

# A Theoretical Model for the Combustion of Droplets in Super-critical Conditions and Gas Pockets

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**Abstract—A Theoretical Model for the Combustion of Droplets in Supercritical Conditions and Gas Pockets.** Supercritical combustion of droplets is studied by means of a physical model which assumes spherical symmetry, laminar conditions, constant pressure and a zero-thickness flame.

Boundary conditions at the infinity state that temperature and composition of the mixture are given and constant.

Initial distributions of temperature and mass fractions of the species are given, as well as the initial conditions at the droplet surface. As combustion proceeds, droplet surface is not considered to exist as a physical boundary allowing unrestricted diffusion of species through it.

With some additional simplifications for the density and transport coefficients, a numerical solution of the problem is obtained.

An analytical solution of the problem is also obtained by means of an asymptotic analysis. This solution applies when the initial temperature of the droplet is small as compared with the temperature of the surrounding atmosphere. It is shown that this is the most important case from the technological point of view.

For this case results show that an apparent droplet exists throughout most of the process, in which its surface is characterized by an abrupt change in temperature and composition of the chemical species.

Results show burning rates, combustion times, flame radius and temperature at the droplet center as function of the principal variables of the process. In particular, the square of the apparent droplet radius is a linear function of time as occurs in subcritical combustion.

It is shown that combustion times are faster in supercritical conditions than in subcritical conditions with the minimum value existing at critical conditions.

A numerical application is carried out for the case of oxygen droplets burning in hydrogen and a comparison is carried out between the theoretical results obtained numerically and analytically as well as with those experimentally obtained.

*Translated abstracts appear at the end of this paper*

## Nomenclature

$c_p$	specific heat at constant pressure;
$D$	diffusion coefficient;
$q_r$	heat of reaction per unit mass of fuel;
$r$	distance to the center;
$t$	time;
$T$	temperature;
$T_0$	initial temperature of the gas pocket;
$V$	velocity;
$x$	non-dimensional distance;
$Y$	mass fraction;

$z$	non-dimensional distance to the gas pocket surface;
$w$	rate of production of species;
	$\varepsilon = T_0/T_\infty$ ;
$\lambda$	heat-transfer coefficient;
$\nu$	stoichiometric ratio;
$\tau$	non-dimensional time;
$\theta$	non-dimensional temperature.

## Subscripts

1	droplet material (fuel on oxidizer);
2	outside material (fuel on oxidizer);
3	combustion products;
$s$	droplet surface;
$f$	flame;
$\infty$	infinity;
0	initial conditions.

## 1. Introduction

SUPERCRITICAL combustion of fuels and propellants in droplet form has become a problem of high technical interest since the operating pressures in the combustion chambers of rocket motors have reached values higher than the critical pressure of several fuels and oxidizers of frequent utilization, such as hydrogen, kerosene and oxygen.

Normally, fuels and propellants are stored in the tanks of the rocket vehicles at temperatures close to boiling temperature at ambient pressure, and vapor pressure in the tanks is maintained at values not very different from one atmosphere. Therefore, propellants may be injected into the combustion chambers at supercritical pressures, but at temperatures considerably smaller than critical temperature.

Surface tension of a droplet is a function of droplet temperature [1], becoming equal to zero as temperature reaches its critical value when it is surrounded by its own vapors. Therefore, a liquid fuel or propellant injected under these conditions will generate a spray of droplets. These droplets will begin vaporizing at supercritical pressure but at subcritical temperature. Droplet temperature will increase until critical temperature is eventually reached and then the surface tension will become very small or zero as well as the heat of vaporization, and then the droplet will become a sphere or fluid particle surrounded by a mixture of the same fluid and combustion product. From here on complete supercritical vaporization or combustion will take place.

It may be shown [2] that a droplet injected at supercritical pressure and at subcritical temperature will reach its critical temperature in a short time. It has also been verified that the amount of fuel vaporized until critical temperature is reached is a small percentage of the total amount of fuel or propellant of the droplet.

