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NOMENCLATURE

B	transfer number
C_p	specific heat at constant pressure, KJ/kg°C
D	diffusion coefficient, cm^2/sec
D_o	dimensionless diffusional oxidant flux
d	diameter, m
e	prescribed value in error
h	mesh size, m
h_{fg}	latent heat of vaporization per unit mass of fuel, KJ/kg
i	stoichiometric ratio
K	burning constant, mm^2/sec
Le	lewis number
M	molecular weight
m	mass flow rate, kg/sec
N	molal diffusion rate, kg/sec mol
P	pressure, N/m^2
Q	heat of combustion, KJ/kg
q	chemical rate of formation, kg/sec
r	radius, m
R_o	universal gas constant, J/kg mol °K
T	temperature, °K
Y	weight fraction
V	atomic volume
v	radial velocity, m/sec

Greek symbols

α	$\frac{M_F h_{fg} P}{\rho C_p R_o}$
β	constant
ρ	density, kg/m^3
λ	thermal conductivity, KJ/mh°c
ν	bulk mass velocity, m/sec

Subscripts

B	boiling
C	flame
F	fuel
Ftotal	total fuel
i	species
L	at droplet surface
l	liquid
N2	nitrogen
o	oxygen
∞	at infinite

CHAPTER 1

INTRODUCTION

The combustion of sprays of liquid fuels is of considerable technological importance to a diversity of applications ranging from steam raising, furnaces, space heating, diesel engines to space rockets. Because of the importance of these applications spray combustion is responsible for a considerable proportion of the total energy requirements of the world.

The study of the behaviour of a single droplet is a pre-requisite for obtaining an insight into the mechanism of spray combustion, since a burning spray may be regarded as an ensemble of individual burning or evaporating particles. Such study will also provide a better understanding of the parameters governing the design of equipment for combustion processes.

Theoretical models of droplet combustion are of great importance since they give insight into the dependence of the rate of combustion on the various physical and chemical processes that occur. Furthermore, they are of great value in the design and modelling of spray combustion systems since it permits the direct ab initio calculation of the rate of droplet burning. Consequently a number of theoretical investigations have been undertaken over the past twenty-five years in parallel with the experimental studies. [1]

The initial basic approach involved a sphericosymmetric model based on a vaporising droplet in which the rate-controlling process is molecular diffusion rather than chemical kinetic factors. This model has developed as a result of work by numerous investigators who have proposed a number of approaches but which all tend to same kind of result. [1]

Generally it is assumed that the droplet is spherical and is a pure liquid. In addition, the following assumptions are generally made in the basic model.

(i) The combustion system has spherical symmetry. The spherical droplet of radius r_L is surrounded by a concentric flame zone of radius r_c. Concentric with the droplet and outside the flame zone lies another outer boundary which is taken to be at infinite distance from the droplet, and the composition of which is that of ambient atmosphere.

(ii) Fuel vapour diffuses from the drop surface to the flame front and oxygen from the boundary in the ambient gas to the flame surface. The resulting combustion products diffuse from the flame to the ambient atmosphere.

(iii) Exothermic chemical reaction between the fuel vapor and oxidant takes place at the surface of stoichiometric composition.

(iv) Combustion occurs under iso-baric, quasi-steady conditions.

(v) Chemical reaction occurs instantaneously and the reaction zone is infinitely thin.

(vi) Part of the heat of combustion is transmitted by conduction to the droplet to affect vaporization while the rest enters the ambient gas.

(vii) The droplet temperature is uniform and is usually taken as boiling point of the liquid T_B, although it may set as 0.9 T_B [2].

(viii) Radiations and thermal diffusion effects are negligible.

In the analyses based on quasi-steady combustion and infinite kinetics it was assumed that soon after ignition the droplet settled down to steady-state conditions, and indeed experimental plots of d^2 against t seemed to confirm this since they became linear after a short time interval. To make any theoretical prediction of burning-rate coefficient and temperature and composition field surrounding a burning droplet it is necessary to use the general continuity equations developed by Hirschfelder et al. [3].

These equations take the general form:

Global mass conservation

$$\frac{\partial\rho}{\partial t} + \frac{\partial r^2\rho v}{\partial r} = 0 \qquad (1.1)$$

which reduced on integration, when $\frac{\partial\rho}{\partial t} = 0$

$$m_F = 4\pi r^2 v\rho = \text{Constant} \qquad (1.2)$$

where m_F is the mass flow of the fuel vapor leaving the surface (i.e. the mass burning rate), r is the radial co-ordinate, ρ the gas density and v the radial velocity.

Species mass conservation

$$\frac{\partial}{\partial t}(\rho Yi) + \frac{1}{r^2}\left\{\frac{\partial r^2}{\partial r}\ \rho v Yi - \rho Di\ \frac{\partial Yi}{\partial r}\right\} = q_i \qquad (1.3)$$

where Yi is the weight fraction, Di is the diffusion coefficient and qi is the chemical rate of formation of species i. This may be rewritten as

$$\frac{\partial\ (\rho Yi)}{\partial t} + \frac{m_F}{4\pi r^2}\frac{\partial Yi}{\partial r} - \rho D_i\frac{1}{r^2}\frac{\partial}{\partial r}\left\{r^2\frac{\partial Yi}{\partial r}\right\} = q_i \qquad (1.4)$$

Conservation of energy

For an adiabatic system this takes the form

$$\frac{\partial}{\partial t}\ \rho\Sigma_i\ (YiHi) + \frac{1}{r^2}\frac{\partial r^2}{\partial r}\left\{\rho v\Sigma_i(YiHi) - \frac{\lambda\partial T}{\partial r}\right\} = \Sigma q_i H_i \qquad (1.5)$$

where Hi is the enthalpy of species i, λ the thermal conductivity of the mixture and T the temperature.

The equation of motion

$$\frac{\partial(\rho v)}{\partial t} + \frac{1}{r^2}\frac{\partial}{\partial r}\ (r^2\rho v^2) = -\frac{\partial p}{\partial r} \qquad (1.6)$$

where p is the pressure, normally it is assumed that combustion occurs under constant pressure.

In the quasi steady state analysis the time dependent terms become zero and the boundary conditions are imposed on the basis of negligible liquid-phase reactions within the droplet and completion of chemical reaction at the outer boundary.

That is, at $r = r_L$, $T = T_L$ and $Y_F = Y_{F,L}$
and at $r = r_\infty$, $T = T_\infty$ and $Y_O = Y_{O,\infty}$
where Y_F and Y_O are the mass fractions of the fuel vapor and oxygen respectively.

Consequently, the major assumption of an 'infinitely rapid chemical reaction rate' is made, that is, the chemical reaction rate is not controlling the rate of disappearance in any way. Usually this assumption is coupled with the use of a simplified chemical reaction of the type

$$\text{Fuel} + \text{oxygen} \rightarrow \text{Products}$$

In this model the flame zone, as a consequence of the infinite rate assumption, is of infinitesimal thickness and would thus be represented by a surface rather than an extended reaction zone. Generally it is necessary to assure that the fuel and oxidant diffuse to the reaction zone in stoichiometric proportions and again, as a consequence of the infinite reaction rate assumption, their concentrations become zero at the reaction interface. When these approximations are made an analytic solution may be obtained. The forms of the final equations depend upon the exact method of solution and in particular if fixed or variable properties are assumed. A typical and widely used solution based on temperature independent transport properties is that given by Wise and Agoston [4] .

$$m_F = 4\pi r_L \bar{\rho}\bar{D} \ln(1+B) \qquad (1.7)$$

where $\bar{\rho}$ is the averaged gas density, $\bar{D}$ the averaged diffusivity and B is the transfer number given by

$$B \equiv \frac{1}{h_{fg}} \left[\bar{C_p}(T_\infty - T_L) + Q\, Y_{o,\infty}/i\right] \qquad (1.8)$$

which in the evaporation limit (i.e. evaporation in hot combustion products) becomes

$$B = \frac{\bar{C}_p (T_\infty - T_L)}{h_{fg}} \qquad (1.9)$$

where $\bar{C_p}$ is the average specific heat, T_∞ the ambient temperature, T_L the temperature at the liquid surface (usually taken as the boiling point of the liquid), although it may be set as $0.9\,T_B$, Q the heat of combustion, h_{fg} the latent heat of vaporisation unit mass evaporating, and i the stoichiometric mixture ratio, (Y_o/Y_F) Stoich.

The quantity of $\bar{\rho}\,\bar{D}$ in Eq. (1.2) is usually replaced, assuming a Lewis number (Le) of unity by $\bar{\lambda}/\bar{C}_p$. In which case, an expression is obtained for burning-rate coefficient, K, thus

$$K = \frac{8\,\bar{\lambda}}{\bar{C}_p\, \rho_l} \ln(1+B) \qquad (1.10)$$

Similarly expressions have been derived for the flame temperature, the mass fraction of fuel vapor at droplet surface ($Y_{F,L}$) and the ratio of flame radius to droplet radius(r_C / r_L). Thus Wise and Agoston [4] obtained

$$T_f - T_L = \frac{Q - h_{fg}}{C_p} \left\{ \frac{1}{1 + i/Y_{O,\infty}} \right\} + \left\{ \frac{T - T_L}{1 + Y_{O,\infty}/i} \right\} \qquad (1.11)$$

$$Y_{F,L} = 1 - \left\{ (1 + Y_{O,\infty}/i) / (1 + B) \right\} \qquad (1.12)$$

$$\frac{r_c}{r_L} = \left\{ \ln(1 + B) \right\} \Big/ \left\{ \ln (1 + Y_{O,\infty}/i) \right\} \qquad (1.13)$$

The simple spherico-symmetric-flame model assumes that λ and C_p are constant and that Lewis number is unity. The results obtained thus markedly depend upon the choice of λ and C_p and since they both depend on both temperature and composition almost any approach is certain to be unsatisfactory. Both λ and C_p are usually evaluated on the basis that the gas composition is air or nitrogen and their values calculated at the arithmetic means of T_f and T_L, although alternatively logarithmic mean is often used. More sophisticated approaches have been adopted, thus Sioui and Roblee [5] used a computer calculation of λ whilst Annamalai et al.[6] used a more accurate analytic type calculation.

Other workers have produced alternative forms of Eqs

(1.7) - (1.13). Bruzutowski [7] has developed a dimensionless form of the quasi-steady droplet combustion theory in which

$$K = \frac{8M_F\lambda W}{\rho C_p h_{fg}} \qquad (1.14)$$

where M_F is the molecular weight of the fuel, W is the dimensionless burning rate given by $\beta D_o + \ln(1 + B_{ev})$ and D_o is the dimensionless diffusional oxidant flux and β is a constant. Likewise he found that

$$\frac{r_c}{r_L} = \frac{1 + \ln(1+B_{ev})}{\beta D_o} \qquad (1.15)$$

The burning rate obtained by these one dimensional, quasi-steady state analyses is in close agreement with the experimental data. [12]. However, the location of the flame based on these analyses does not agree well with the experimental results - e.g. the experimentally observed value of r_c/r_L lies between 6-10 for hydrocarbon fuels while the quasi-steady state analyses predict it between 25-30. [14]

In the present study, a new model has been proposed for the burning of a single fuel oil droplet based on one dimensional, quasi-steady state and molecular diffusion controlled analyses. The process is numerically calculated with a high speed digital computer. The main advantage of this model is that there is a close agreement between the calculated and the observed value of the flame radius.

