \frac{\partial C_i}{\partial r}) \tag{3}$$

respectively, for $i = 1,2$, where a denotes the thermal diffusivity and D is the mass diffusivity. The initial and boundary conditions are

at $t = 0$: $\quad T_i = T_\infty$; $\quad C_i = C_\infty$ $\tag{4}$

at $r = R_1$: $\quad k_1 \frac{\partial T_1}{\partial r} = \rho_\ell \dot{R}_1 [L + C_{p\ell}(T_1 - T_\infty)]$ $\tag{5-a}$

$$C_1 - C_s = b(T_1 - T_s); \quad -D_1 \frac{\partial C_1}{\partial r} = [\rho_\ell + (E_1 - 1)C_1]\dot{R} \tag{5-b}$$

at $r = R_2$: $\quad T_1 = T_2$; $\quad k_2 \frac{\partial T_2}{\partial r} - k_1 \frac{\partial T_1}{\partial r} = D_1 H \frac{\partial C_1}{\partial r}$ $\tag{6-a}$

$$C_2 = 0; \quad D_2 \frac{\partial C_2}{\partial r} = -\gamma \, D_1 \frac{\partial C_1}{\partial r} \qquad (6\text{-}b)$$

at $r = \infty$: $\quad T_2 = T_\infty; \quad C_2 = C_\infty$ $\qquad\qquad\qquad (7)$

with b defined as $M_1 L C_s / (\bar{R} T_s^2)$. Here, M denotes the molecular weight; k, thermal conductivity; ρ, density; C_p, specific heat; L, latent heat of vaporization; C_s and T_s, concentration and temperature, respectively, over the droplet surface under saturation state; H, heat of combustion; γ, stoichiometric mass ratio; and $\bar{R}$, universal gas constant. The subscripts ℓ and s signify the liquid drop and saturated state, respectively. The first expression of Eq. (5-b) describes a relation between liquid temperature and composition at the droplet surface. In its derivation, use is made of the Clausius-Clapeyron equation and heat of mixing is neglected.

A similarity transformation is performed on Eqs. (2) through (7) according to

$$T_i^*(N_i) = [T_i(r,t) - T_\infty]/\Delta T; \quad C_i^*(N_i S_i) = [C_i(r,t) - C_\infty]/C_\infty \qquad (8)$$

$$N_i = \frac{r}{2(a_i t)^{1/2}}; \quad R_i = (-1)^i 2B_i(a_i t)^{1/2} \qquad (9)$$

Here, $\Delta T = T_\infty - T_s$ and $S_i = L_{ei}^{1/2}$, where $L_{ei} = a_i / D_i$ is the Lewis number. The superscripts $\cdot$ and $\cdot\cdot$ signify derivatives with respect to N_i. Both B_1 and B_2 are positive constants to be determined.

The resulting second-order ordinary differential equations are integrated twice subject to the appropriate boundary conditions. It yields

$$T_1^* = \frac{-I(E_1,B_1,N_1)}{[1+WC\phi_1(E_1,B_1)]Ja}; \quad T_2^* = -\frac{I(E_1,B_1,B_2A)\,I(E_2,B_2,N_2)}{[1+WC\phi_1(E_{12}B_1)]\,\phi_2(E_2,B_2)Ja} \qquad (10)$$

$$C_1^* = \frac{(m_2-W)\,I(E_1,B_1S_1,N_1S_1)}{1+W\phi_1(E_1,B_1S_1)}; \quad C_2^* = -\frac{I(E_2,B_2S_2,N_2S_2)}{\phi_2(E_2,B_2S_2)} \qquad (11)$$

in which

$$I(E_i,Y,y) = (-1)^i 2Y^3 \exp[Y^2 + 2(-1)^i E_i Y^2] \int_{(-1)^i y}^{\infty} x^{-2} \exp(-x^2 - 2E_i Y^3 x^{-1})dx \qquad (12)$$

$$\phi_i(E_i,Y) = I(E_i,Y,Y) \qquad (13)$$

Here, $A = (a_2/a_1)^{1/2}$; $Ja = \rho_1 C_{p1} \Delta T / \rho_\ell L$; $m_1 = b\Delta T/C_\infty$