This important case in which combustion begins at critical temperature will be specially considered in this study, although physical model of the process will be applicable throughout the complete supercritical region. Actually, some simplifications introduced in the values of the transport coefficients and on the density of the mixture will give a better quantitative approximation in the supercritical region far from the critical conditions, for which the process will be similar to the case of the combustion of a gas pocket within a reacting gaseous environment.

Supercritical vaporization or combustion of droplets is a process which differs essentially from droplet vaporization or combustion in subcritical conditions.

In the first place, since the latent heat of vaporization is zero, classical quasi-stationary theories utilized

to study subcritical combustion [3, 4] cannot be applied since they give an infinite value for the burning rate of a droplet as the heat of vaporization becomes equal to zero. Therefore, in supercritical conditions diffusion is the rate controlling process and the heat flux reaching the droplet surface is only utilized for increasing the droplet temperature.

On the other hand, a real droplet does not exist, since when it reaches critical conditions it becomes a sphere of a fluid surrounded by a mixture of the same fluid with inert gases.

Therefore, the existence of the droplet with a physical surface throughout the combustion process, as it has been considered by a number of investigators, can only be physically admitted by assuming that the diffusion coefficients depend strongly on the concentration of the species around critical conditions, assumption which has not yet been justified. This case is amply discussed in ref. [5].

Some studies already exist on supercritical combustion. Spalding [6], carried out a study by assuming that at critical conditions the droplet is transformed into a point-source of fluid, and a study of similar nature was performed by ourselves [7]. However, these studies give little information on the real nature of the supercritical combustion process.

Rossner [8], performed an interesting study as an expansion on his work on chemical releases [9]. The assumptions introduced in his model lead to the solution of a pure diffusion problem for which an analytical solution exists. Some interesting conclusions were derived, but this treatment only gives a good approximation of the problem when the process is far from critical conditions, as it was stated by the author. In practice, the real combustion process always begins at critical temperature as it has been already discussed.

An excellent experimental study on supercritical combustion of the droplets burning in a still atmosphere has been carried out by Faeth and collaborators [10].

The principal conclusions of this work were that burning rate of the droplets attains a minimum value around critical conditions and that droplet temperature increases rapidly once the critical conditions are reached.

Lazar and Faeth [11], carried out another work on this field including a theoretical treatment, but utilizing a stationary model.

All these theoretical and experimental studies refer to the case of vaporization or combustion of droplets within a stagnant atmosphere, that is to say, disregarding forced convection effects. This is the preliminary basic study but in any further studies on the

combustion processes of droplets in actual combustion chambers conditions forced convection effects should be taken into account. Due to the absence of surface tension, forced convection effects might be specially significant, since the droplets might change considerably in shape or they might even be shattered by the shearing aerodynamic forces originated by the motion of the droplets with respect to the reacting gaseous atmosphere. Some preliminary experimental works already exist on this subject [12, 13].

## 2. Model of the Process and General Equations

Model of the process will be based on assuming that the droplet burns or vaporizes in a still atmosphere. Spherical symmetry will be assumed and, therefore, convection effects will be disregarded.

Pressures will be taken as constant throughout the process and laminar conditions will be considered.

Three chemical species will only be considered: 1, fuel or oxidizer in the droplet; 2, oxidizer or fuel surrounding the droplet, and 3, combustion products.

Based on these assumptions, general equations of the process are those of a laminar diffusion flame with spherical symmetry, which are as follows:

(a) *Conservation of mass for the mixture*

$$\frac{1}{K4\pi r^2} \frac{\partial \dot{m}}{\partial r} + \frac{\partial \rho}{\partial t} = 0 \quad (1)$$

in which:

$$\dot{m} = 4\pi r^2 \rho v \quad (2)$$

where  $v$  is the radial velocity of the mixture.

(b) *Conservation of mass for the species*

$$\rho \frac{\partial Y_i}{\partial t} + \rho v \frac{\partial Y_i}{\partial r} - \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \rho D \frac{\partial Y_i}{\partial r} \right) = w_i \quad (3)$$

where  $w_i$  is the reaction rate of species  $i$ .

