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Using a Simulation by 'Cellular Automata' as a help for Turbulent Combustion Modelling

R. BORGHI and R. SAID

Laboratoire de thermodynamique UA No. 230 CNRS Universite de Rouen, Mont-Saint-Aignan-France.

ABSTRACT

The modelling of turbulent combustion is a crucial problem for the numerical simulation of flames and combustion chambers. A crucial point, in this respect, is the relevance of u_L/u' (the laminar flame velocity divided by a characteristic turbulence velocity) as a parameter involved in the mean reaction rates $\overline{\dot{w}}$ and turbulent burning velocity u_T, for premixed flames of the type called "wrinkled". In order to get more insight on this problem a very simple numerical simulation, similar to a "cellular automaton" as introduced by Von Neuman forty years ago, has been imagined. Two situations have been investigated : in the case of the propagation of a turbulent flame the well known linear relation between u_T/u_L and u'/u_L is recovered ; in the case of the combustion in a statistically homogeneous medium, a law for $\overline{\dot{w}}$ is found, with u'/u_L explicitly occuring, which gives the Eddy break up formulation for $u'/u_L \gg 1$ and takes a form similar to the model ESCIMO of D.B. Spalding when $u'/u_L \ll 1$.

I - CRUCIAL PROBLEMS IN TURBULENT PREMIXED COMBUSTION MODELLING

I.1. The turbulent combustion in a premixed medium is a complicated phenomenon with multiple aspects. Within a laminar premixed flow, the combustion takes the form of a continuous flame front which moves with, respect to the flow itself with a usually well known velocity. In laminar perturbed flows, this flame front is curved and strained in a complex way and can be extinguished within certain circumstances : the detailed study of all phenomena appearing here is not completely performed, and comprises many difficulties (P. Clavin, 1985). In turbulent flows the flame fronts are continuously displaced, stretched, curved ; they are interacting between them ; they can be also extinguished at some place for some times. The important parameters, relevant to the study of the structure of turbulent premixed flames are : η/e_L (η is the Kolmogorov microscale of the turbulence, e_L the thickness of the laminar flame front), τ_t/τ_c (τ_t is an integral time scale of the turbulence, τ_c a global chemical time scale for the chemical reactions occuring within the flame), and u'/u_L (u' is a velocity scale of the turbulence, for instance the square rootof the turbulence kinetic energy, u_L the laminar flame velocity with respect to the fresh mixture). A detailed discussion on the structure of turbulent premixed flames can be found in Borghi (1985). Roughly speaking, one can distinguish between wrinkled turbulent flame when $\eta < e_L$, τ_c being much lower than τ_t, and non wrinkled (or thickened) turbulent flames when $\eta > e_L$ (τ_c being closer of, or higher than τ_t).

The prediction of the properties of turbulent flames needs basic informations concerning a "turbulent flame velocity", analogous to the laminar one (this is just a rough analogy), or better, concerning a mean volumetric combustion rate. Our present knowledge of the structure of premixed turbulent flames is not enough to lead to firm conclusions on these two quantities, even if we assume that the turbulence (that is the fluctuations of velocities) is perfectly known, and even in the simple limiting case of wrinkled flames.

I.2. The "turbulent flame velocity". Very old empirical relations concerning u_T, the "turbulent flame velocity", found : $u_T = u_L + c\,u'$, with $c \simeq 2$ (1) (Damköhler, 1940, Schelkin, 1968). More recent experiments lead to a similar dependance, but with c function of the turbulence Reynolds number R_t (R.G. Abdel, 1984), with a wide scatter, however. A theoretical study of Clavin and Williams (Clavin, 1979) leads to a quadratic dependance, in the limit $u'/u_L \ll 1$:

$$u_T/u_L = 1 + \alpha (u'/u_L)^2 \qquad (2)$$

with no dependance of the scale in α. A recent numerical simulation by Ashurst and Barr (W.T. Ashurst, 1983) agrees with the linear dependance on u' and the dependance on R_t, but the right value of c is not clear.