$W = 1 + E_1$; $C = (C_{p\ell}/C_{p1})-1$; $K = Ak_1/k_2$

$$Q_1 = \frac{D_1 H C_\infty}{k_2 \Delta T} (\frac{a_2}{D_1})^{1/2} \;\; ; \;\; Q_2 = \gamma D_r; \;\; m_2 = \rho_\ell/C_\infty; \;\; D_r = (D_1/D_2)^{1/2}$$

Ja is the Jakob number for droplet evaporation. The constants B_i are evaluated from

$$\frac{(m_2-W)\phi_1(E_1,B_1S_1)}{[1+W\phi_1(E_1,B_1S_1)]} - C_s^* = \left\{ \frac{-\phi_1(E_1,B_1)}{[1+WC\phi_1(E_1,B_1)]Ja} + 1 \right\} m_1 \tag{14-a}$$

$$(K/A)(B_1/B_2)^3 \exp[B_1^2(1-2E_1)-(B_2A)^2-2E_1B_1^3(B_2A)^{-1}]$$

$$-I(E_1,B_1,B_2A)/\phi_2(E_2,B_2) = S_2Q_1Ja[1+WC\phi_1(E_1,B_1)]/Q_2\phi_2(E_2,B_2S_2) \tag{14-b}$$

It is obvious that the radius-time histories given in Eq. (9) for the droplet and flame front do not satisfy the initial conditions $R_1(0)=R_2(0)=R_0$, where R_0 is the initial drop radius. This anomaly arises from the complete neglect of the equations of motion for the gas mixtures which is justified in the succeeding section. As a remedy, one writes the radius-time history as

$$R_i = R_0 + (-1)^i 2B_i(a_i t)^{1/2} \tag{15}$$

which is mathematically inapplicable to the very beginning of a combustion event.

Results and Discussion

Equations (11) and (12) describe the unsteady distribution of temperature and composition, respectively in the gaseous space on both sides of the combustion flame. Both the temperature and concentration fields are functions of the physical properties and the parameters B_i's.

The constant B_1 is evaluated by means of Eq. (14-a) through successive approximation. With the substitution of B_1, Eq. (14-b) may be solved for B_2 in a similar manner. To avoid such a tedious procedure in evaluating B_1 and B_2, the functions ϕ_1, ϕ_2 and I, as defined by Eqs. (12) and (13), are presented in graphical form in Figs. 2, 3 and 4, respectively for values spanning the range of potential application. n, defined as AB_2/B_1, signifies the flame-front standoff ratio in the quasi-steady analysis since the instantaneous radii of the liquid droplet and flame front are respectively $-2B_1(a_1 t)^{1/2}$ and 2 $B_2(a_2 t)^{1/2}$ in the absence of the heat-up period. Now, B_1 can be directly evaluated from Fig. 2, but B_2 and n determined from Figs. 3 and 4 must still satisfy Eq. (14-b).

It can be shown that for any values of B_i and $E_i = 0$

$$\phi_i(0,B_i) = (-1)^i 2B_i^2 (1 - \pi^{1/2} B_i \exp B_i^2 \, \text{erfC} \, B_i) \tag{16}$$

However, for small values of Y, referring to B_2 or $B_2 S_2$, the function ϕ_2 can be approximated by

$$\phi_2(E_2,Y) \cong 2Y^2 \tag{17}$$

where Y is large, a good approximation can be obtained through an asymptotic expansion as

$$\phi_2(1,Y) \cong (\pi/3)^{1/2} Y \tag{18}$$

Both approximations are plotted in Fig. 3.