CHAPTER 2

MATHEMATICAL FORMULATIONS

The following assumptions are made in the diffusion model:

i) The combustion system has spherical symmetry as shown in Fig.1. The spherical droplet of radius r_L is surrounded by a concentric flame zone of radius r_C

ii) The flame is assumed to be supported by exothermic reaction of fuel and oxygen in the flame zone, the oxidant diffusing in from the outer boundary to the flame zone whilst the fuel vapor diffuses from the droplet surface.

iii) Inside the flame zone fuel vapor diffuses from the droplet surface to the flame zone whilst nitrogen diffuses from the flame zone to the droplet surface. Heat is transferred by conduction from the flame zone to the droplet to provide the latent heat of vaporization of the liquid surface.

iv) Thermal diffusion and radiation effects are neglected.

v) The surface temperature T_L at the droplet is taken to be 0.9 T_B (the boiling point of the liquid).

vi) Combustion occurs under iso-baric, quasi-steady conditions.

vii) The experimental value of the flame temperature has been used for determining the burning rate and the flame location of the fuel droplet. This condition makes it possible to separate the region inside the flame zone from that outside of the flame zone.

First consider the governing equations of partial pressure concentration, temperature and velocity of the mixture surrounding the droplet under these assumptions.

The mass transfers of fuel vapor and nitrogen in the flame zone are mainly controlled by the molecular diffusion due to difference in partial pressure concentration. Ficks law of diffusion for fuel into component nitrogen could be written in spherical coordinates as [9]

$$m_F = - D_{FN2} \frac{M_F}{R_0 \bar{T}} 4 \pi r^2 \frac{dP_F}{dr} \tag{2.1}$$

if isothermal diffusion is considered where M_F is molecular weight of fuel, R_0 the universal gas constant, r is the radius coordinate, P_F the partial pressure concentration of fuel, $\bar{T}$ the average temperature, D the diffusion coefficient. Similarly Ficks law for diffusion of nitrogen into fuel could be written as

$$m_{N2} = - D_{N2F} \frac{M_{N2}}{R_0 \bar{T}} 4 \pi r^2 \frac{dP_{N2}}{dr} \tag{2.2}$$

Notice the different subscript on the diffusion coefficient. Now consider a physical situation called equimolal counter diffusion as in Figure 2. N_F and N_{N2} represent the steady state molal diffusion rates of components fuel and nitrogen respectively. In this steady-state situation each molecule of fuel is replaced by a molecule of nitrogen, and vice versa. The molal diffusion rates are given by

$$N_F = \frac{m_F}{M_F} = -D_{FN2}\frac{4\pi r^2}{R_o\bar{T}}\frac{dP_F}{dr} \qquad (2.3)$$

$$N_{N2} = \frac{m_{N2}}{M_{N2}} = -D_{N2F}\frac{4\pi r^2}{R_o\bar{T}}\frac{dP_{N2}}{dr} \qquad (2.4)$$

The total pressure of the system remains constant at steady state, so that

$$P = P_F + P_{N2}$$

or $$\frac{dP_F}{dr} + \frac{dP_{N2}}{dr} = 0$$

or $$\frac{dP_F}{dr} = -\frac{dP_{N2}}{dr} \qquad (2.5)$$

Since each molecule of fuel is replaced by a molecule of nitrogen, we may set the molal diffusion rates equal.

$$N_F = -N_{N2}$$

or $$-D_{FN2}\frac{4\pi r^2}{R_o\bar{T}}\frac{dP_F}{dr} = -D_{N2F}\frac{4\pi r^2}{R_o\bar{T}}\frac{dP_F}{dr} \qquad (2.6)$$

where Eq. (2.5) has been used to express the pressure gradient of nitrogen component. We thus find that

$$D_{FN2} = D_{N2F} = D \qquad (2.7)$$

The calculation of D may be made with Eq.(2.8) given below [8]

$$D = 435.7 \frac{T^{3/2}}{P(V_F^{1/3} + V_{N2}^{1/3})^2} \sqrt{\frac{1}{M_F} + \frac{1}{M_{N2}}} \qquad (2.8)$$

where V_F and V_{N2} are the atomic volumes of fuel and nitrogen respectively.We may integrate the Eq.(2.1) between r_C and r_L to obtain the mass flux of fuel component

$$-\frac{R_o m_F \bar{T}}{4\pi D M_F} \int_{r_L}^{r_c} \frac{dr}{r^2} = \int_{(P_F)_{r_L}}^{(P_F)_{r_c}} d(P_F) \qquad (2.9)$$

or

$$(P_F)_{r_c} - (P_F)_{r_L} = \frac{R_o m_F \bar{T}}{4\pi D M_F} \left[\frac{1}{r_c} - \frac{1}{r_L} \right] \qquad (2.10)$$

or

$$\frac{m_F}{4\pi r^2} = \frac{D M_F}{R_o r^2 (1/r_c - 1/r_L) \bar{T}} \left[(P_F)_{r_c} - (P_F)_{r_L} \right] \qquad (2.11)$$

The diffusion of nitrogen inward is given by

$$m_{N2} = -\frac{D M_{N2}}{R_o \bar{T}} 4\pi r^2 \frac{dP_{N2}}{dr} \qquad (2.12)$$

Since the nitrogen cannot penetrate the fuel droplet, this must be balanced by the bulk mass transfer outward so that

$$\rho A \nu = \rho_{N2} (4\pi r^2) \nu \tag{2.13}$$

where ν is the bulk mass velocity, outward.

Combining Eqs. (2.12) and (2.13), we find

$$-\frac{4\pi D\, M_{N2}}{R_o\, \bar{T}} r^2 \frac{dP_{N2}}{dr} = -4\pi r^2 \frac{P_{N2}\, M_{N2}}{R_o\, \bar{T}} \nu \tag{2.14}$$

$$\nu = \frac{D}{P_{N2}} \frac{dP_{N2}}{dr} \tag{2.15}$$

The mass diffusion of fuel vapor outward is

$$m_F = -\frac{4\pi D\, M_F}{R_o\, \bar{T}} r^2 \frac{dP_F}{dr} \tag{2.16}$$

and the bulk transport of fuel is

$$\rho_F (4\pi r^2) \nu = \frac{P_F M_F}{R_o\, \bar{T}} 4\pi r^2 \frac{D}{P_{N2}} \frac{dP_{N2}}{dr} \tag{2.17}$$

The total mass transport is sum of those given in Eqs(2.16) and (2.17). Adding these quantities and making use of Eq.(2.15) gives

$$m_{Ftotal} = -\frac{4\pi DM_F}{R_o\bar{T}} r^2 \frac{dP_F}{dr} + \frac{M_F}{R_o\bar{T}} 4\pi D r^2 \frac{P_F}{P_{N2}} \frac{dP_{N2}}{dr} \qquad (2.18)$$

or

$$m_{Ftotal} = -\frac{4\pi DM_F}{R_o\bar{T}} r^2 \left[\frac{dP_F}{dr} - \frac{P_F}{P_{N2}} \frac{dP_{N2}}{dr}\right] \qquad (2.19)$$

Substituting Eq.(2.5) into Eq.(2.19)

$$m_{Ftotal} = -\frac{4\pi DM_F}{R_o\bar{T}} r^2 \frac{dP_F}{dr} \left[1 + \frac{P_F}{P_{N2}}\right] \qquad (2.20)$$

or

$$m_{Ftotal} = -\frac{4\pi DM_F}{R_o\bar{T}} r^2 \frac{P}{P-P_F} \frac{dP_F}{dr} \qquad (2.21)$$

Boundary condition:

$P_F(r_L)$ = saturation pressure of fuel corresponding to 0.9 T_B

The mass-flow rate produced by the phase change of liquid to vapor is given by continuity equation:

$$m_{F\text{total}} = -(4\pi r_L^{\,2})\,\rho_l\,\frac{dr_L}{dt} \qquad (2.22)$$

and due to conduction heat transfer

$$m_{F\text{total}} = \frac{(4\pi r_L^{\,2})}{h_{fg}}\,\lambda\,\left.\frac{dT}{dr}\right|_{r=r_L} \qquad (2.23)$$

Substituting Eq.(2.5) into Eq.(2.21) will yield

$$m_{F\text{total}} = \frac{4\pi D M_F}{R_o\,\bar{T}}\,r^2\,\frac{P}{P-P_F}\,\frac{dP_{N2}}{dr} \qquad (2.24)$$

Substituting Eq(2.23) and Eq.(2.24) in Eq.(2.15) will give

$$\nu = \frac{T\,R_o\lambda\,(r_L/r)^2}{P\,M_F\,h_{fg}}\,\left.\frac{dT}{dr}\right|_{r=r_L} \qquad (2.25)$$

Energy equation in steady, one-dimensional and spherical coordinates can be written as

$$\rho\,C_p\,\nu\,\frac{dT}{dr} = \frac{\lambda}{r^2}\,\frac{d}{dr}\left(r^2\,\frac{dT}{dr}\right) \qquad (2.26)$$

Putting Eq.(2.25) into Eq.(2.26) will give

$$\rho C_p \frac{T R_o \lambda}{P M_F h_{fg}} \left(\frac{r_L}{r}\right)^2 \left(\frac{dT}{dr}\right)_{r=r_L} \frac{dT}{dr} = \frac{\lambda}{r^2}\frac{d}{dr}\left(r^2 \frac{dT}{dr}\right) \tag{2.27}$$

or $$\left(\frac{r_L}{r}\right)^2 \left(T\frac{dT}{dr}\right)_{r=r_L} \frac{dT}{dr} = \alpha\left[\frac{d^2T}{dr^2} + \frac{2}{r}\frac{dT}{dr}\right] \tag{2.28}$$

where $\alpha = \dfrac{M_F h_{fg} P}{\rho C_p R_o}$

Boundary Conditions:

At $r = r_L$ $T = 0.9\ T_B$

At $r = r_c$ $T = T_f$ (2.29)

CHAPTER 3

NUMERICAL ANALYSIS

The analysis of single fuel droplet combustion is based on a one-dimensional, quasi-steady, molecular diffusion-controlled phenomenon. The solution of the system involves simultaneous solution of Eqs. 2.21, 2.22, 2.25, 2.28, and boundary conditions. Due to non-linearity of the system, the problem is solved by numerical method. This method is based on finite difference techniques which are ideally suited for solution by means of high speed, digital computers. However, before a numerical method can be applied to a given problem, some preliminary steps are necessary. The purpose of these preliminary steps is to approximate the differential equation by a set of algebraic equations. This is accomplished by replacing continuous domain by a pattern of discrete points within the domain and introducing finite difference approximations between the points.

