

BURNING TIME OF A SPRAY OF LIQUID DROPLETS WITH UNIFORM INITIAL DIAMETER. AN ELEMENTAL AND PEDAGOGICAL APPROACH.

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***Abstract.** An adaptation of the classical model of single droplet is proposed to obtain a simple model for the combustion of clouds of liquid droplets. The main objective is not the development of a rigorous model to simulate all the physical and chemical phenomena competing in the control of this combustion phenomena but rather to give the students a simple tool to enable them to reach a quick understanding of the importance of the effects involved in the reaction.*

***Keywords.** droplet combustion, liquid spray combustion.*

1. Introduction

Models for single droplet evaporation and burning are commonly represented in many combustion textbooks. They all rely on the initial development by Spalding in 1953 (Williams, 1976; Glassman, 1977; Kanury, 1979; Spalding, 1979; Kuo, 1986; Turns, 1996; Borman and Ragland, 1998) and give the students a thorough insight on the important physical parameters conditioning such important evaporation and combustion mechanism.

A step further should try, in a simple way, to present the students an analysis of group combustion of droplets, including some effects dependent upon the reactor model being adopted. Models for group droplet combustion show how complex these phenomena are, and how difficult is to explain in a simple way, the important mechanisms and their effects upon the overall reaction rate. These studies are usually oriented towards the solution of practical situations, for the simulation of heat release and pollutants formation rates and involve such a large number of variables, Chiu and Chigier (1995), and heterosized sprays (Williams, 1976), that normal graduate students will have enormous difficulties to follow and accept them.

In this work a simple approach for the combustion of a spray of liquid droplets is proposed; it is based on the application of the single droplet evaporation and combustion rate to two basic furnace configurations, the well stirred reactor and the isothermal plug flow reactor. This approach is rather questionable, as there is no empirical justification for researchers and designers to use results from single droplet studies and burning tests to make reliable predictions in spray flames, Chigier (1979). The objective here is only pedagogical. To arrive at such simple analytical treatment some simplifications were carried out, but the overall results may lead the students to a stronger comprehension of the main parameters controlling the group combustion of liquid droplets.

The simplest single droplet evaporation and combustion model considers spherically symmetrical burning in a stagnant medium, there is no relative velocity between the droplet and the free stream as well as no buoyancy, i.e., there are no convection effects, Faeth (1979). It is also assumed that droplets are of single component fuel and that interaction between closely spaced droplets is ignored, in other words, the spray is considered to be diluted and droplet breaking phenomena is ignored. For larger droplets the assumption of the above conditions as a simplified approach for real combustion may also be subject of criticism. However, this approximation will make the analysis straightforward and coherent with the desire for simplicity.

2. Well stirred furnace

The simplest furnace model is the well stirred reactor in which perfect mixing is achieved inside the control volume, Turns (1996). It is assumed that the spray droplet combustion will take place in a reactor where average temperature as well as reactants concentration are known. The mass flow rate of air is also known. In practical terms a good example of batch combustion of sprays is the Diesel engine combustion; in industrial systems other situations like this are not very common, spray combustion is mainly a steady state phenomenon, Williams (1976).

The basic assumptions for the model to be developed are the following:

- The furnace gas is at an average temperature T_{∞} during the combustion process;

- The oxygen mass concentration, $Y_{O_{\infty}}$, is known and assumed uniform inside the furnace, although changing with the evolution of the combustion process;
- The furnace is assumed a well stirred reactor, and the output burned gas composition is the same as in the furnace interior.