The ϕ_1 function has the upper and lower limits which are parallel as shown in Fig. 2. The lower limit coincides with the quasi-steady approximation.

Figure 4 illustrates that the upper limits of the I function for a given E_1 and any values of B_1. The lower limit corresponds to the abscissa, n = 1 at which the flame front coincides with the droplet surface.

(i) Effects of radial convection

One finds through an examination of Eqs. (1), (2) and (3) that $E_i = 0$ corresponds to the case of no convection in the unsteady transport fields external to a burning droplet. In other words, the difference between the non-zero and zero E_i curves in Figs. 2 through 4 is a measure of the effects of convective motion on the evaporation rate and flame movement. Figure 4 reveals that in the absence of radial convection, fast droplet evaporation as indicated by large values of B_1 results in a combustion with n close to unity. In other words, the flame front where chemical reaction takes places stays close to the droplet surface during the process of combustion.

(ii) High ambient-gas temperature case

When the difference in temperature between the drop and the surrounding gas mixture is considerable, $1/m_1$ approaches zero and the LHS of Eq. (14-a) vanishes. The rate of decrease in size of the drops is then determined by heat transfer processes within the flame surface. B_1 is evaluated by

$$\phi_1(E_1,B_1) = \frac{Ja}{1-J_b} \tag{19}$$

where $J_b = (C_{p\ell} - C_{p1}) \Delta T / L$ indicates the contribution due to initial heating. When $J_b \ll 1$, Eq. (19) reduces to $\phi_1(E_1,B_1) = Ja$.

(iii) Oxidizer-diffusion controlling case

The temperature field inside the flame boundary T_1^* may have already attained a 'steady state at the initiation of drop combustion since the heat capacity of the fuel vapor-gas mixture is very small, implying a small value of K. In addition, the flame-front standoff ratio is much larger than unity. Hence, the first term of Eq. (14-b) can be neglected. The transport phenomena of the gas mixture inside the flame surface would play a minor role on drop combustion, or conversely, the drop burning is controlled by heat and mass transfer in the oxidizer-inert gas mixture. The theory is called the oxidizer transfer model [18], in contrast to the present analysis known as the fuel vapor-oxidizer transfer model. Out of the total heat H that is produced in droplet burning, the fraction L is consumed for droplet evaporation. The remaining fraction (H-L) is dissipated outward into the hot environment. Hence, H in the definition of Q_1 should be replaced by (H-L), i.e. $Q_1 = D_1(H-L)/k_2\Delta T \, (a_2/D_1)^{1/2}$. In addition, the interfacial temperature $T_2^*(B_2)$ corresponds to T_f^*, where $T_f^* = (T_f-T_\infty)/\Delta T$ and T_f is the adiabatic flame temperature. This is equivalent to replacing $-I(E_1,B_1,B_2A)/\{[1+WC\phi_1(E_1,B_1)]Ja\}$ by T_f^* in Eq. (14-b), which is then reduced to

$$(T_f-T_\infty)/C_\infty = Q_3\phi_2(E_2,B_2)/\phi_2(E_2,B_2S_2) \qquad (20)$$

wherein $Q_3 = (H-L)/(\gamma\rho_2 C_{p2})$. For $Le_2 = 1$ or $S_2 = 1$, Eq. (20) is further simplified as

$$T_f-T_\infty = Q_3 C_\infty \quad . \qquad (21)$$

This equation is identical with that obtained in reference 18 which has neglected the convective contribution to the transport phenomena.