It is very clear that if the turbulence intensity is very large ($u'/u_L \gg 1$), if the Damköhler number τ_t/τ_c is infinite (the reactions are very fast with respect to the turbulence), and if the turbulence Reynolds number $R_T = u' l_t/\nu$ (where l_t is the spatial integral scale of the turbulence and ν the viscosity) is very large, as usualy stated, a simple dimensional reasoning lead to : $u_T = \beta u'$, with $\beta = c^{3/4}$ (3)
On the other hand, if we use the dimensional estimation of $u_L \propto (\nu/\tau_c)^{1/2}$ (with Schmidt and Lewis number close to unity), we obtain $R_T = (u'/u_L)^2 \tau_t/\tau_c$ (4)
One can remark then that very large values of both R_T and τ_t/τ_c can coexist with finite values of u'/u_L ; in such a case, a formula where β in (3) is a function of u'/u_L is expected, without appearence of the scale l_t, because $R_T \gg 1$: the formula (1), with c constant, or (2) could be such a formula. A contrary, if R_T is finite, that imply that both u'/u_L and τ_t/τ_c are finite (excluding the case where one of them is zero, which is not interesting) ; in such a case β in (3) can depend on R_T and τ_t/τ_c, or equivalently through (4) on R_T and u'/u_L, leading perhaps to a formula like (1) with c depending on R_T. Taking into account such a discussion, formulas (1) or (2) cannot be contradictory. In addition, in the case where τ_t/τ_c is finite but $u'/u_L \gg 1$, the relation (4) shows that $R_T \gg 1$ is implied and we could expect a formula in the form $u_T/u' = f(\tau_t/\tau_c)$ (5)
Such a relation is numerically obtained by a presumed pdf method, for instance the one used in (R. Borghi, 1986). The particular simulation that we shall describe later will be devoted to the particular case $\tau_t/\tau_c \gg 1$ and u'/u_L finite : it will be interesting to compare the relations (1) or (2) with the simulations.

I.3. The "mean reaction rate". More interesting for numerical simulations is the mean volumetric combustion rate in a turbulent medium. By definition, the volumetric combustion rate is the mass of products given by unit of time and volume by the chemical reactions (a similar rate can also be defined for the temperature or the mass of reactants). In the case of a laminar flow, this rate is just given by the chemistry, as a function of temperature and concentrations (for instance with Arrhenius laws) ; in the case of a turbulent flow, the mean combustion rate is the average value of the previous one, taking into account the random fluctuations of temperature and concentra-

tions. Due to the strong non linearity of the chemical rates, the mean value is completely different from the value computed with the mean concentrations and temperature ; and the first studies on this phenomenon lead to the prevision that, in case of very fast chemistry, $\tau_t/\tau_c \gg 1$, the mean combustion rate would be controlled only by the turbulent fluctuations. That prevision has been demonstrated recently by Bray and Moss (K.N.C. Bray, 1980) for a premixed turbulent flame, and by Bilger (Bilger, 1980) for a diffusion flame.

In fact, the demonstration is only partial in the case of premixed flames. One find that $\bar{\dot{w}}$ is proportional to the destruction rate of the fluctuations of a combustion degree :

$$\bar{\dot{w}} \propto \overline{D\, \partial c'/\partial x_k \cdot \partial c'/\partial x_k} \qquad (6)$$

(C, the combustion degree, is zero in the fresh mixture and 1 in the burnt gases, and D is the diffusivity coefficient for C, probably close to ν).
Using now a classical closure relation in turbulent non reacting flows, it comes that :

$$\bar{\dot{w}} \propto \bar{\rho}\, \widetilde{c''^2}/\tau_t = \bar{\rho}\, \tilde{c}(1-\tilde{c})/\tau_t \qquad (7)$$

where $\tilde{c} = \overline{\rho c}/\bar{\rho}$ and $\widetilde{c''^2} = \tilde{c}(1-\tilde{c})$
is due to the fact, if $\tau_t/\tau_c \gg 1$ and $R_T \gg 1$, only perfectly burnt gases, C=1, or perfectly fresh gases, C=0, can be found in the reacting medium.