In the following development it is intended to arrive at an expression for the combustion of a spray of uniformly sized droplets. Some mathematical simplifications will have to be done in order to allow further analytical treatment of the model equations. Henceforth the development is based upon the combustion rate equation of a single droplet of diameter d as given by Kanury (1977),

$$\dot{M}_w = \frac{2 \alpha_{tg} \rho_g}{d} \ln (B + 1) \quad (1)$$

where,

$$B = \frac{[-\Delta h] f Y_{O_{\infty}} + c_{pg} (T_{\infty} - T_B)}{h_{LV} + c_L (T_B - T_R)} \quad (2)$$

is the mass transfer number (Kanury, 1977) or Spalding number (Turns, 1997), whereas the complete combustion time of such isolated droplet of initial diameter d_i will be given by,

$$t_b = \frac{d_i^2}{\frac{8 \rho_g \alpha_{tg}}{\rho_L} \ln (B + 1)} \quad (3)$$

In the previous equations f is the stoichiometric fuel/oxygen ratio (Kanury, 1977), c_L , h_{LV} , Δh are respectively the specific heat, the latent heat of vaporization and the entalpy of combustion for the droplet liquid, whereas α_{tg} , c_{pg} and ρ_g are respectively the thermal difusivity, the constant pressure specific heat and the density of the gas phase around the droplet. T_{∞} is the average furnace temperature, T_R and T_B are the droplet temperature and the boiling temperature of the droplet liquid.

But the objective is the evaluation of the combustion of a cloud or spray of droplets. For each droplet belonging to the spray its mass reduction with the time is a function of the combustion rate,

$$-\rho_L \frac{\pi d^2}{2} \frac{d(d)}{dt} = \dot{M}_w \pi d^2 \quad (4)$$

This equation is the same whether or not the droplet is isolated or belonging to a cloud of droplets, i.e. no restrictions concerning its environment were imposed. The combination of Eqs. (1) and (4) gives,

$$\frac{d(d)}{dt} = -\frac{4 \rho_g \alpha_{tg}}{\rho_L d} \ln (B + 1) \quad (5)$$

An oxygen mass balance of the furnace must now be done. The difference in oxygen mass flow rates between the furnace entrance ($U_i A_i \rho_{O_i}$) and exit ($U_e A_e \rho_{O_{\infty}}$), is the oxygen that was consumed in the combustion reaction by the N_d droplets composing the spray, and then,

$$U_i A_i \rho_{O_i} - U_e A_e \rho_{O_{\infty}} = N_d \left[-\frac{d}{dt} \left(\frac{\rho_L \pi d^3}{6} \right) \right] \quad (6)$$

This number of droplets in the spray is a function of the total mass, and can be obtained through the initial mass of the spray, m_c , and uniform droplet initial diameter,

$$N_d = \frac{m_c}{\rho_L \frac{\pi d_i^3}{6}} \quad (7)$$

Introducing this definition of droplet number into Eq. (6) and derivating it in order of time,

$$U_i A_i \rho_{O_i} - U_e A_e \rho_{O_\infty} = -\frac{3 m_c d^2}{f d_i^3} \frac{d(d)}{dt} \quad (8)$$

The mass balance for a single droplet of the cloud, Eq. (5) as well as the overall oxygen mass balance for the reactor, inside which the cloud is being consumed, Eq. (8) must be coupled together. The transfer number B which is a function of the oxygen concentration inside the furnace is also known. The solution of these two differential equations depends on the solution of Eq. (5) in order to Y_{O_∞} , using Eq. (2) and introducing the result into Eq. (8). A single differential equation could then be obtained and its integration would give the required spray burning time. There is however no possibility to get a simple analytical expression for Y_{O_∞} from Eq. (2), unless an approximation is used.

As the range of B values for the combustion of various liquids in air is in a very limited interval [3; 9] (Glassman, 1977; Kanury, 1977 and Kuo, 1986), the following approach is suggested,

$$\begin{aligned} \ln \left(\frac{[-\Delta h] f Y_{O_\infty} + c_{pg}(T_\infty - T_B)}{h_{LV} + c_l(T_B - T_R)} + 1 \right) &= \\ = \ln \left[\frac{c_{pg}(T_\infty - T_B)}{[h_{LV} + c_l(T_B - T_R)]} + 1 \right] &+ \frac{[-\Delta h] f Y_{O_\infty}}{[h_{LV} + c_l(T_B - T_R)] \left[\frac{c_{pg}(T_\infty - T_B)}{[h_{LV} + c_l(T_B - T_R)]} + 1 \right]} \end{aligned} \quad (9)$$