(iv) Transient effects

The quasi-steady model [17,19] yields

$$B_1^2 = \ln(1+B)/2W; \quad n = 1+\gamma(\rho_1/\rho_2)\ln(1+B)/A^2 \qquad (22-a)$$

in which B is the transfer number defined as $C_{p1}\Delta T_f/L$ and $\Delta T_f = T_f - T_s$. For B less than unity, Eq. (22-a) can be approximated by

$$B_1 = (Ja^*/2)^{1/2}, \quad n = 1+\gamma(\rho_\ell/\rho_2)Ja^*/A^2 \qquad (22-b)$$

where Ja^* is the Jakob number for droplet combustion defined as $\rho_1 B/\rho_\ell$. The lower broken line in Fig. 2 represents the quasi-steady result. The deviation of the zero E_1 curve from the quasi-steady approximation is attributed to the contribution of the transient term. Similarly, the difference in the values

of B_2 or n between the present analysis and the quasi-steady model is a mea-
sure of transient effects. In reference to Eq. (17) and the definition of
E_1, it is seen from Fig. 2 that the quasi-steady model is an accurate approxi-
mation only when ρ_g is much less than ρ_ℓ and the degree of superheat ΔT is
sufficiently small.

(v) Effects of gas inertia

The role of gas inertia on drop evaporation is found to be negligible in
comparison with heat transfer effects [15]. This conclusion is still valid
here in the presence of combustion. The relative importance of effects of gas
inertia and heat transfer on the movement of the flame front will be estab-
lished in the following: with the aid of Eq. (1-b), the equation of motion
for the oxidizer-inert gas mixture is integrated from the flame surface R_2
to infinity. Neglecting the effect of viscosity, it yields

$$R_2 \ddot{R}_2 + \frac{3}{2} \dot{R}_2^2 = \frac{g_c}{\rho_2}[p_2(R_2) - p_2(\infty)] \tag{23}$$

in which g_c expresses the conversion factor and p_2 is the gas pressure. The
equation of state for an ideal gas $p_2 = \rho_2 \bar{R} T_2$, where $\bar{R}$ is the universal gas
constant, is then combined with Eq. (23). It yields, in dimensionless form

$$\frac{1}{X}[R_2^* \ddot{R}_2^* + \frac{3}{2}(\dot{R}_2^*)^2] = T_2^*(R_2^*) - T_2^*(\infty) \tag{24}$$

Here $R_2^* = R_2/R_r$; $t^* = a_2 t/R_r^2$; $T_2^*(R_2^*) = \dfrac{T_2(R_2)-T_\infty}{\Delta T}$; $T_2^*(\infty) = \dfrac{T_2(\infty)-T_\infty}{\Delta T}$

$$X = \frac{g_c \bar{R} R_r \, T}{m_2 a_2^2}$$

R_r is the reference flame radius; and $T_2(\infty)$, a prescribed temperature of the
oxidizer-inert gas mixture at a large distance from the flame surface at T_2
(R_2). For a step change in $T_2(R_2)$ from $T_\infty = 293°K$ to $T_f = 2300$ °K and $T_2(\infty)$
remaining at T_∞, X takes the values of 3.0×10^6 for $R_r = 3$ mm in the atmospheric
environment. One may then conclude that the effect of gas inertia on the
flame-front movement, as expressed by the LHS of Eq. (23), is entirely neglig-
ible as compared to that of heat transfer processes. Hence, the equations
of motion for the gas mixtures may be omitted in the formulation of the prob-
lem.

Conclusions

The equations governing spherically-symmetric, unsteady transport pheno-
mean in the gas phases are solved exactly including the effects of droplet
heating. The results which predict the mass burning rate and the temporal

motion of the flame obey the square law. Their radius time history is revised to take the form of Eq. (15) but is inapplicable in the short initial stage of droplet combustion. The evaporation and flame movement constants B_i and the flame-front standoff ratio n are presented in graphical form for convenience in practical uses. The effects of radial convection resulting from unequal fluid densities, transient terms and gas inertia are established. The quasi-steady approximation is in considerable error for large superheats and large vapor densities, while the oxidizer diffusion model is an accurate approximation when the Lewis numbers of the gas mixtures are unity.