(c) *Energy*

$$\rho \frac{\partial T}{\partial t} + \rho v \frac{\partial T}{\partial r} - \frac{1}{r^2} \frac{\partial}{\partial r} \left( r^2 \frac{\lambda}{c_p} \frac{\partial T}{\partial r} \right) = \frac{q_r w_p}{c_p} \quad (4)$$

in which  $q_r$  is the heat of reaction and  $w_p$  is the reaction rate of the combustion products.

In order to simplify the problem a zero-thickness flame theory will be admitted. It has been shown [3] that it gives an excellent approximation of the process provided that the droplet is not too small or the pressure is not too low.

Therefore, in the outer region from the flame only combustion products (3) and oxidizer (or fuel) (2) will exist. In the inner region only fuel (or oxidizer) from the droplet (1) and combustion products (3) will exist.

For simplicity, the specific heats will be taken constant and equal for all chemical species. The diffusion coefficients and thermal conductivity will be taken as functions of the temperature only, disregarding their variation with the mixture composition.

Finally, the product of the density times the temperature will be taken as constant. This assumption will introduce some errors in the process of supercritical droplet combustion near critical conditions but it will be a good assumption for the case of supercritical combustion of droplets far from critical conditions or for the case of gas pockets.

## 3. Boundary and Initial Conditions

At the infinity it will be assumed that the temperature and composition of the gaseous atmosphere are given and constant, that is:

$$r = \infty \begin{cases} T = T_\infty \\ Y_{1\infty} = 0 \\ Y_2 = Y_{2\infty} \\ Y_3 = Y_{3\infty} \end{cases} \quad (5)$$

At the origin of coordinates, we will have:

$$r = 0 \begin{cases} \frac{\partial T}{\partial r} = 0 \\ \frac{\partial Y_i}{\partial r} = 0 \end{cases} \quad (6)$$

In order to solve the problem initial conditions:

$$t = 0 \begin{cases} T = T_0(r) \\ Y_i = Y_{i0}(r) \end{cases} \quad (7)$$

will have to be given. The velocity  $V$  has to fulfill conditions:

$$\begin{aligned} r = 0 & \quad V = 0 \\ r = \infty & \quad V = 0 \end{aligned} \quad (8)$$

and its initial distribution has to satisfy Eqs. (1) to (4) with conditions (7). Actual initial conditions are difficult to precise since they will depend on the previous history of the process before reaching critical conditions.

The problem will be solved by taking the following initial step functions:

$$t = 0 \begin{cases} r < r_{s0} & T = T_0, & Y_1 = 1, & Y_2 = 0 \\ r > r_{s0} & T = T_\infty & Y_1 = Y_{1\infty}, & Y_2 = Y_{2\infty} \end{cases} \quad (9)$$

It will be shown that final results do not depend essentially on these initial conditions.

Finally, at the flame front it will be stated the continuity of temperature and that the mass fractions of fuel and oxidizer are equal to zero and that their fluxes reach the flame front at the stoichiometric ratio.

#### 4. Solution of the System

By multiplying Eq. (1) by  $T$  and adding it to Eq. (4) and applying the thin flame theory, it results:

$$\frac{\partial(T\rho r^2)}{\partial t} + \frac{\partial(T\rho Vr^2)}{\partial r} - \frac{\partial}{\partial r} \left( r^2 \frac{\lambda}{c_p} \frac{\partial T}{\partial r} \right) = 0 \quad (10)$$

Since  $T\rho = \text{constant}$ , it is obtained by integrating with respect to  $r$ :

$$\rho Vr^2 T = r^2 \frac{\lambda}{c_p} \frac{\partial T}{\partial r} + H(t) \quad (11)$$

By using boundary conditions (7) and (8), and by expressing the continuity of velocity and temperature across the flame, it is obtained:

$$H(t) = 0 \quad \text{inside the flame} \quad (12)$$

$$H(t) = \frac{\lambda}{c_p} r_f^2 \left[ \left( \frac{\partial T}{\partial r} \right)_f^- - \left( \frac{\partial T}{\partial r} \right)_f^+ \right] \quad \text{outside the flame.} \quad (13)$$