In many real situations the sensible heat term is smaller than the latent heat term, $[h_{LV} + c_l(T_B - T_R)] \approx h_{LV}$. For the sake of simplicity a function $J(T)$ can be defined such as

$$J(T) = \frac{c_{pg}(T_\infty - T_B)}{h_{LV}} + 1 \quad (10)$$

and then,

$$\ln \left(\frac{[-\Delta h] f Y_{O_\infty} + c_{pg}(T_\infty - T_B)}{h_{LV} + c_l(T_B - T_R)} + 1 \right) = \ln [J(T)] + \frac{[-\Delta h] f Y_{O_\infty}}{h_{LV} J(T)} \quad (11)$$

From the droplet mass balance,

$$\frac{d(d)}{dt} = -\frac{4 \rho_g \alpha_{tg}}{\rho_L d} \ln [J(T)] - \frac{4 \rho_g \alpha_{tg}}{\rho_L d} \frac{[-\Delta h] f Y_{O_\infty}}{h_{LV} [J(T)]} \quad (12)$$

which is solved in order of Y_{O_∞} ,

$$Y_{O_\infty} = \frac{h_{LV} [J(T)]}{[-\Delta h] f} \ln [J(T)] - \frac{\rho_L h_{LV} [J(T)]}{4 \rho_g \alpha_{tg} [-\Delta h] f} d \frac{d(d)}{dt} \quad (13)$$

Introducing this last result into Eq. (8) and considering that $\rho_O = \rho_g Y_O$, the final differential equation is,

$$\left[\frac{U_e A_e \rho_L h_{LV} [J(T)] d}{4 \alpha_{tg} [-\Delta h] f} + \frac{3 m_c d^2}{f d_i^3} \right] d(d) = \left\{ -U_i A_i \rho_g Y_{O_i} + \frac{U_e A_e \rho_g h_{LV} [J(T)] \ln [J(T)]}{[-\Delta h] f} \right\} dt \quad (14)$$

which can then be integrated between the following limits,

$$\begin{aligned} t = 0 & & d = d_i \\ t = t_\phi & & d = (1 - \phi)^{1/3} d_i \end{aligned}$$

where φ is the burned mass fraction and t_φ is the corresponding burning time. The result is then,

$$t_\varphi = \frac{[J(T)]U_e A_e \rho_L h_{LV} d_i^2 \left[1 - (1 - \varphi)^{2/3}\right] + 8 \alpha_{ig} [-\Delta h] m_c \varphi}{8 \rho_g \alpha_{ig} [-\Delta h] f U_i A_i Y_{oi} + 8 \rho_g \alpha_{ig} U_e A_e h_{LV} [J(T)] \ln [J(T)]} \quad (15)$$

The first term of the numerator accounts for the effect of the diffusion control on the combustion time, while the second term of the numerator accounts for the effect of the assumed furnace model, in this case a well stirred reactor.

In the real situation, droplets compete among themselves for the available oxygen and the droplet combustion is a group phenomena, not an individual process, as could be considered from the extrapolation of the single droplet combustion equations to group combustion. To account for the interdroplet combustion a simple approach can be adopted, by affecting the reaction zone oxygen concentration with a multiplying correcting factor η (Annamalai, 1995). Another approach considers that usually the furnace is a perfectly stirred reactor, but not a well stirred reactor (Hottel, 1961), and a bypass factor $0 \leq \chi \leq 1$ can be applied to the oxygen concentration, to account for a less perfect comburent access to the reaction zone. Finally, a reasonable simplification for the furnace flow will be to assume that $U_i A_i \approx U_e A_e \approx U_f A_f$, such that the burning time for the mass fraction φ will then be,

$$t_\varphi = \frac{[J(T)]U_f A_f \rho_L h_{LV} d_i^2 \left[1 - (1 - \varphi)^{2/3}\right] + 8 \alpha_{ig} [-\Delta h] m_c \varphi}{8 \rho_g \alpha_{ig} [-\Delta h] f U_f A_f \eta (1 - \chi) Y_{oi} + 8 \rho_g \alpha_{ig} U_f A_f h_{LV} [J(T)] \ln [J(T)]} \quad (16)$$