Acknowledgment

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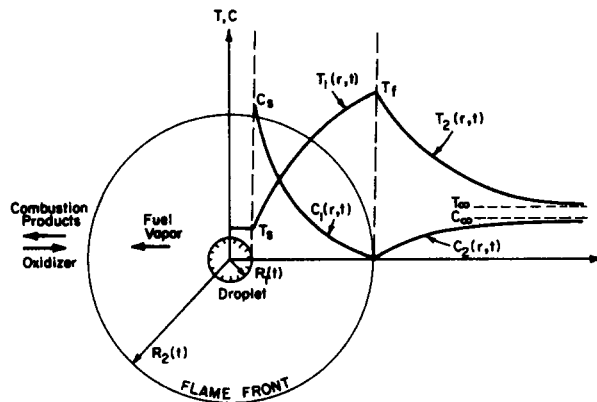
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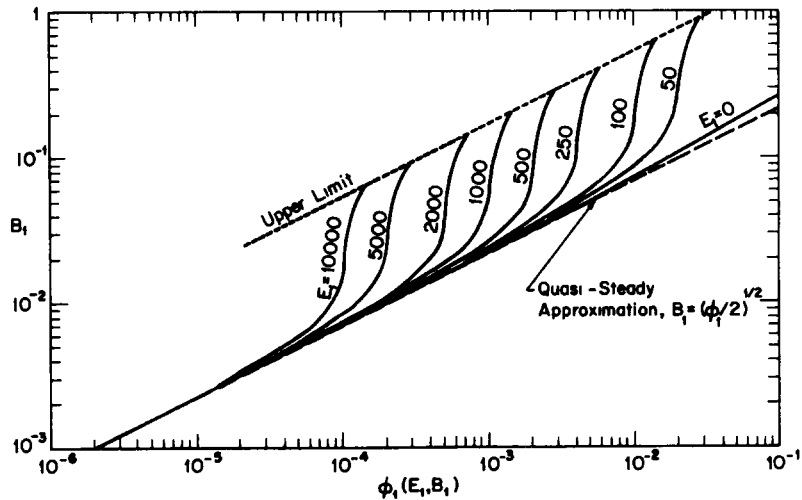

Fig. 1. Schematic diagram of burning fuel drop
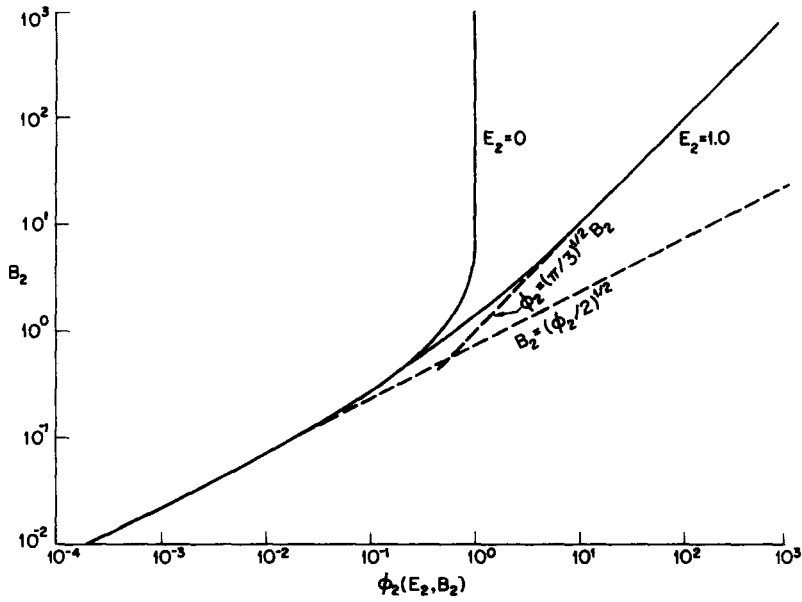

Fig. 2 ϕ_1 versus B_1

Fig. 3 ϕ_2 versus B_2

Fig. 4 $-I$ versus n