But other closure relations could be used, arguing that the random fluctuations of C are here "reacting fluctuations" ; instead of τ_t , depending only on the turbulence, one could imagine that u'/u_L has to take place here. The formula (7) is, in fact, used in many turbulent combustion model (R. Borghi, 1986, D.B. Spalding, 1971), but other formulas have been proposed. In (P.A. Libby, 1980), for instance, Libby and Bray obtain :

$$\bar{\dot{w}} \propto \bar{\rho}\, \tilde{c}(1-\tilde{c})\, u_L/\ell_t \qquad (8)$$

where ℓ_t is an integral length scale of the turbulence.

Similarly, D.B. Spalding, who has been the inventor of a formula equivalent to (7) , called the Eddy Break up model, studied recently another model, ESCIMO (D.B. Spalding, 1978) ; a simplified version of it led to the simple formula

$$\bar{\dot{w}} \propto \bar{\rho}\, \left((1-\tilde{c})/\tau_t - u_L/\lambda_0\right) \qquad (9)$$

where λ_0 is particular length scale of the turbulence, not well defined. (see Borghi (1985)).

II - THE "CELLULAR AUTOMATA"

II.1. The principles . In order to visualize the various phenomena involved, we have imagined a statistical simulation code of the type called "cellular automaton" . Our purpose was not to simulate the turbulent motions of fluid particles but given such movements, to simulate the turbulent combustion itself, and particularly the influence of turbulent dispersion with respect to the laminar flame propagation. It is not intended that this simulation do represent accurately the reality ; it is just intended that the right phenomena and parameters will be put into evidence more clearly. The proposed simulation involves three steps, and can be developed on a line with only one dimensional displacements, or within a plane or a three dimensional space. We have developped here only the one and two dimensional versions. Let us begin with a line ; this line is divided into a number of adjacent sites ; within each site there is one "fluid particle", which can be either burned (black) or unburned (white) ; no partially burned particles are allowed, because we assume always that the reactions are very fast, $\tau_c/\tau_c \gg 1$. The simulation comprises three steps,

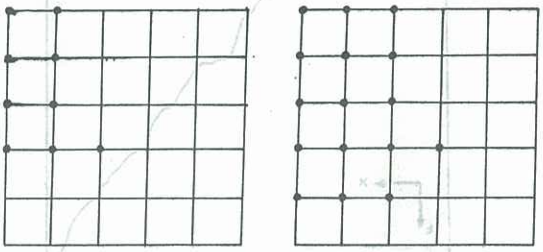
i) the first step is a random displacement of all fluid particles, based on a random choice of a turbulent velocity v with a rms value u' and a zero mean value.

ii) the second step is a combustion step between fluid particles. After the step 1, some sites get occupied by two (or more) particles ; in such a case we choose to "coalesce" all particles in only one, which is burned if one of the particles on the site was burned.

Similarly we have to look at unoccupied sites ; the choice is here to fill this site with a burned particle if one neighbour is burned, or with an unburned particle if all the neighbours are unburned.

iii) the third step is a propagation step. It consists in the movement, with a prescribed velocity u_L of the boundary between burned and unburned particles (that is the flame front), from the burned side to the unburned one.