The above equation is simple to use but the error that is obtained with the suggested approach has to be quantified. The easiest way to do it will be to compare the burning time of a single droplet equation according to the basic theory, (Kanury, 1977), Eq. (17),

$$t_{b\varphi} = \frac{\left[1 - (1 - \varphi)^{2/3}\right] d_i^2}{\frac{8 \rho_g \alpha_{ig}}{\rho_L} \ln (B + 1)} \quad (17)$$

with the burning time obtained through the approximation suggested by Eq. (9),

$$t_{a\varphi} = \frac{\left[1 - (1 - \varphi)^{2/3}\right] d_i^2}{\frac{8 \rho_g \alpha_{ig}}{\rho_L} \left[\ln J + \frac{[-\Delta h] f Y_{O_\infty}}{h_{lv} J} \right]} \quad (18)$$

3. Isothermal plug flow furnace

The objective of the next analysis is to develop a simple expression for the approximate furnace length, when there is continuous combustion of a spray of liquid droplets in a one-dimensional furnace. The furnace is characterized by having an isothermal plug flow, i.e., for a given cross section of the furnace, the reactant mixture properties will remain constant and there will only be changes in the longitudinal direction. For the sake of simplicity of analysis there are other conditions inside the furnace that will not follow the plug flow conditions; besides the assumption of constant temperature, gas phase density and pressure inside the furnace are also considered. The furnace is composed by a series of elemental control volumes and each elemental control volume can be considered a small well-stirred reactor, inside of which the mass fraction of oxygen is constant and equal to Y_{O_∞} . For this generic elemental volume, analogously to what was developed in the well-stirred furnace, Eq. (12) also applies for a single droplet. On the other end, the mass balance for the elemental volume follows a development similar to that adopted for the well-stirred reactor,

$$U_f A_f \rho_g (Y_{O_\infty})_x - U_f A_f \rho_g (Y_{O_\infty})_{x+dx} = -\frac{3 \dot{m}_{cx} d^2}{f d_{ix}^3} d(d) \quad (19)$$

and as the number of liquid droplets per unit time can be related to the mass flow rate of introduced liquid fuel (\dot{m}_c or \dot{m}_{cx} for an elemental volume at distance x from the entrance), as well as to their initial diameter (d_i or d_{ix}),

$$\dot{m}_{cx} = \frac{\dot{N}_g \rho_L \pi d_{ix}^3}{6} \quad (20)$$

the volume element mass balance of oxygen is finally,

$$dY_{o\infty} = \frac{\dot{N}_d \rho_L \pi}{2 f U_f A_f \rho_g} d^2 d(d) \quad (21)$$

Equation (21) can be integrated to obtain an equation for the evolution of the oxygen concentration along the furnace assuming constant overall properties for the gaseous phase

$$\int_{Y_{oi}}^{Y_{o\infty}} dY_{o\infty} = \frac{\dot{N}_d \rho_L \pi}{2 f U_f A_f \rho_g} \int_{d_i}^d d^2 d(d) \quad (22)$$

Using the definition of \dot{N}_d the result is,

$$Y_{o\infty} = Y_{oi} + \frac{\dot{m}_c}{f U_f A_f \rho_g} \left[\left(\frac{d}{d_i} \right)^3 - 1 \right] \quad (23)$$