To solve this problem numerically the flame radius is chosen initially relative to droplet radius and the flame zone; i.e. the space between the flame surface and droplet surface is subdivided into twenty small but finite sub-volumes and each assigned a reference number (Figure 3).

The first order differential $\frac{dT}{dr}$ is written in central difference as follows:

$$\frac{dT_i}{dr} = \frac{T_{i+1} - T_{i-1}}{2.h} \qquad (3.1)$$

The second order differential $\frac{d^2T}{dr^2}$ is written in finite-difference form as follows:

$$\frac{d^2T_i}{dr^2} = \frac{T_{i+1} - 2T_i + T_{i-1}}{2.h^2} \qquad (3.2)$$

Replacing the terms (3.1) and (3.2) into Eq. (2.28) the following finite difference equation is obtained.

$$\frac{r_L^2 T_1 (T_2 - T_1)(T_{i+1} - T_{i-1})}{2h^2 \alpha (r_L + ih)^2} = \frac{T_{i+1} - 2T_i + T_{i-1}}{h^2} + \frac{2(T_{i+1} - T_{i-1})}{2(r_L + ih)h} \qquad (3.3)$$

or solving for Ti

$$T_i = \frac{T_{i+1}}{2} + \frac{T_{i-1}}{2} + \frac{(T_{i+1} - T_{i-1})}{2(r_L + ih)}.h - \frac{r_L^2 . T_1 . (T_2 - T_1)(T_{i+1} - T_{i-1})}{4(r_L + ih)^2 \alpha} \qquad (3.4)$$

BOUNDARY CONDITIONS

$$T_1 = 0.9\, T_B \qquad (3.5)$$

$$T_{21} = T_f$$

The preceeding equation has been solved by Gauss-Seidel method

The solution begins with assumed values of T_i^0 and known values at the boundary. The iterative Eqs. 3.4 and 3.5 are used to sweep all nodal points and to calculate a new set of values of T_i^1. This sequence is a cyclic, single-step process which is repeated over and over to calculate successively T_i^2, T_i^3, etc., using in each sweep the known set of temperatures T_i^t to calculate a new set T_i^{t+1}. Finally, there obtain

$$T_i^{t+1} - T_i^t \leqslant e$$

at all points, where e is prescribed value of the error in the temperature. When this condition has been met, the iteration has converged to the solution of finite difference approximation. The flow diagram showing the computational sequence is shown in Fig. 17.

The physical properties of fuel used in these calculations are shown in Table 1. The values of Cp, λ and ρ are evaluated at the arithmetic mean of flame temperature and droplet surface temperature while the value of diffusion coefficient D is evaluated at the arithmetic mean temperature between the two nodes [10, 11].

The partial pressure distribution of fuel can be obtained by Eq. (2.21) based on finite difference technique. Eq. (2.21) can be expressed in finite difference form as follows:

$$\frac{P_{F_i} - P_{F_{i-1}}}{h} = -\frac{m_{ftotal}\,\bar{T}_i R_o}{4\pi D_i M_F r^2} \; \frac{P - \dfrac{(P_{F_{i+1}} + P_{F_{i-1}})}{2}}{P} \qquad (3.6)$$

or

$$P_{F_i} = P_{F_{i-1}} - \frac{h\, m_{ftotal}\,\bar{T}_i R_o}{4\pi D_i M_F r^2} \; \frac{2P - P_{F_{i+1}} - P_{F_{i-1}}}{2P} \qquad (3.7)$$

where Ti is the average temperature between the two nodes and Di diffusion coefficient corresponding to Ti.

BOUNDARY CONDITION

$P_F(1)$ = saturation pressure of fuel corresponding to 0.9 T_B (3.8)

The preceding equation has also been solved by the Gauss-Seidel Method [9] in the manner of Eq.(3.4).

The partial pressure distribution of the fuel gives the correct location of the flame. The flame location can be interpolated using the Lagrange interpolation method [13] from the partial pressure distribution of fuel (P_F) at a point where all the fuel is consumed (P_F=0). The value of the chosen flame radius is then compared with the interpolated flame radius. If the chosen flame radius is larger than the interpolated flame radius, the chosen flame radius is increased by a small value as any small increase in the chosen flame radius results in an increase in the interpolated flame radius. With this new value of the chosen flame radius the temperature and partial pressure distribution of fuel is calculated and flame radius interpolated at point (P_F=0). The procedure is repeated till the value of chosen flame radius becomes smaller than interpolated flame radius. At this point, the chosen flame radius is the correct location of the flame and is printed.

The velocity distribution is then obtained from Eq.(2.25). The radius of fuel droplet is calculated at each stepwise increase of time from Eq.(2.22). The droplet burning time is the time when the radius of droplet becomes zero.

CHAPTER 4

RESULTS AND DISCUSSIONS

Figures 4 to 16 show the results of the numerical analysis on the combustion of a single fuel droplet of benzene and toluene based on diffusion model. Figures 4 - 5 depict the temperature distribution in the diffusion zone for benzene and toluene respectively. The temperature increases rapidly near the droplet surface and then approaches gradually a value equal to the flame temperature at the flame surface. The temperature distribution is also plotted when the droplet radius becomes a half of the initial value and is found to be similar in time as well as in space.

The partial pressure distribution of fuel is plotted in Figures 6 - 7 for benzene and toluene respectively. The partial pressure of the fuel decreases rapidly near the droplet surface and then gradually becomes zero at the location of the flame surface. The partial pressure distribution of fuel in the diffusion zone is also shown when the radius of the droplet becomes a half of the initial value.

Figures 8 - 9 show the partial pressure distribution of nitrogen in the diffusion zone for benzene and toluene respectively. The parital pressure of nitrogen increases rapidly near the droplet surface and then gradually becomes a value equal to atmospheric pressure at the flame surface. The partial pressure distribution of nitrogen in the diffusion zone is also plotted when the radius of the droplet becomes a half of the initial value.

Figures 10 - 11 show the velocity distribution of benzene and toluene fuel vapors in the diffusion zone. The velocity of the fuel vapor decreases rapidly near the droplet surface and then gradually decreases to a very small value at the flame surface. The velocity distribution of fuel vapor is also plotted when the radius of the droplet becomes a half of the initial value and is found to increase with time near the droplet surface and remains nearly constant near the flame surface.

The droplet diameter vs. time history of a burning droplet is shown in Figures 12 - 13 for benzene and toluene respectively. The plots of d_L^2 against time are nearly linear by the theory of diffusion model and are in close agreement with experimental data [12]. The burning constant can be evaluated by using Eq.(4.1)

$$K = d_L^2/t_b \tag{4.1}$$

where t_b is the burning time of the fuel droplet. The value of the burning constant obtained by the diffusion model is compared with the experimental works of Godsave and Goldsmith [12] and is found to be in agreement as shown in Table 2.

Figures 14 - 15 plot the total diffused mass of fuel vapors of benzene and toluene against time for 2 mm. diameter droplet. The mass flow rate of the fuel vapor diffusing towards the flame front is nearly proportional to the droplet radius and decreases almost linearly with time.

Figure 16 shows the plot of the ratio of the flame radius to the droplet radius against time for 2 mm diameter fuel droplet. The ratio of the flame radius to the droplet radius remains nearly constant and lies in the range 7 to 10 which is nearly equal to the value obtained by the experimental works [12, 14] as shown in Table 3.

CHAPTER 5

CONCLUSION

The process of burning of a fuel droplet in quiescent air is formulated by making use of a diffusion model and calculated numerically, treated as a one-dimensional, quasi-steady, and molecular diffusion-controlling phenomenon. The value of the ratio of flame radius to the droplet radius calculated by the diffusion model is in close agreement with experimental data. The following important results are obtained by this analysis:

a) The burning rate (the mass flow rate of fuel vapor diffusing towards the flame front) is nearly proportional to the droplet radius.

b) The plot of d_L^2 against time gives approximately a linear relationship throughout the course of burning and the burning constant can be predicted.

c) The flame is located nearly at the same position relative to the droplet surface.

d) The value of the ratio of the flame radius to droplet radius is in the range of 7 - 10.

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TABLE 1

PROPERTIES OF FUEL

	BENZENE	TOLUENE
†ρ (Kg/m^3)	0.50	0.85
ρ_l (Kg/m^3)	874	870
†Cp (Kcal/Kg°C)	0.9	1.02
†λ (Kcal/mh°C)	0.0396	0.0414
T_L (°C)	80	110
h_{fg} (Kcal/Kg)	94	84
D (cm^2/sec)	0.088	0.084
M_F (mol)	78	92
T_f (°K)	2237	2600

† The values are evaluated at the arithmetic mean of droplet surface and flame temperature [10,11].

TABLE 2

BURNING CONSTANTS FOR FUELS

FUEL	BURNING CONSTANT mm^2/Sec.		INVESTIGATOR	DIFFUSION MODEL mm^2/Sec.
	CALCULATED	MEAN EXPERIMENTAL		
Benzene	1.12	0.97	Godsave	0.71
Benzene	1.12	0.99	Goldsmith	
Toluene	1.11	0.66	Godsave	0.70
Toluene	1.11	0.77	Goldsmith	

TABLE 3

COMPARISON OF EXPERIMENTAL DATA WITH DIFFUSION MODEL

(material: benzene)

[14]

TECHNIQUE	CONDITION	d_L (mm)	$\frac{r_c}{r_L}$
Stationary suspended drop	Unsteady, natural convection	1.5	3.0
Droplet in Zero "g" State	Unsteady, no convection	0.95	6-10
Quasi - Steady State Theory	Quasi-Steady, no convection	Any size	29.0
Diffusion model	Quasi-Steady, no convection	Any size	7-10