In the one dimensional version, each of the steps described here are very clear ; in the steps 2 and 3, we have to look only at two neighbours. For the two dimensional version : each step needs additional choice. First, we have to choose a lattice in order to represent the plane ; here, we have chosen a square lattice the simplest one, but it has particular symetry properties ; it is fully possible that an hexagonal lattice, where each site is related to six other would be more satisfactory . Second, we have to define in a precise way the neighbours ; with a square lattice, we can call neighbours only the four closest sites (it is the von Neumann neighbourhood), or the eight closest sites (the Moore neighbourhood). Third, the propagation step is not so simple, because the velocity of propagation would be normal to the flame front itself ; in the frame work of a square lattice, we have adopted the following procedure :



Propagation using Neumann neighbours

figure 1

each unburned site must get burning if there is at least one burned site in his neighbouhood (fig. 1).

There is a length scale defined by the lattice (say Δx) ; there is also a time scale Δt ; Δt^{-1} is the frequency with wich the three steps are repeated. The random walks of each particles are taken independant of the other ; that means that the spatial correlation scale is Δx ; the velocities are randomly chosen, each Δt , independant to the previous ones ; that means that the correlation time is Δt . In order to represent turbulent movements, it is necessary then that $\Delta x/\Delta t = u'$; when the lattice is regular, it follows that the simulated turbulence is homogeneous and isotropic. We intend to vary the parameter u'/u_L from $u'/u_L \gg 1$ to $u'/u_L \ll 1$; the situation $u' = 0$ is easily recovered without the step 1, and the situation $u_L = 0$, without the step 3. Of course each $u_L \Delta t$ is not necessarily commensurate with Δx , and so only discrete value of u'/u_L can be tried ; there is no problem at each step if $u_L \Delta t$ is a multiple of Δx ; if $u_L \Delta t = \Delta x/n$ $(n > 1)$, the step 3 is performed only every n steps.

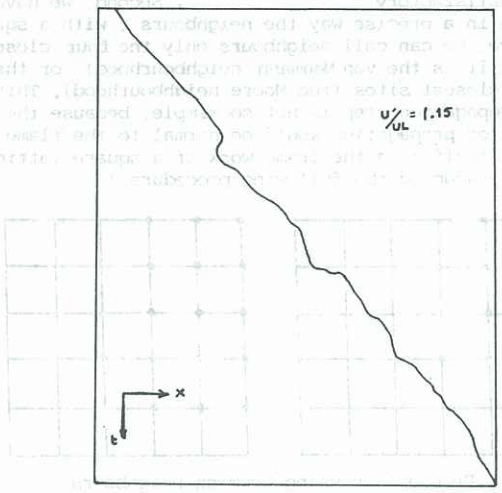
II.2. Physical interpretations. The physical significance of step 1 is clearly the turbulent diffusion. Simulations of turbulent dispersion of fluids particles or solid (or liquid) particles have been proposed recently, with very similar Lagrangian methods.

The physical significance of step 3 is clearly the laminar propagation of a flame. We have chosen here that the velocity of the flame is constant, irrespective to the curvature of the front, without local extinctions.

The second step represents just a simple interpolation when we are concerned with the filling of an unoccupied site. But it represent, when two particles interact, a physical process : it is the volumetric burning of a bulk of fluid ; clearly, we can expect than this

phenomenon actually occur when two flame fronts are to close toghether; it is necessary in order to avoid that the flame surface by unit of volume does not increase to infinity due to turbulent dispersion. The particular rule chosen for this step, that is that one burned particle suffices always to ignite the other, is consistent with our hypothesis that τ_c/τ_t is infinitely small.