This last equation, showing the dependence of the oxygen concentration throughout the furnace on the liquid fuel mass flow rate and size, is now introduced in the droplet mass balance, Eq. (12) resulting on,

$$dt = - \frac{\rho_L h_{LV} U_f A_f d_i^3}{4 \alpha_{ig} [-\Delta h]} \frac{d}{f U_f A_f \rho_g Y_{oi} d_i^3 + \dot{m}_c (d^3 - d_i^3)} d(d) \quad (24)$$

which can be integrated to give the combustion time for fraction φ ,

$$t_\varphi = \frac{\rho_L h_{LV} U_f A_f d_i^3}{24 \alpha_{ig} [-\Delta h] \alpha^{1/3} \dot{m}_c^{2/3}} \left\{ 2\sqrt{3} \left[\arctg \left(\frac{2 \dot{m}_c^{1/3} d_i}{\sqrt{3} \alpha^{1/3}} - \frac{1}{\sqrt{3}} \right) - \arctg \left(\frac{2 \dot{m}_c^{1/3} (1-\varphi)^{1/3} d_i}{\sqrt{3} \alpha^{1/3}} - \frac{1}{\sqrt{3}} \right) \right] + \ln \left[\frac{(\alpha^{1/3} - \dot{m}_c^{1/3} d_i) + \alpha^{1/3} \dot{m}_c^{1/3} d_i}{(\alpha^{1/3} - \dot{m}_c^{1/3} d_i (1-\varphi)^{1/3})^2 + \alpha^{1/3} \dot{m}_c^{1/3} d_i (1-\varphi)^{1/3}} \frac{(\alpha^{1/3} + \dot{m}_c^{1/3} d_i (1-\varphi)^{1/3})^2}{(\alpha^{1/3} + \dot{m}_c^{1/3} d_i)^2} \right] \right\} \quad (25)$$

where $\alpha = (f U_f A_f \rho_g Y_{oi} - \dot{m}_c) d_i^3$.

Once again, the inter-droplet competition for the available oxygen, may be accounted for. If the inter-particle competition is to be considered, then α is slightly different because of the oxygen mass fraction correction factor η , must be introduced,

$$\alpha = (f U_f A_f \rho_g \eta Y_{oi} - \dot{m}_c) d_i^3 \quad (26)$$

Admitting that, $t_b = L_f / U_f \Rightarrow L_f = t_b U_f$, the furnace length is calculated through,

$$L_f = \frac{\rho_L h_{LV} U_f^2 A_f d_i^3}{24 \alpha_{ig} [-\Delta h] \alpha^{1/3} \dot{m}_c^{2/3}} \left\{ 2\sqrt{3} \left[\arctg \left(\frac{2 \dot{m}_c^{1/3} d_i}{\sqrt{3} \alpha^{1/3}} - \frac{1}{\sqrt{3}} \right) - \arctg \left(-\frac{1}{\sqrt{3}} \right) \right] + \ln \left[\frac{(\alpha^{1/3} - \dot{m}_c^{1/3} d_i) + \alpha^{1/3} \dot{m}_c^{1/3} d_i}{(\alpha^{1/3} + \dot{m}_c^{1/3} d_i)^2} \right] \right\} \quad (27)$$

4. Results

Before presenting the results of this simplified approach it is convenient to quantify the errors inherent to the proposed development. The simplest way to do it will be through the comparison of the single droplet combustion time obtained from the approximated result vis a vis the result obtained with the conventional theory. As the basic principle intrinsic to the present analysis was to accept it on the grounds of a pedagogical approach, this evaluation methodology, although rather simplified, is adopted.

4.1. Single droplet burning

In the next figure burning times for a single droplet calculated with the correct Eq. (17) as well as with the approximated Eq. (18) are compared.