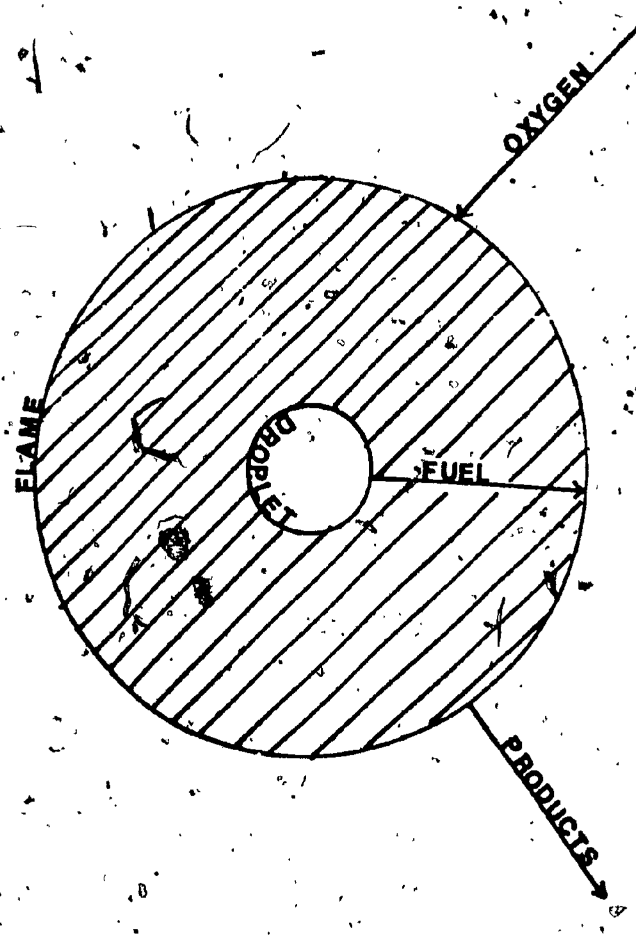


Figure 1. DIFFUSION MODEL FOR DROPLET COMBUSTION

▨ DIFFUSION ZONE

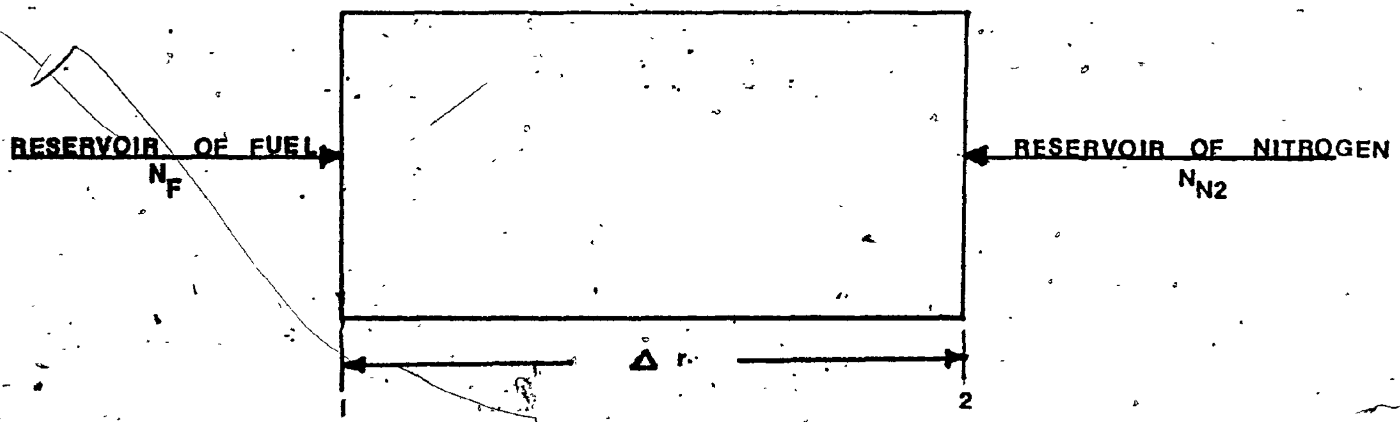


Figure 2. SKETCH ILLUSTRATING EQUIMOLAL DIFFUSION

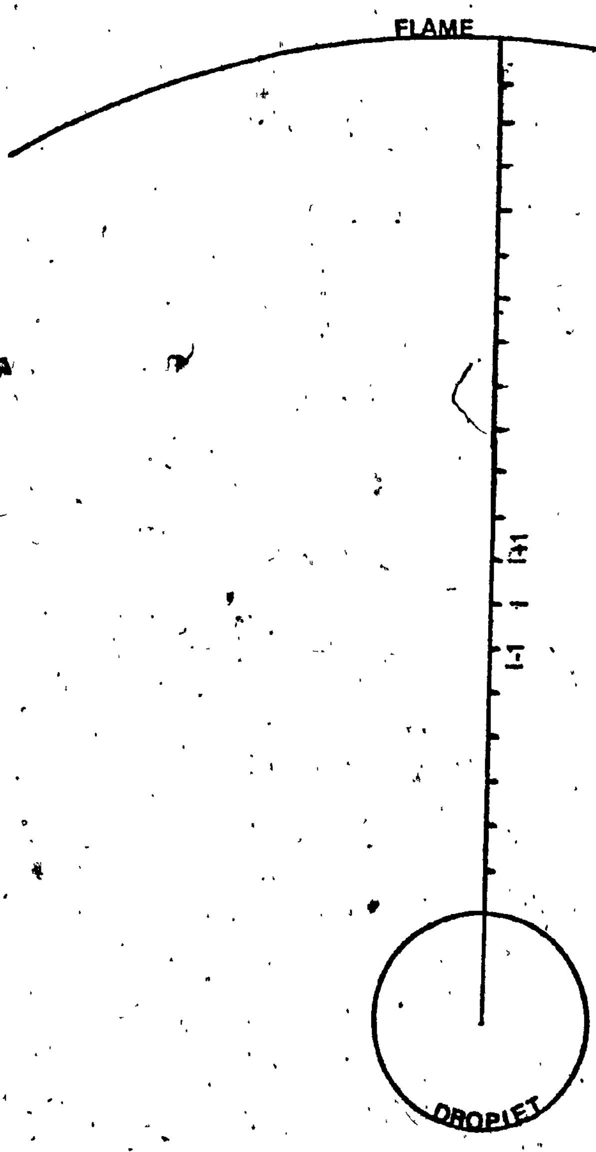


Figure 3. SKETCH SHOWING NODAL POINTS FOR ONE DIMENSIONAL GAUSS-SIEDEL METHOD.

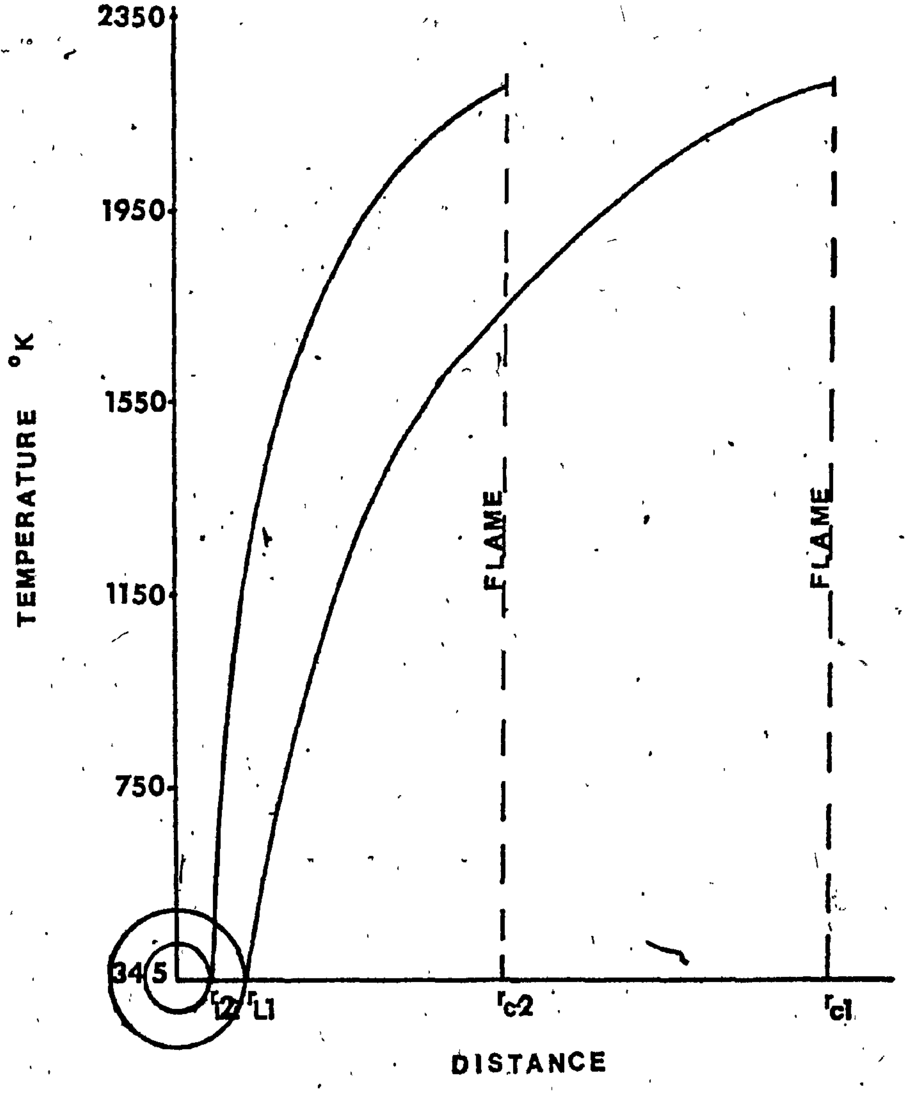


FIGURE 4. TEMPERATURE DISTRIBUTION FOR BENZENE DROPLET

$r_{L1} = 1$ mm. $\quad \frac{r_{c1}}{r_{L1}} = 9.15 \quad \frac{r_{c2}}{r_{L2}} = 9.24$

$r_{L2} = 0.5$ mm. $\quad \left.\frac{dT}{dr}\right|_{r = r_{L1}} = 7.7\text{x}10^6 \quad \left.\frac{dT}{dr}\right|_{r = r_{L2}} = 14.5\text{x}10^6$