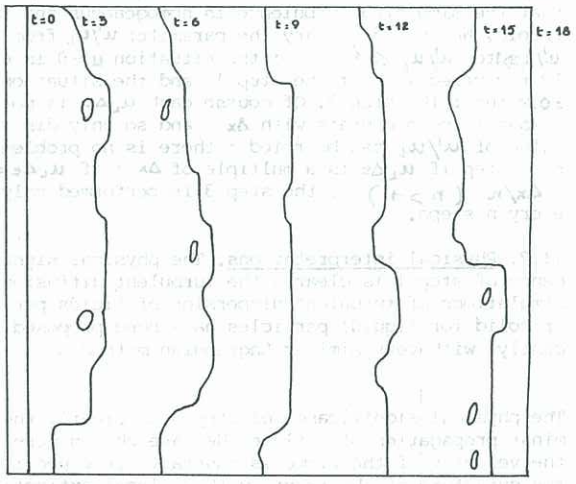
II.3. Some examples of simulations. The figure 2 shows the case of a one-dimensional propagation of flames, for a certain u'/u_L ; each line corresponds to a certain value of time. One see clearly the influence of the turbulence : the front is strongly convoluted, some pockets appear, the mean velocity of propagation is increased. This is more and more evident, as u'/u_L is higher and higher.



Propagation of a flame in one-dimension

Figure 2

The figure 3 show the propagation of a flame in a two-dimensional medium ; at t=0 only a small strip of the plane is burned ; here are superimposed two frames, at two different times. The simulations have been made with 53 fluid particles and sites in one dimension, and 20x40 sites and fluid particles in two dimensions, on a Apple II microcomputer. The lattice being limited, we have assumed as boundary conditions a reflexion condition. We can follow then the flame propagation only a certain time, depending on u_L/u'.



Propagation of a flame in
two-dimension using Moore-neigbours
$u'/u_L = 1.15$

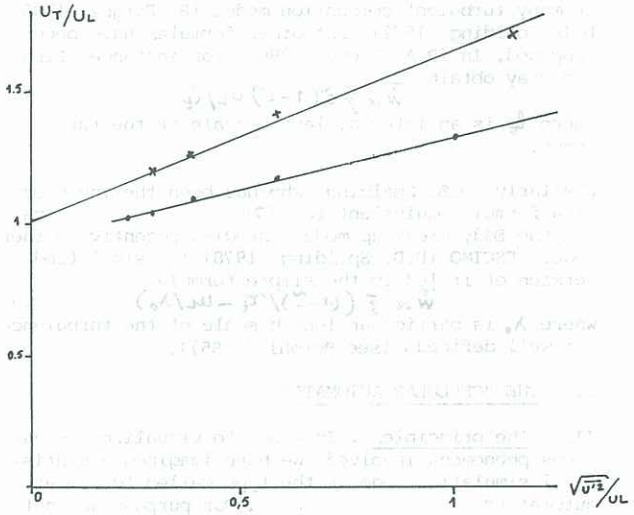
Figure 3

III - RESULTS AND DISCUSSIONS

III.1. We have now to extract quantitative results from the numerical simulations. We have first calculated u_T, the turbulent propagation velocity, given an initial distribution of fluid particles, with only a black strip on the left side, the flame develops with an irregular front ; inaddition, each realization is different. We have to compute u_T as a mean value of the front velocity : the mean value has been taken here over the whole propagation and for 30 realizations.

In order to compute $\bar{\dot{w}}$, the initial distribution of black and white particles has been taken random, but homogeneous, with a given number of black particles corresponding to 25 % of the total number. At each time step, the reaction rate $\dot{w}$ can be computed as the increase (within one time step) of the number of burned particles : the mean value can be calculated over a number of realizations (usually 30) for the same time step. Similarly a combustion degree can be compuded as the fraction of black particles, and averaged over many realizations to give $\bar{c}$; we have not distinguished here between different averages as we are interested only in qualitative results.

III.2. The turbulent flame speed. The figure 4 shows the curves u_T/u_L as a function of u'/u_L , as obtained for one-dimensional and two dimensional simulations.