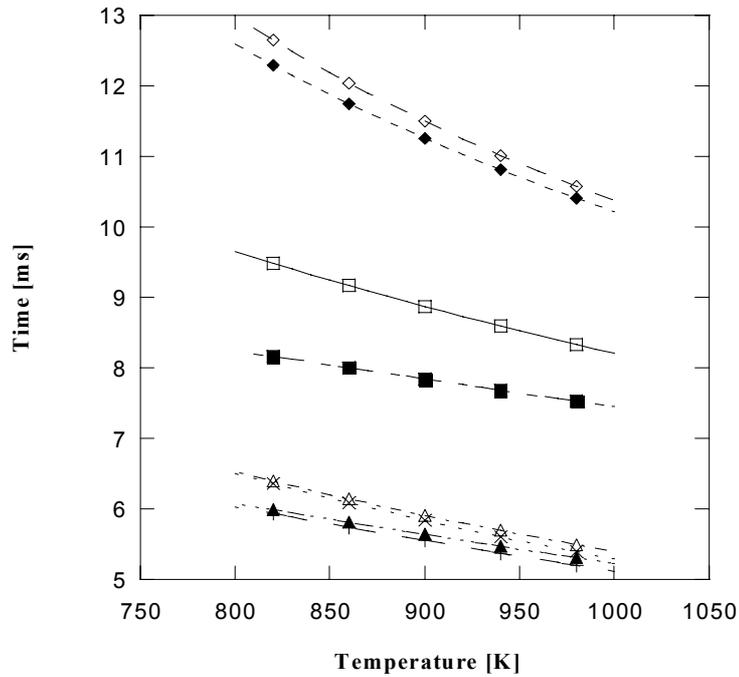


Figure 1. Burning time for single droplets calculated through the correct (\square Methanol, \diamond Ethanol, \times Octane, Δ Heptane) and the approach (\blacksquare Methanol, \blacklozenge Ethanol, \blacktimes Octane, \blacktriangle Heptane) equations. Initial droplet size $50 \mu\text{m}$ and $Y_{O_{\infty}} = 8\%$.

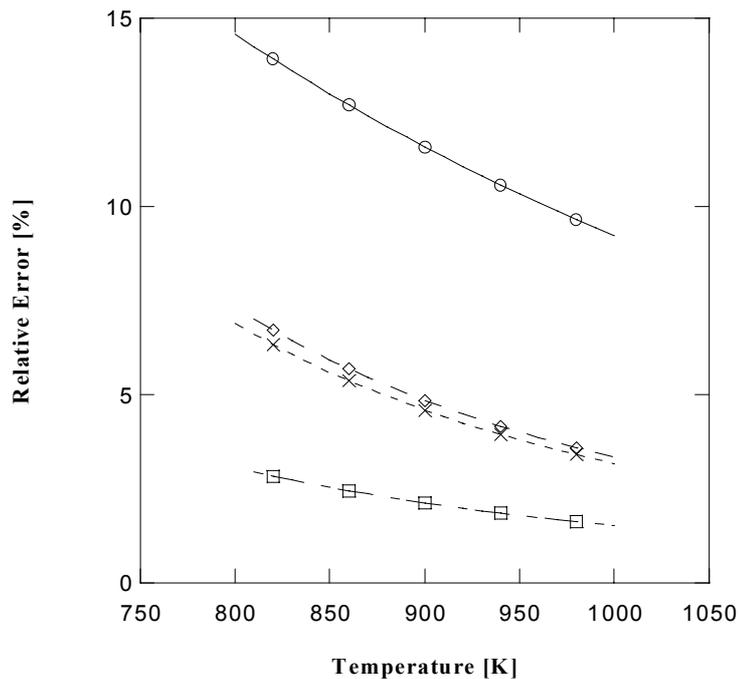


Figure 2 – Relative error in the calculation of the burning time of a single droplet (\circ Methanol, \square Ethanol, \diamond Octane, \times Heptane) using the approach versus the correct equation.

The relative errors of the results plotted in Fig. (1) are shown in Fig. (2). Here it is found that these errors are quite acceptable from an engineering point of view, although they concern exclusively single droplet combustion. They can however give a clue on the order of magnitude of expected deviations that will be obtained for the calculation of burning time of clouds of particles through the recommended approximations, either for well stirred or plug flow reactors.

4.2. Well stirred furnace

For the batch combustion of a cloud of 0.1 kg of 50 μm droplets results are shown in Fig. (3). Here it is shown the effect of the temperature as well as the type of fuel on the combustion time. Higher temperatures and lighter molecules allow a faster combustion.