Eqs. (11), (12) and (13) allow the elimination of the mixture velocity, which make feasible numerical integration of the system. Introducing the dimensionless variables:

$$x = \frac{r}{r_{s0}} \quad (14)$$

$$\theta = \frac{T}{T_\infty} \quad (15)$$

$$\tau = \frac{D_\infty}{r_{s0}^2} t, \quad (16)$$

and taking the Lewis–Semenov number equal to one; system of equations reduce to:

(a) Inside the flame:

$$\frac{1}{\theta^2} \frac{\partial \theta}{\partial \tau} = \frac{1}{x^2} \frac{\partial}{\partial x} \left[ x^2 \sigma(\theta) \frac{\partial \theta}{\partial x} \right] \quad (17)$$

$$\frac{1}{\theta^2} \frac{\partial Y_1}{\partial \tau} = \frac{1}{x^2} \frac{\partial}{\partial x} \left[ x^2 \sigma(\theta) \frac{\partial Y_1}{\partial x} \right] \quad (18)$$

(b) Outside the flame

$$\frac{1}{\theta^2} \frac{\partial \theta}{\partial \tau} = \frac{1}{x^2} \frac{\partial}{\partial x} \left[ x^2 \sigma(\theta) \frac{\partial \theta}{\partial x} \right] - \frac{K(t)}{\theta^2} \frac{1}{x^2} \frac{\partial \theta}{\partial x} \quad (19)$$

$$\frac{1}{\theta^2} \frac{\partial Y_2}{\partial \tau} = \frac{1}{x^2} \frac{\partial}{\partial x} \left[ x^2 \sigma(\theta) \frac{\partial Y_2}{\partial x} \right] - \frac{K(t)}{\theta^2} \frac{1}{x^2} \frac{\partial Y_2}{\partial x} \quad (20)$$

in which:

$$\sigma(\theta) = \frac{\rho^2 D}{\rho_\infty D_\infty} \frac{\lambda T_\infty}{\lambda_\infty T} \quad (21)$$

$$K(\tau) = \frac{H(t)}{\rho_\infty D_\infty r_{s0} T_\infty} \quad (22)$$

As a consequence of taking the Lewis–Semenov number equal to one, there exists a direct relationship between mass fraction and temperature which facilitate numerical integration of the system.

Temperature at the flame is obtained directly, resulting:

$$\theta_f = \frac{(\alpha c_p T_\infty / q_r) - (Y_{2\infty} / \nu)}{(\alpha c_p T_\infty / q_r)} \quad (23)$$

in which:

$$\alpha = \frac{1 + Y_{2\infty} / \nu}{(c_p T_\infty / q_r) (1 - \epsilon) - 1} \quad (24)$$

#### 5. Asymptotic Analysis

Considering the case in which supercritical combustion begins at critical temperature, this initial critical temperature  $T_0$  is considerably smaller than temperature  $T_\infty$  of the surrounding atmosphere, which will be close to the adiabatic combustion temperature.

Therefore, parameter:

$$\epsilon = \frac{T_0}{T_\infty} \ll 1 \quad (25)$$

will be small and this permits an asymptotic treatment of the problem.

This asymptotic study is shown in full in ref. [12].

This study is based on the existence of three regions in the flow field:

*Inner region*

In this region in a first order approximation it is taken:

$$\frac{\partial \theta}{\partial \tau} \simeq 0(\epsilon^2) \rightarrow 0; \quad \theta = \epsilon \quad (26)$$

for values of  $x$  of order one

### Outer region

In this region the characteristic time is of order  $1/\varepsilon$ , the temperature is of order one, and in times of order unity temperature and mass fractions reach stationary distributions.

Therefore, disregarding the non-stationary terms and taking  $\alpha(\theta)$  equal to unity, it is obtained in this region:

$$\theta = \frac{A_1}{x} + B_1 \quad (\text{inside the flame}) \quad (27)$$

$$\frac{\theta}{A_2} - \frac{K(t)}{A_2^2} \ln(K - A_2\theta) = \frac{1}{x} + B_2 \quad (\text{outside the flame}) \quad (28)$$

in which  $A_1 A_2 B_1$  and  $B_2$  are integration constants.