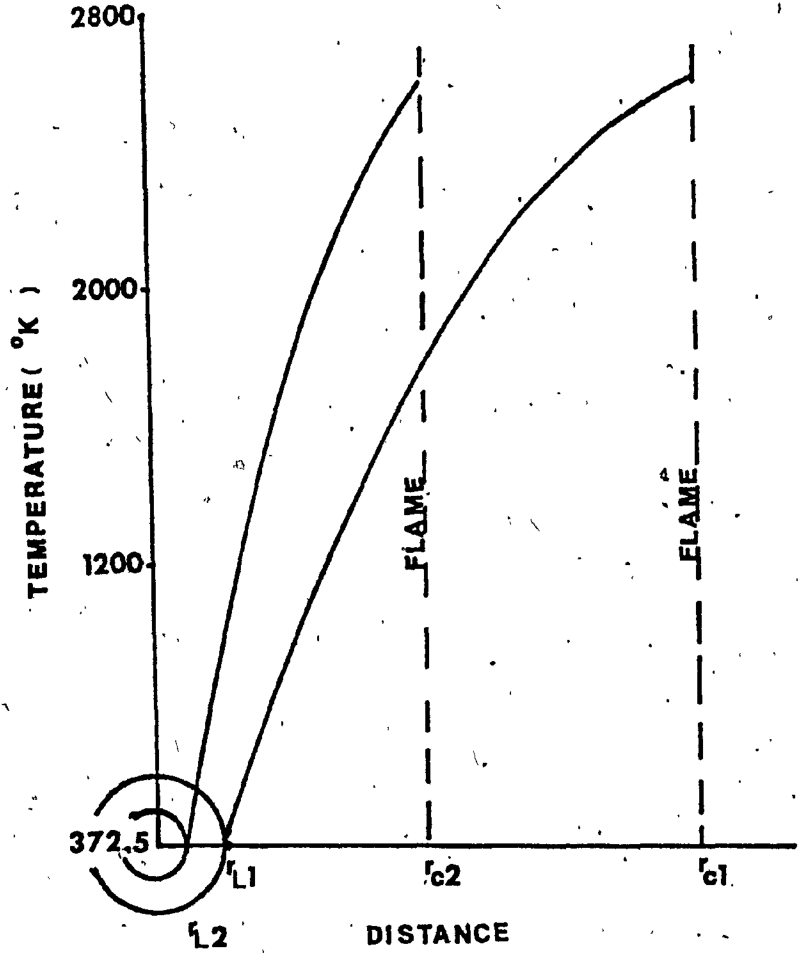


FIGURE 5. TEMPERATURE DISTRIBUTION FOR TOLUENE DROPLET

r_{L1} = 1 mm. $\frac{r_{c1}}{r_{L1}} = 7.3$ $\frac{r_{c2}}{r_{L2}} = 7.37$

r_{L2} = 0.5 mm. $\left.\frac{dT}{dr}\right|_{r=r_{L1}} = 6.3\times10^{6}$ $\left.\frac{dT}{dr}\right|_{r=r_{L2}} = 12.6\times10^{6}$

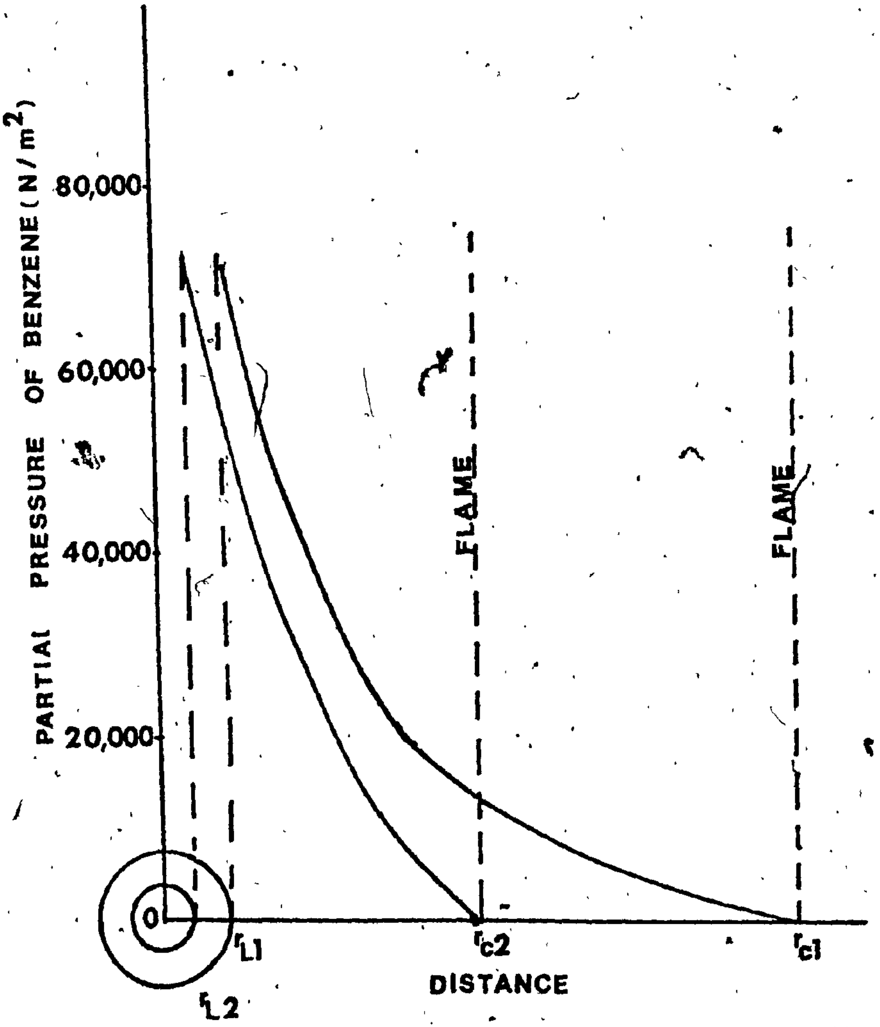


FIGURE 6. PARTIAL PRESSURE DISTRIBUTION OF FUEL FOR BENZENE DROPLET

r_{L1} = 1 mm. r_{c1}/r_{L1} = 9.15

r_{L2} = 0.5 mm. r_{c2}/r_{L2} = 9.24

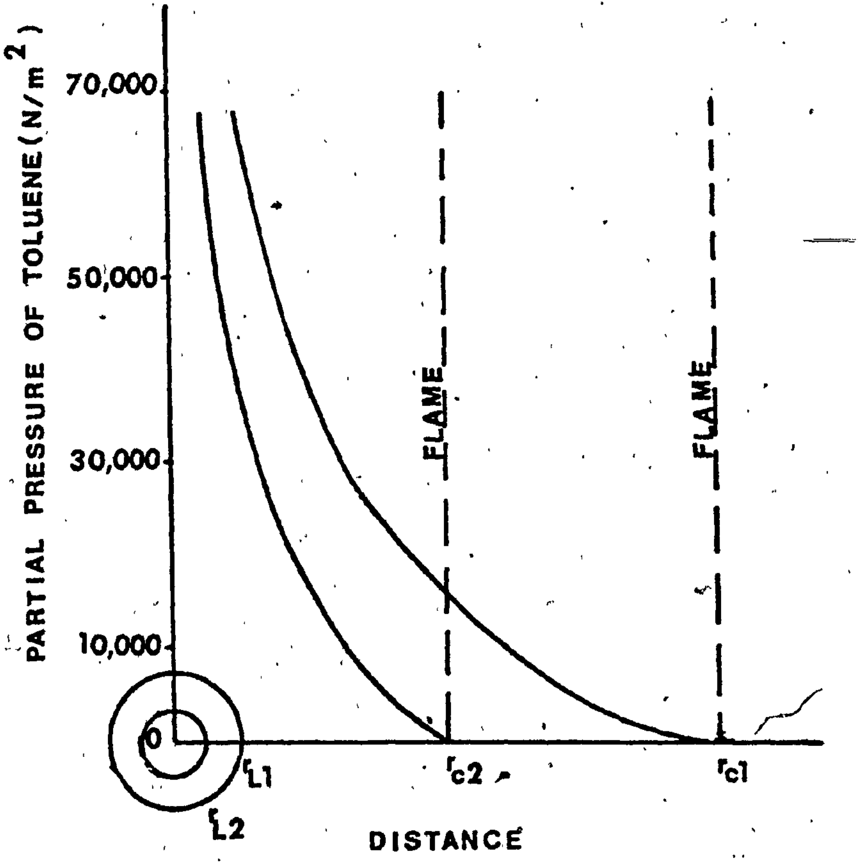


FIGURE 7. PARTIAL PRESSURE DISTRIBUTION OF FUEL FOR TOLUENE DROPLET

r_{L1} = 1 mm. r_{c1}/r_{L1} = 7.3

r_{L2} = 0.5 mm. r_{c1}/r_{L2} = 7.37

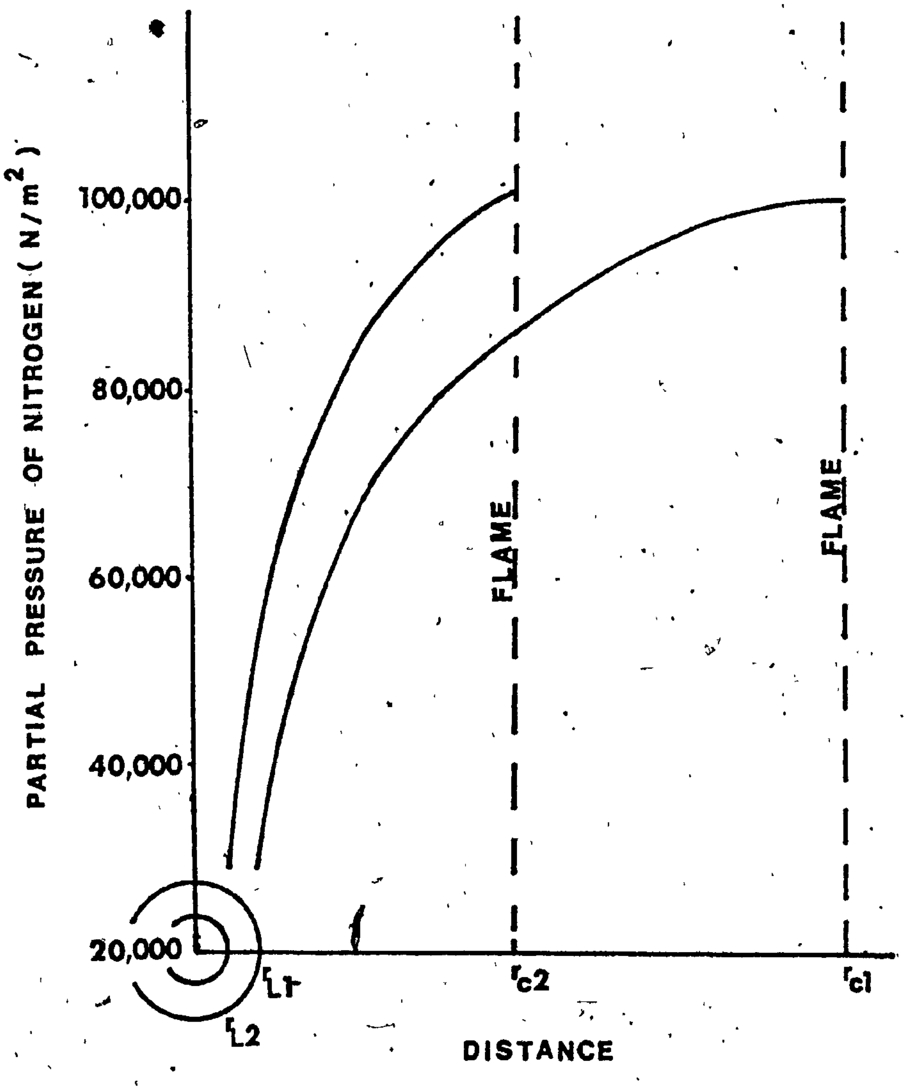


FIGURE 8. PARTIAL PRESSURE DISTRIBUTION OF NITROGEN FOR BENZENE DROPLET.