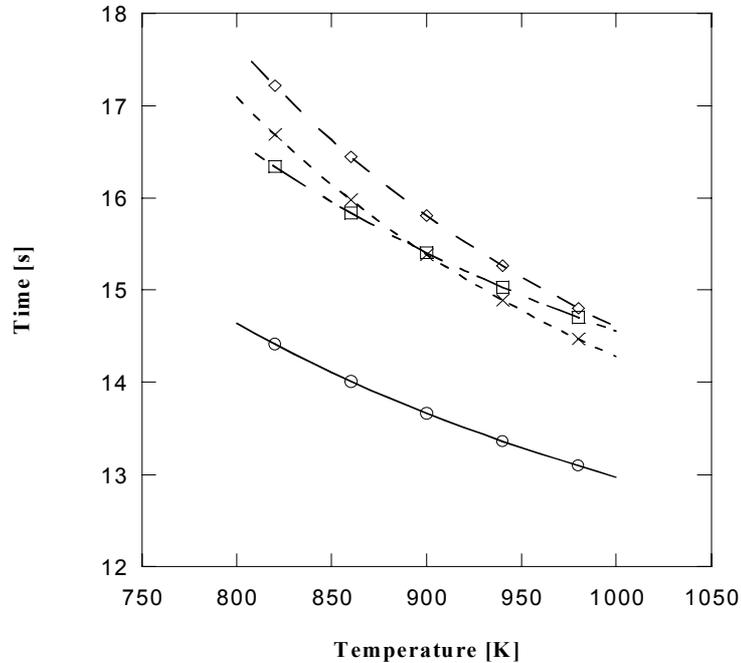


Figure 3 – Combustion time for clouds of 50 μm droplets. Batch size, 0.1 kg. Other conditions are, $Y_{O_{\infty}} = 8\%$, $\eta = 0.8$, $\chi = 0.3$, $\phi = 0.9$, $\dot{m}_{ar} = 0.5 \text{ kg/s}$ and $A_f = 2 \text{ m}^2$. (O Methanol, \square Ethanol, \diamond Octane, \times Heptane).

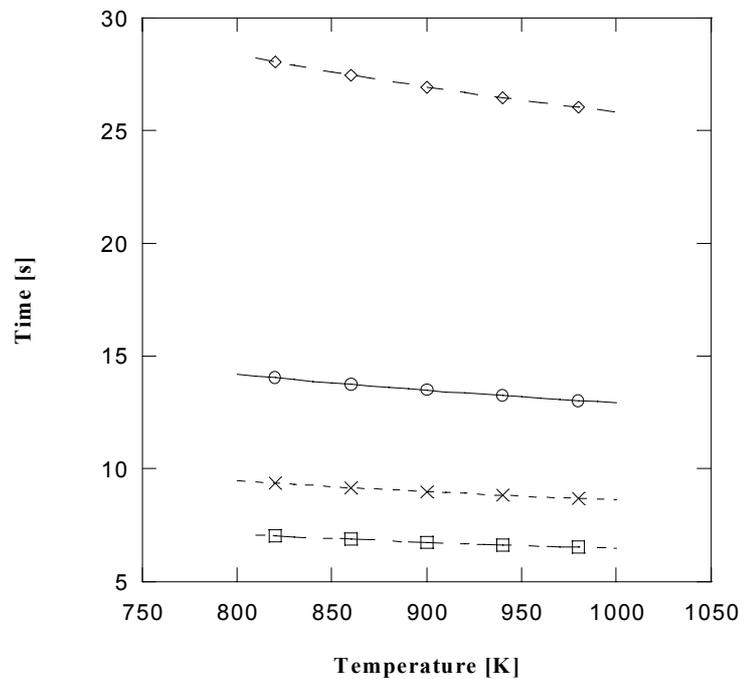


Figure 4 - Combustion time for clouds of 50 μm droplets of octane. The characteristics of the different situations are shown in Tab. (1).