### Transition region

In this region the stationary and non-stationary terms are of the same order. By introducing the non-dimensional variables:

$$z = \frac{x - x_s(\tau)}{\mu(\varepsilon)}; \quad \mu(\varepsilon) \ll 1 \quad (29)$$

$$\tau_1 = \mu_1(\varepsilon) \tau; \quad \mu_1(\varepsilon) \ll 1 \quad (30)$$

$$\theta_1 = \frac{\theta}{\varepsilon} \quad (31)$$

the problem reduces to the solution of equation:

$$\frac{dx_s}{d\tau_1} \frac{1}{\theta_1^2} \frac{\partial \theta_1}{\partial z} = \frac{\partial^2 \theta_1}{\partial z^2} \quad (32)$$

which may be integrated, resulting:

$$(\theta_1 - 1) + \ln(\theta_1 - 1) = - \left( \frac{dx_s}{d\tau_1} \right) z + B \quad (33)$$

where  $B$  is an integration constant:

By matching solutions and utilizing boundary conditions and conditions at the flame front, the values of the integration constants and functions  $\mu(\varepsilon)$  and  $\mu_1(\varepsilon)$  are obtained, as well as solutions of  $\theta$  in terms of  $\tau$  and  $x$ .

The most important final results are the values of the combustion or extinction time  $\tau_{\text{ext}}$  and the flame to droplet radius ratio. They are given by the explicit expressions:

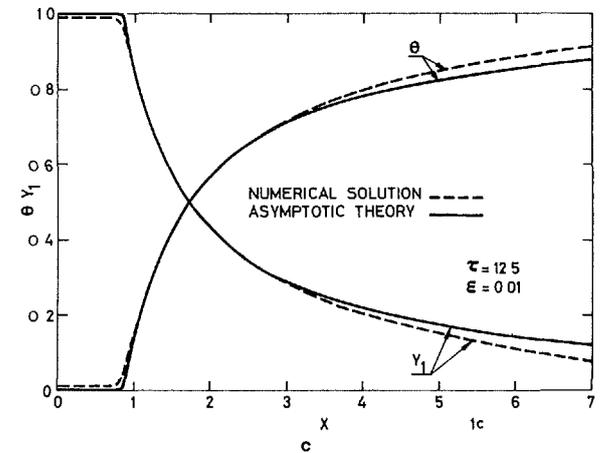
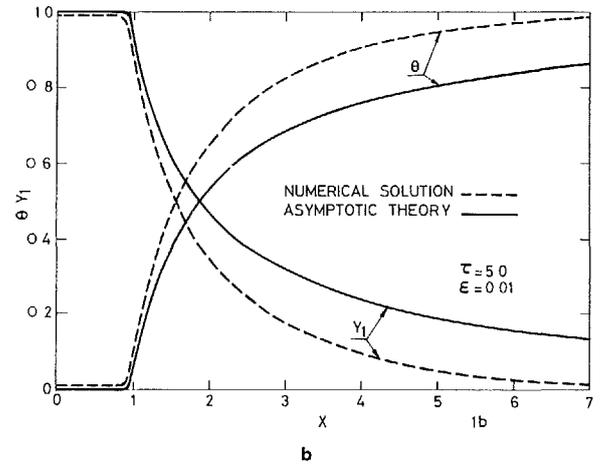
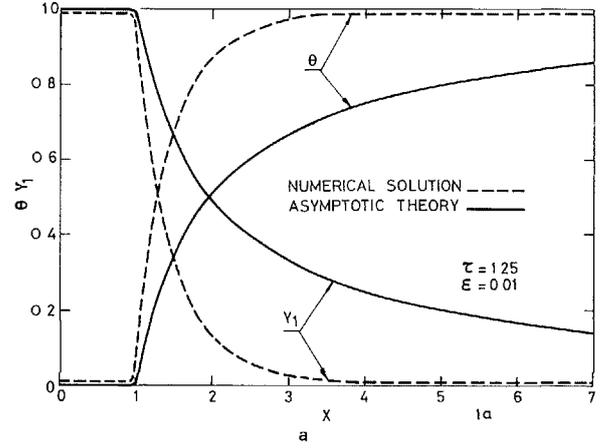