r_{L1} = 1 mm r_{c1}/r_{L1} = 9.15

r_{L2} = 0.5 mm. r_{c2}/r_{L2} = 9.24

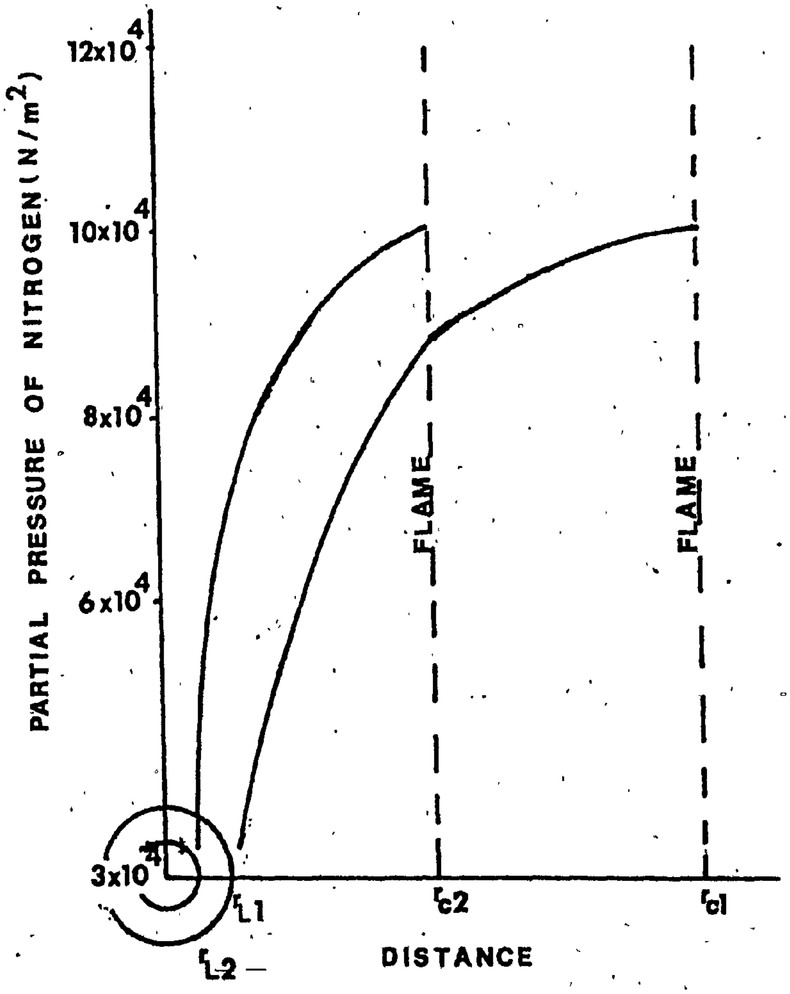


FIGURE 9. PARTIAL PRESSURE DISTRIBUTION OF NITROGEN FOR TOLUENE DROPLET

r_{L1} = 1 mm. r_{c1}/r_{L1} = 7.3

r_{L2} = 0.5 mm. r_{c2}/r_{L2} = 7.37

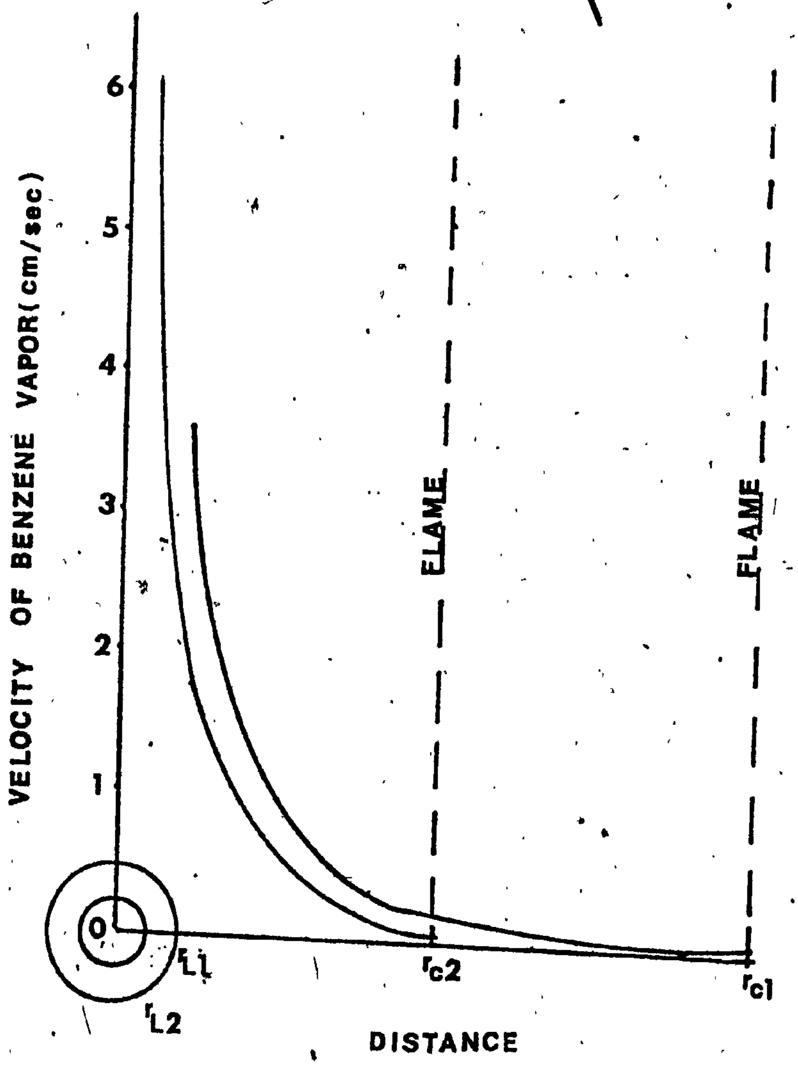


FIGURE 10. VELOCITY DISTRIBUTION OF FUEL VAPOR FOR BENZENE DROPLET

r_{L1} = 1 mm. r_{c1}/r_{L1} = 9.15

r_{L2} = 0.5 mm. r_{c2}/r_{L2} = 9.24

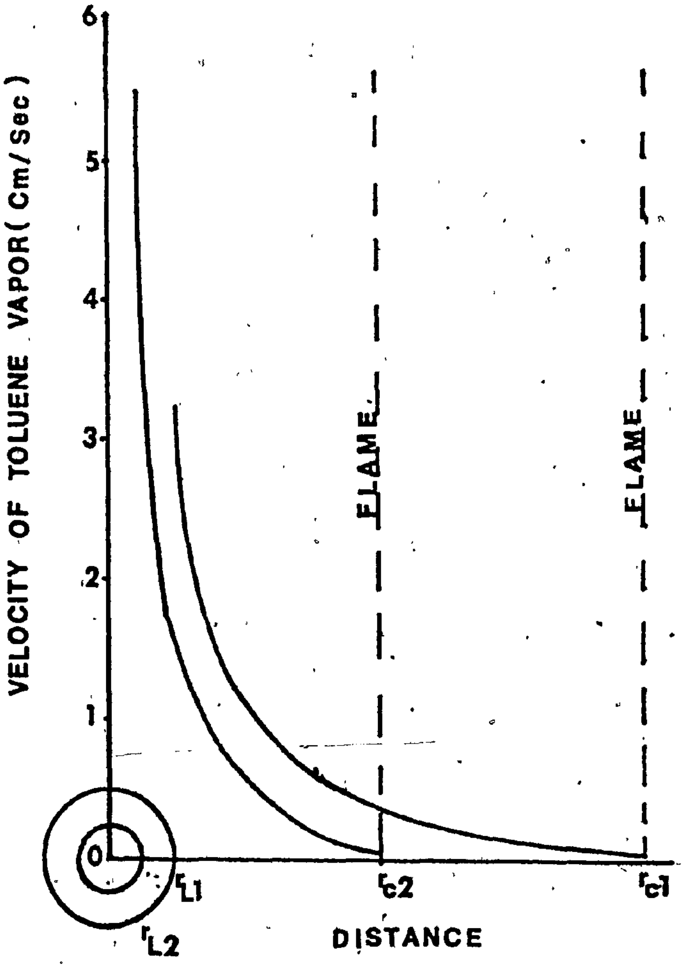


FIGURE 11. VELOCITY DISTRIBUTION OF FUEL VAPOR FOR TOLUENE DROPLET