Considering only one type of fuel Fig. (4) presents the influence of several physical parameters on the cloud burning time.

Table 1. Conditions for the situations shown in Fig. (4).

Symbol	$Y_{O_{\infty}}$ (%)	η (-)	χ (-)	ϕ (-)	\dot{m}_c (kg)	\dot{m}_{air} (kg/s)	A_f (m ²)
○	8	0.8	0.3	0.9	0.1	0.50	0.2
□	8	0.8	0.3	0.9	0.05	0.50	0.2
◇	8	0.8	0.3	0.9	0.1	0.25	0.2
×	8	0.8	0.3	0.6	0.1	0.50	0.2

The important parameters controlling the combustion are essentially the batch size and air flow rate available for combustion, i.e., the cloud behaves as an agglomerate and the individual characteristics of the droplets become hidden under the weight of the cloud. The extension of individual droplet burning model towards the full cloud situation gives a result well inside the expected experimental trends, Chiu and Chigier (1995), a collective phenomena resulting from inter-drop interactions.

4.3. Isothermal plug flow

Finally in Fig. (5) are shown the results of the furnace length calculations for steady state burning of several fuels and physical conditions as detailed in Tab. (2). The inter-droplet competition factor and the oxygen by-pass factor are identical to the values used in the previous figure, respectively $\eta = 0.8$ and $\chi = 0.3$, whereas the burned fraction was now $\phi = 0.8$. The furnace section area was maintained at 0.2 m².

Table 2. Conditions for the situations shown in Fig. (5).

Symbol	Fuel	\dot{m}_c (kg/s)	\dot{m}_{air} (kg/s)	d_i (μ m)
○	Methanol	0.05	5	50
□	Ethanol	0.05	5	50
◇	Octane	0.05	5	50
×	Heptane	0.05	5	50
+	Methanol	0.05	10	20
△	Ethanol	0.05	10	20
●	Octane	0.05	10	20
■	Heptane	0.05	10	20

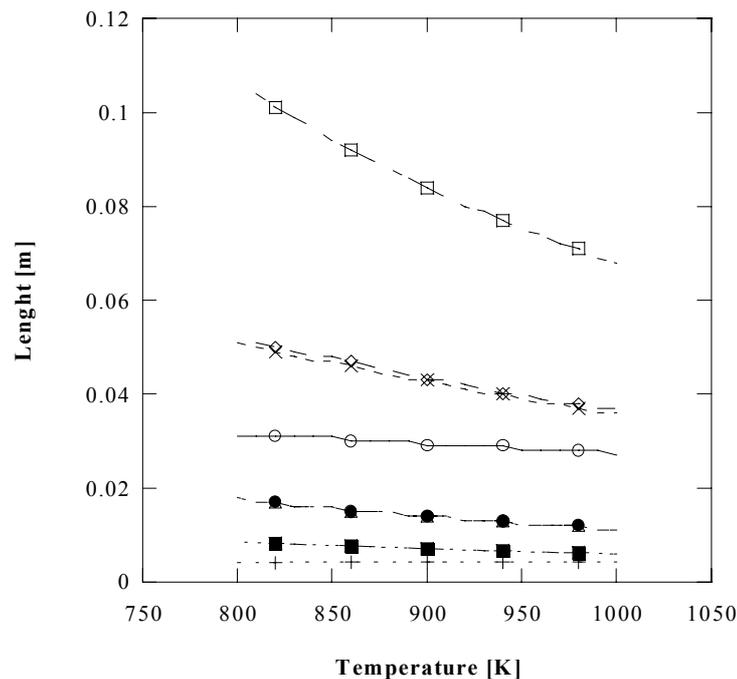


Figure 5 – Furnace length for 80 % combustion of several fuels. Conditions according to Tab. (2).

5. Conclusions

A simple adaptation of the classical single droplet burning equation was applied to cloud burning conditions. Well stirred and plug flow situations were considered. The main objective is to provide a quick pedagogical approach to a complex problem.

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