FIG. 1. a, b, c. Temperature and mass fraction profiles at different times. No combustion.

$$\tau_{\text{ext}} = \frac{1}{2\varepsilon \left[ 1 + \frac{q_r}{c_p T_\infty} \ln \left( 1 + \frac{Y_{2\infty}}{v} \right) \right]} \quad (34)$$

$$\frac{x_f}{x_s} = \frac{\left(1 + \frac{Y_{2\infty}}{\nu}\right) \left[ \frac{q_r}{c_p T_\infty} \ln \left(1 + \frac{Y_{2\infty}}{\nu}\right) + 1 \right]}{\frac{q_r}{c_p T_\infty} \ln \left(1 + \frac{Y_{2\infty}}{\nu}\right) \left(1 + \frac{Y_{2\infty}}{\nu}\right) + \left(1 - \frac{q_r}{c_p T_\infty}\right) \frac{Y_{2\infty}}{\nu}} \quad (35)$$

## 6. Results and Conclusions

Numerical results were restricted, for simplicity, to the case of no combustion, which is a vaporization process in subcritical conditions and that corresponds to a pure mixing process in supercritical conditions.

Some of the results obtained are shown in Figs. 1, 2 and 3, in which the corresponding analytical results are also, for comparison, included.

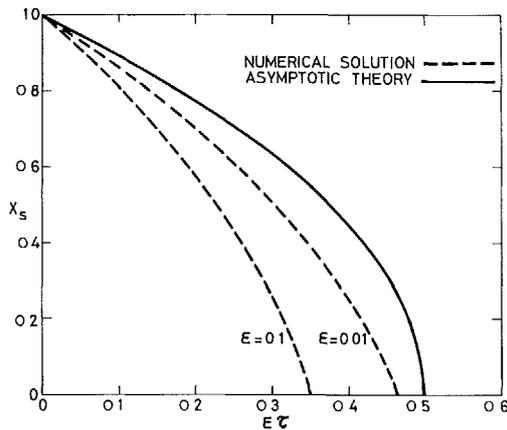


FIG. 2. Apparent droplet radius as function of time. No combustion.

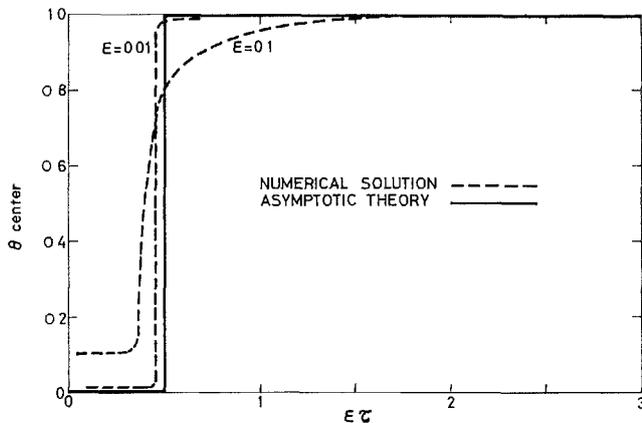


FIG. 3. Temperature at the center as function of time. No combustion.

The most interesting conclusion is that when the initial temperature of the droplet is small as compared with the temperature of the surrounding atmosphere ( $\epsilon \ll 1$ ) an apparent droplet exists throughout most of the process. (Figs. 1 and 2). This droplet practically keep its initial temperature and composition during the process and its surface is characterized by an abrupt change in the temperature and mass fraction profiles. This result is physically explained by the strong dependency of the transport coefficients on temperature.

Figs. 1 and 2 also show that when  $\epsilon$  is small the analytical and numerical solution practically coincide.

Results for the combustion case were analytically obtained.