r_{L1} = 1 mm. r_{c1}/r_{L1} = 7.3

r_{L2} = 0.5 mm. r_{c2}/r_{L2} = 7.37

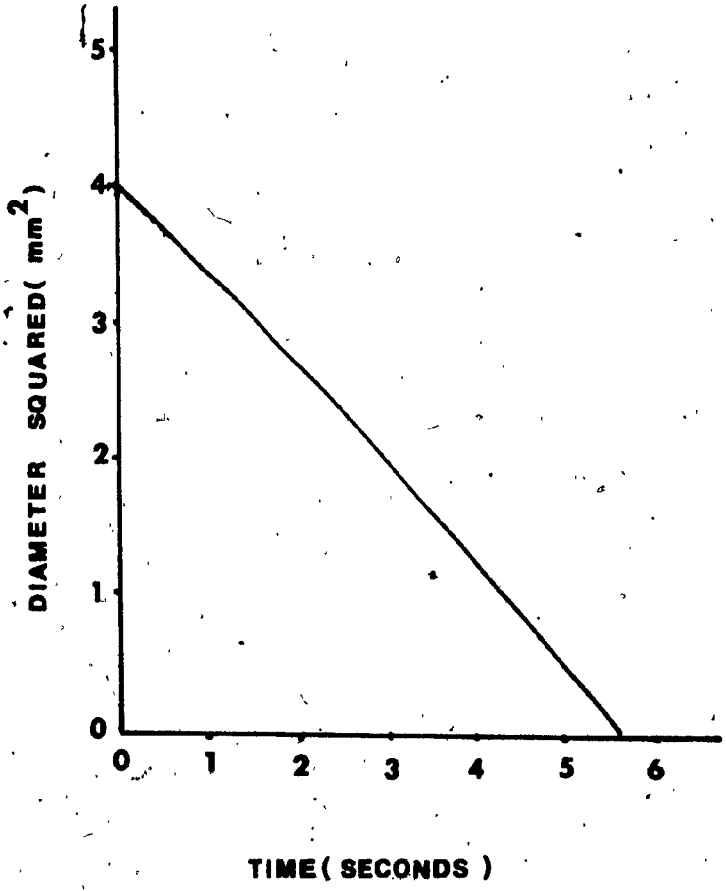


FIGURE 12. d_L^2 VS. TIME FOR BENZENE DROPLET OF 2-mm. DIAMETER

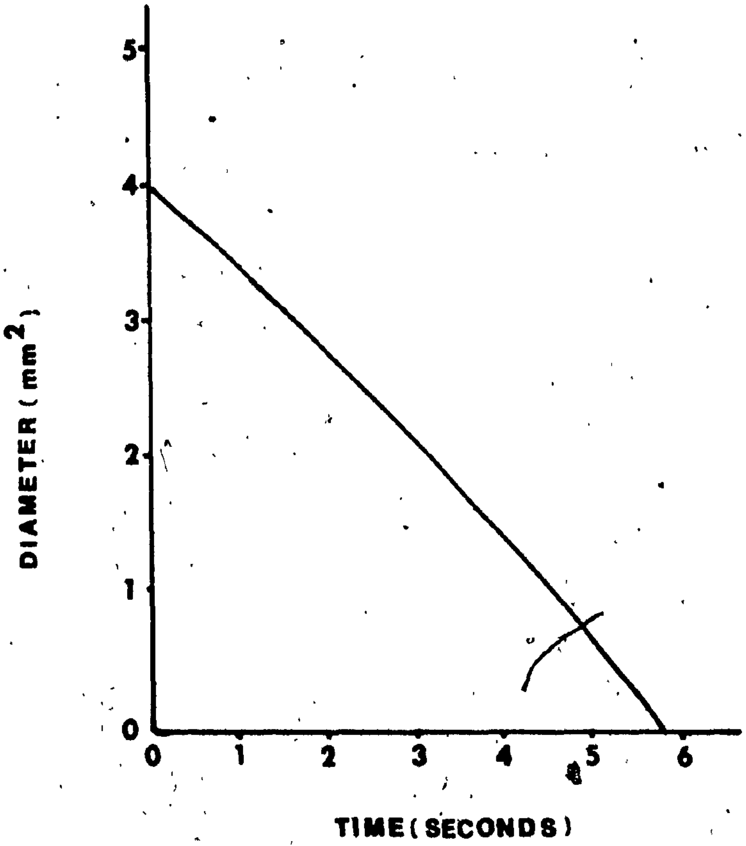


FIGURE 13. d_L^2 VS. TIME FOR TOLUENE DROPLET OF 2 mm. DIAMETER

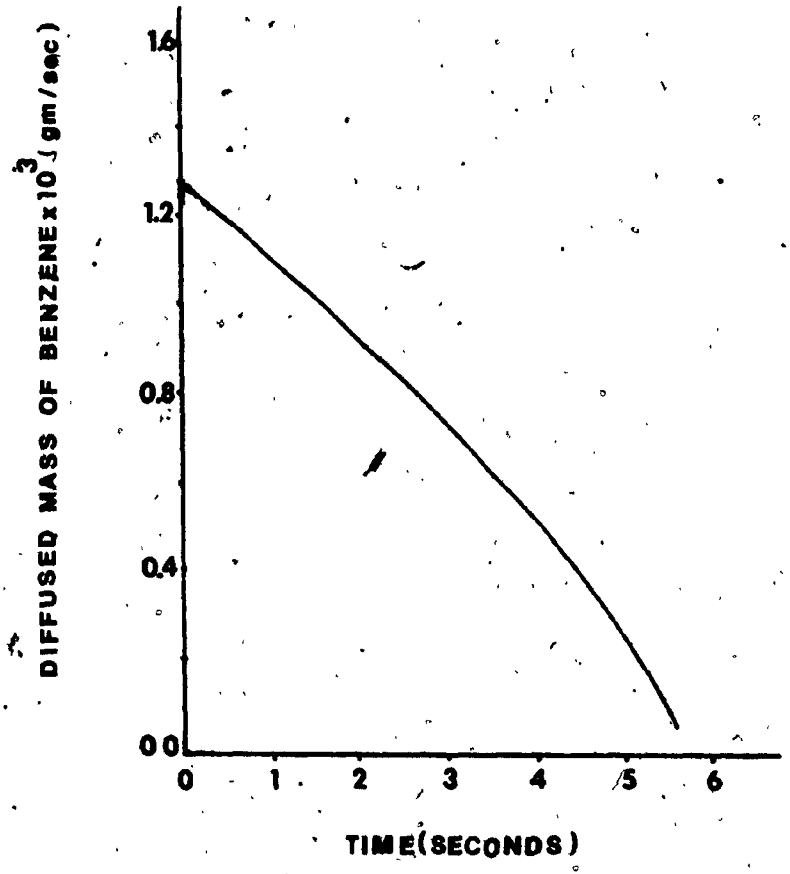


FIGURE 14. DIFFUSED MASS OF FUEL FOR BENZENE DROPLET

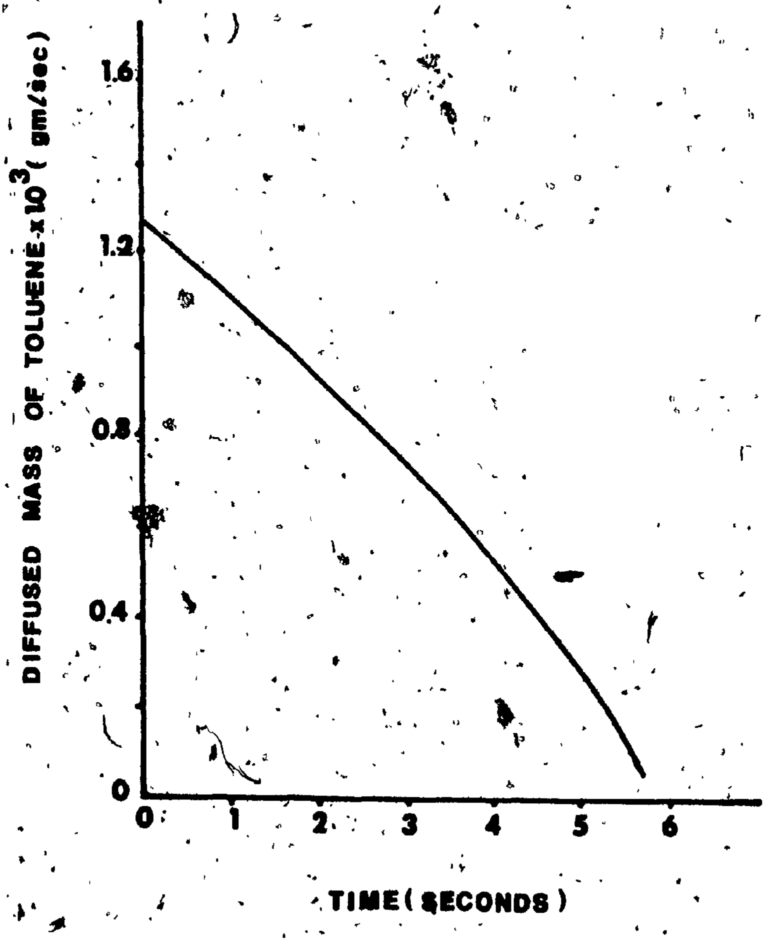


FIGURE 15. DIFFUSED MASS OF FUEL FOR TOLUENE DROPLET

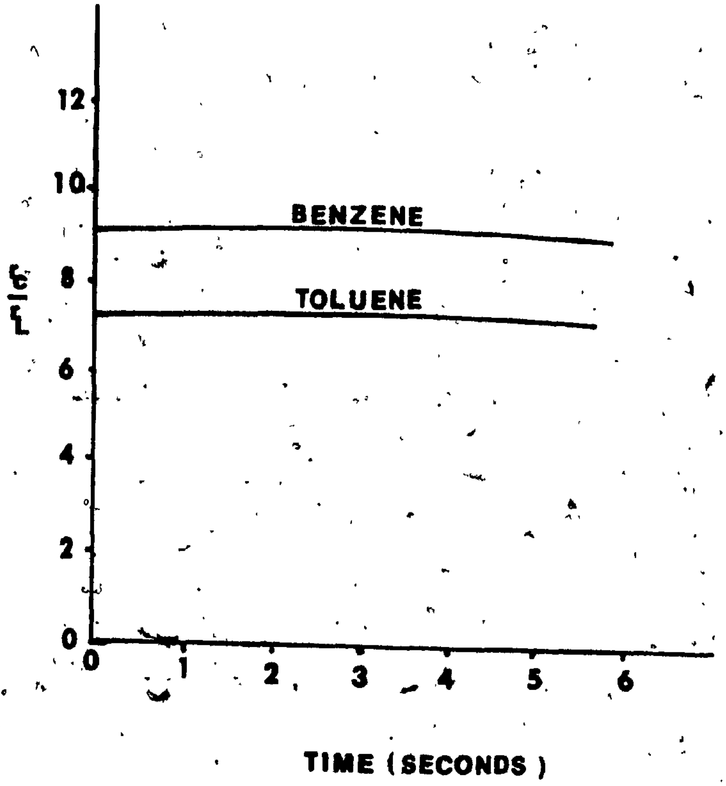
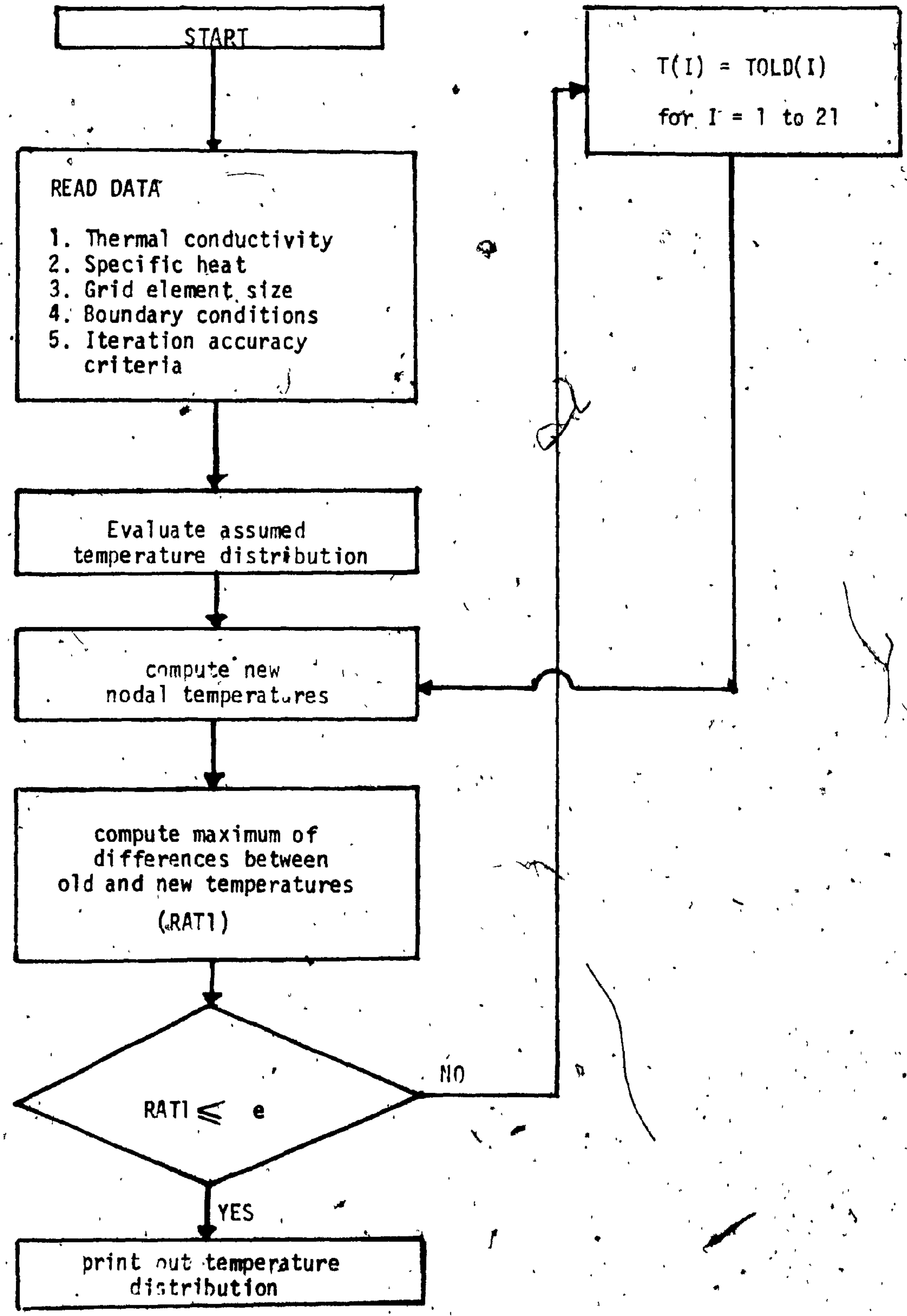