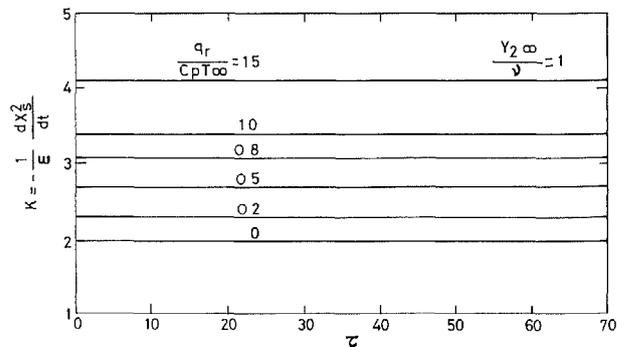
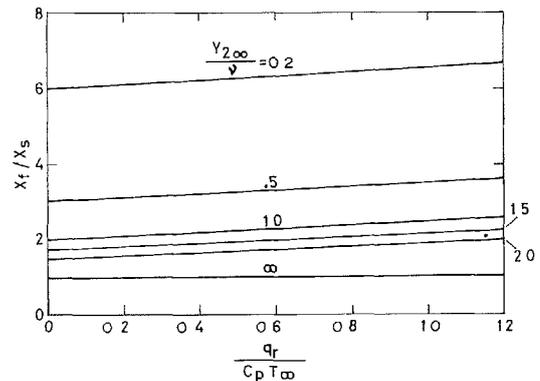


FIG. 4. Combustion case. Asymptotic theory. 4a Flame to droplet radius ratio. 4b Combustion rate constant

An interesting conclusion is that, when referred to the apparent droplet radius, burning rate defined as:

$$k = \frac{r_0^2}{t_{\text{ext}}} = -\frac{dr^2}{dt} \quad (36)$$

does not depend on time as occurs in subcritical conditions.

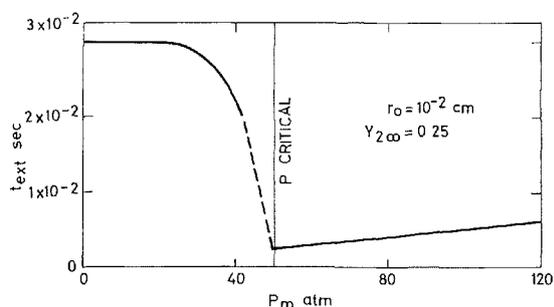


FIG. 5. Droplet lifetime for supercritical combustion of  $O_2$  droplets in  $H_2$ . Constant initial pocket radius.

The ratio of the flame radius to the droplet radius is also constant, but the rapid initial transient conditions in which the flame radius grows until it reaches the quasi-stationary value given by (35) is not considered in our asymptotic treatment. Values of burning rates and ratio of flame radius to droplet radius are shown in Fig. 4.

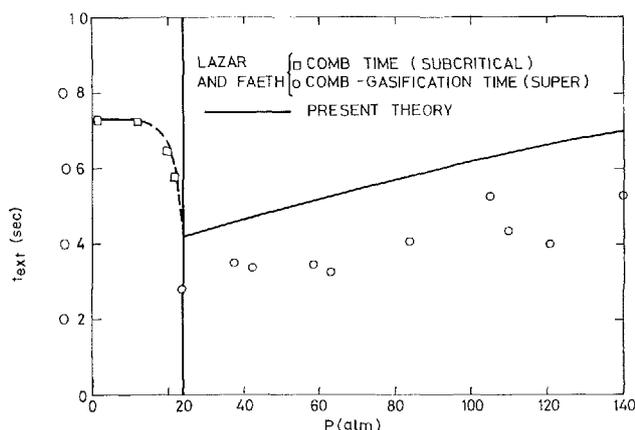


FIG. 6. Droplet lifetime for supercritical combustion of  $n$ -Decane in air. Constant initial mass of fuel equivalent to a liquid droplet of  $875 \mu$ . Comparison with experimental results

A droplet burns faster in supercritical condition as compared with a droplet of equal initial radius at subcritical conditions, with the minimum burning time occurring at critical conditions. However, if

two droplets, of equal initial mass are compared, supercritical combustion may be faster or not than subcritical combustion depending on the values of the physical variables of the process.