FIGURE 16. RATIO OF FLAME RADIUS TO DROPLET RADIUS VS. TIME FOR 2 mm. DIAMETER DROPLET

FIGURE 17. FLOW DIAGRAM FOR GAUSS-SIEDEL METHOD



APPENDIX A

```
C-----------------------------------------------------------------------
C     THIS IS A PROGRAM TO CALCULATE THE BURNING TIME AND FLAME LOCATION
C     OF A SINGLE FUEL DROPLET OF BENZENE
C-----------------------------------------------------------------------
      PROGRAM DROPLET(INPUT,OUTPUT)
      DIMENSION Q(21),CONS(21),V(21)
      DIMENSION RATP(21),YPFOLD(21)
      DIMENSION T(21),TOLD(21),RAT(21),YPF(21),YPN(21)
      DIMENSION R(21),EL(21)
C-----------------------------------------------------------------------
C     READING THE PROPERTIES OF THE FUEL
C-----------------------------------------------------------------------
      TF=2237.
      TO=345.
      DENLIQ=874.
      RK=0.000011
      CP=0.9
      FD=0.088/10000
      FM=78
      HFG=94.
      RHO=0.50
      RO=0.001
      ORT=0.0
      DELRS=0.00005
      P=101300
      UGAS=8315.
      TIME=0.0
      DELT=1.0
C-----------------------------------------------------------------------
C     SETTING THE CONVERGENCE PARAMETERS
C-----------------------------------------------------------------------
      EPI=10.
      RATP1=10.
      RAT1=1.
      EPSI=1.
C-----------------------------------------------------------------------
C     CHOOSING THE INITIAL VALUE OF FLAME RADIUS IN TERMS OF DROPLET
C     RADIUS.
C-----------------------------------------------------------------------
 18   CONTINUE
      DELX=RO*6/20
 40   CONTINUE
      DO 100 I=1,21
      R(I)=RO+DELX*(I-1)
 100  CONTINUE
C-----------------------------------------------------------------
C     TO EVALUATE THE TEMPERATURE DISTRIBUTION
C-----------------------------------------------------------
C-----------------------------------------------------------------------
C     THE INITIAL TEMPERATURE DISTRIBUTION IS SPECIFIED. IT IS SIMPLY
C     THE AVERAGE OF THE FLAME AND DROPLET SURFACE TEMPERATURE
C-----------------------------------------------------------------------
      DO 1 I=2,20
      T(I)=(TO+TF)/2.
      TOLD(I)=T(I)
 1    CONTINUE
      T(1)=TO
```

```
      T(21)=TF
    5 CONTINUE
C-----------------------------------------------------------------
C     THE NODAL TEMPERATURES ARE COMPUTED FROM THE TEMPERATURE
C     DISTRIBUTION EQUATION DEVELOPED EARLIER
C-----------------------------------------------------------------
      ALPHA=(P*FM*HFG)/(RHO*CP*UGAS)
      DO 2 I=2,20
      T(I)=((T(I+1)-T(I-1))*DELX)/(2*(RO+DELX*(I-1)))+T(I+1)/2.+
     $T(I-1)/2.-((RO**2.)*(T(2)-T(1))*(T(I+1)-T(I-1))*T(1))/
     $(ALPHA*((RO+DELX*(I-1))**2.)*4.)
C-----------------------------------------------------------------
C     THE MAXIMUM OF THE ABSOLUTE VALUES OF THE DIFFERENCES BETWEEN THE
C     OLD AND NEW TEMPERATURE DISTRIBUTIONS IS DETERMINED.IF IT IS LESS
C     THAN THE CONVERGENCE CRITERION EPSI,THE TEMPERATURE DISTRIBUTION
C     IS FINAL,IF NOT,THE OLD VALUES OF T ARE REPLACED BY NEW ONES AND
C     THE COMPUTATION IS RETURNED TO STATEMENT 5 FOR AN ADDITIONAL
C     ITERATION.
C-----------------------------------------------------------------
      RAT(I)=ABS(TOLD(I)-T(I))
      IF(RAT(I).GT.RAT(I-1)) RAT1=RAT(I)
      TOLD(I)=T(I)
    2 CONTINUE
      IF(RAT1.LE.EPSI) GO TO 4
      GO TO 5
    4 CONTINUE
      DELTEM=(T(2)-T(1))/DELX
      FMTOT=4.*3.14*RO**2.*RK*DELTEM/HFG
C-----------------------------------------------------------
C     THE PARTIAL PRESSURE OF FUEL AND NITROGEN IS EVALUATED AS A
C     FUNCTION OF RADIUS BETWEEN FLAME AND DROPLET SURFACE
C-----------------------------------------------------------
      YPF(1)=72937.5
C-----------------------------------------------------------------
C     THE INITIAL PRESSURE DISTRIBUTION FOR FUEL AND NITROGEN IS
C     SPECIFIED.
C-----------------------------------------------------------------
      DO 10 I=2,21
      YPF(I)=YPF(1)/2.
      YPFOLD(I)=YPF(I)
   10 CONTINUE
   80 CONTINUE
      DO 11 I=1,20
      D(I)=FD*(((T(I+1)+T(I))/596.)**1.5)
   11 CONTINUE
      D(21)=D(20)
      DO 25 I=1,21
      CONS(I)=4.*3.14*D(I)*FM/UGAS
   25 CONTINUE
C-----------------------------------------------------------------
C     THE NODAL PRESSURES ARE CALCULATED FROM THE PRESSURE DISTRIBUTION
C     EQUATIONS DEVELOPED EARLIER.
C-----------------------------------------------------------------
      DO 14 I=2,21
      YPF(I)=YPF(I-1)-(DELX*FMTOT*T(I)*(2.*P-(YPF(I+1)+YPF(I-1))))/
     $(CONS(I)*((DELX*(I-1)+RO)**2.)*P*2.)
C-----------------------------------------------------------------
```

```
C      THE MAXIMUM OF THE ABSOLUTE VALUES OF THE DIFFERENCES BETWEEN THE
C      OLD AND NEW PRESSURE DISTRIBUTIONS IS DETERMINED.IF IT IS LESS
C      THAN THE CONVERGENCE CRITERION EPI, THE PRESSURE DISTRIBUTION
C      IS FINAL,IF NOT,THE OLD VALUES OF P ARE REPLACED BY NEW ONES AND
C      THE COMPUTATION IS RETURNED TO STATEMENT 80 FOR AN ADDITIONAL
C      ITERATION.
C-----------------------------------------------------------------------
      RATP(I)=ABS(YPFOLD(I)-YPF(I))
      IF(RATP(I).GT.RATP(I-1)) RATP1=RATP(I)
      YPFOLD(I)=YPF(I)
   14 CONTINUE
      IF(RATP1.LE.EPI) GO TO 15
      GO TO 80
   15 CONTINUE
      DO 16 I=1,21
      YPN(I)=P-YPF(I)
   16 CONTINUE
C-----------------------------------------------------------------------
C      VELOCITY DISTRIBUTION IS EVALUATED FROM THE EQUATIONS DEVELOPED
C      EARLIER.
C-----------------------------------------------------------------------
      DO 101 I=1,21
      V(I)=(T(1)*UGAS*RK*(RO**2.)*(T(2)-T(1)))/
     $(P*FM*HFG*DELX*((RO+DELX*(I-1))**2.))
  101 CONTINUE
C-----------------------------------------------------------------------
C      THE FLAME RADIUS IS ALSO EVALUATED BY USING LAGRANGE INTERPOLATION
C      FROM THE PARTIAL PRESSURE DISTRIBUTION OF FUEL ASSUMING THAT ALL
C      FUEL IS CONSUMED AT THE FLAME SURFACE.IF THE DIFFERENCE BETWEEN
C      THE CHOSEN FLAME RADIUS AND THE INTERPOLATED RADIUS IS NEGATIVE,
C      THE CHOSEN FLAME RADIUS IS INCREASED IN STEPS OF DELRS AND THE
C      COMPUTATION IS RETURNED TO STATEMENT 40 AND THE PROCESS IS
C      REPEATED TILL THE THIS DIFFERENCE BECOMES POSITIVE.THE CORRECT
C      LOCATION OF FLAME IS THEN PRINTED.
C-----------------------------------------------------------------------
      CALC=0.0
      YPFK=0.0
      DO 105 I=1,21
      DIV=1.
      PROD=1.
      DO 110 J=1,21
      IF(J.EQ.I) GO TO 110
      DIV=DIV*(YPF(I)-YPF(J))
      PROD=PROD*(YPFK-YPF(J))
  110 CONTINUE
      EL(I)=PROD/DIV
      CALC=CALC+EL(I)*R(I)
  105 CONTINUE
      FLRAD=RO+DELX*20.
      IF(FLRAD-CALC) 202,202,203
  202 GO TO 250
  203 FLRAD=FLRAD+DELRS
      DELX=(FLRAD-RO)/20
      GO TO 40
  250 CONTINUE
C-----------------------------------------------------------------------
C      PRINTING THE FLAME RADIUS, DROPLET RADIUS AND RATIO BETWEEN THEM
```