These conclusions are shown in Figs. 5 and 6 in which numerical applications corresponding to the case of oxygen droplets burning in hydrogen and decane droplets burning in air are shown. In Fig. 6 experimental results obtained by Faeth [10] are also shown. It may be pointed out that an excellent qualitative agreement exists between these experimental results and those analytically obtained.

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**Résumé—Un modèle théorique pour la combustion de gouttes dans des conditions super critiques et dans des des poches gazeuses.** La combustion supercritique de gouttes est étudiée grâce à un modèle physique qui suppose une symétrie sphérique, des conditions laminaires, une pression constante et une flamme d'épaisseur nulle.

Les conditions limite à l'infini énoncent que la température et la composition du mélange sont données et constantes.

Les distributions initiales de température et de fractions de masse des espèces sont données, comme le sont aussi les conditions initiales à la surface de la goutte. A mesure que la combustion se fait, la surface de la goutte n'est pas considérée exister en tant que limite physique permettant une diffusion non restreinte des espèces par elle.

Avec quelques simplifications supplémentaires pour la densité et les coefficients de transport, une solution numérique du problème est obtenu.

Une solution analytique du problème est également obtenu par analyse asymptotique. Cette solution s'applique lorsque la température initiale de la goutte est faible par rapport à la température de l'atmosphère environnante. Il est montré que c'est le cas le plus important du point de vue technologique.

Pour ce cas, les résultats montrent qu'une goutte apparente existe durant tout le processus, et dans laquelle sa surface est caractérisée par un changement soudain de température et de composition de l'espèce chimique.

Les résultats montrent les taux de combustion, les temps de combustion, le rayon de la flamme et sa température au centre de la goutte en fonction des variables principales du processus. En particulier, le carré du rayon de la goutte apparente est une fonction linéaire du temps comme dans une combustion subcritique.

Il est montré que les temps de combustion sont plus courts dans des conditions super critiques que dans des conditions subcritiques avec une valeur minimale aux conditions critiques.

Une application numérique est menée pour le cas de gouttes d'oxygène brûlant dans de l'hydrogène et l'on compare les résultats théoriques, numériques et analytiques, et aussi expérimentaux.

#### **Резюме—Теоретическая Модель Горения Капель в Сверхкритических Условиях и с Учетом Догорания.**

Сверхкритическое горение капелек исследуется с помощью физической модели, которая предполагает сферическую симметрию, ламинарность течения, постоянство давления и нулевую толщину фронта пламени. Граничными условиями на бесконечности являются заданные температура и состав смеси, которые считаются постоянными.

Начальное распределение температуры, концентрации компонент и начальные условия у поверхности капелек также заданы. В процессе протекания горения поверхность капелек не считается существующей в виде физической границы, допуская неограниченную скорость диффузии компонент. С некоторыми добавочными упрощениями для плотности и коэффициентов переноса задача решается численно. Получено также аналитическое решение проблемы при помощи методов асимптотического анализа. Это решение применимо, когда начальная температура капелек мала при сравнении с температурой окружающей среды. Указывается, что это самый важный случай с практической точки зрения.

Для этого случая из расчетов следует, что идеализированная капелек существует в течение почти всего процесса, в течении которого ее поверхность описывается моделью с разрывом изменения непрерывности температуры и состава компонент химической реакции.

Приводятся значения скорости горения, продолжительности сгорания, радиуса пламени и температуры в центре капелек в зависимости от основных переменных величин, участвующих в процессе. В частности, квадрат радиуса кажущейся капелек является линейной функцией времени, что характерно для субкритического горения.

Отмечается, что время горения при сверхкритических условиях меньше, чем при субкритических; минимальная величина соответствует критическим условиям. Приводятся численные примеры для случая капелек кислорода, горящих в водороде, и проводится сравнение между теоретическими результатами, полученными как численно, так и аналитически — с опытными данными.