The turbulent flame speed
(·) for one-dimension (+) for two-dimension

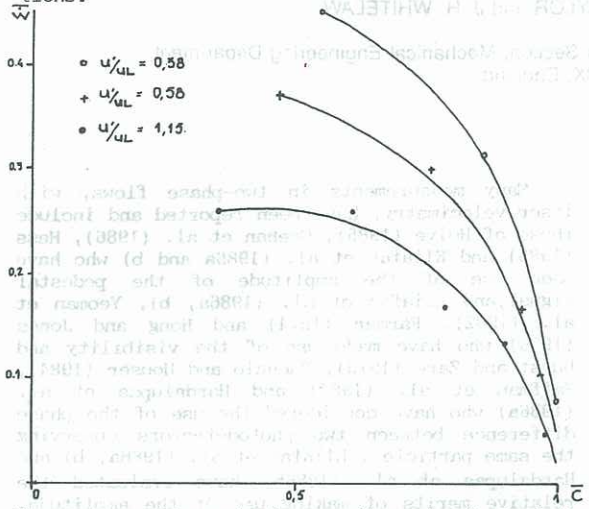
Figure 4

The first result is that we obtain clearly a linear relation, in agreement with relation (1), and in contradiction with relation (2) ; the constant C, the slope of the curve, is found here of about 0.3 ± 0.05 in the one-dimensional case, and 0.45 ± 0.07 in the two-dimensional case. These figures are far from 2, the value often found in experiments ; Ashurst and Barr, in (W.T. Ashurst, 1983), have found values between 0.5 and 0.9 in their various calculations.

In fact, experimental values of u_T are very difficult to define ; there are many possibilities to "measure" them, each being approximately equivalent, but with a multiplicative constant. In addition, in real flows, the combustion influences the turbulence, through several different (and opposite in sign) phenomena ; in our simulation, no effect of such a type is taken into account. Ashurst and Barr have tried to explain the differences in values of C by the effect of Reynolds number : as we have said in the first part, the Reynolds number dependance of C can occur only if τ_c/τ_t is not infinitely small ; that cannot be the case in our simulation, and probably also in their ones (at least their computation with a zero thickness flame).

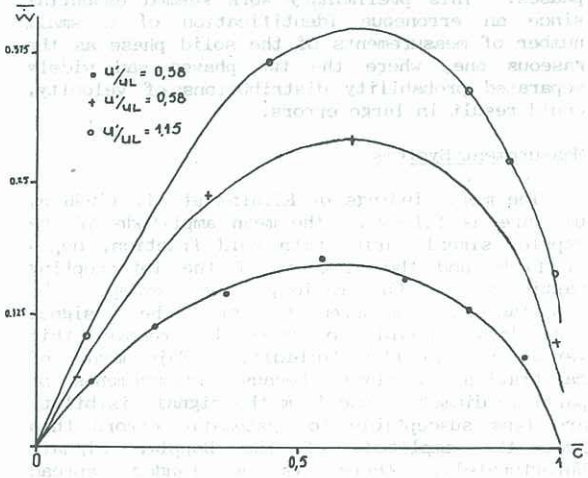
III.3. The mean reaction rate. A mean reaction rate can be calculated, from the simulation, as explained, for each time step, during the combustion of a statistically homogeneous medium. We have then plotted $\tilde{\dot{w}}$ as a function of $\tilde{c}$ instead of time.

The figure 5 shows, for the one dimensional simulation $\tilde{\dot{w}}(\tilde{c})$ for different values of u'/u_L ; the figure 6 shows the same quantity for two dimensional simulations.



The mean reaction rate for one-dimensional simulation

Figure 5



The mean reaction rate for two-dimensional simulations

Figure 6

A clear qualitative difference is seen at the first sight : a monotonic shape of $\tilde{\dot{w}}(\tilde{c})$, always decreasing when $\tilde{c}$ increases to 1, is found for one dimensional calculations. It is not the case for the two-dimensional simulation, where $\tilde{\dot{w}}$ increases with $\tilde{c}$ at small $\tilde{c}$, and decreases if $\tilde{c}$ is large enough. The reality, which is three-dimensional, can be expected very much similar to two-dimensional simulation. A clear influence of u'/u_L on the shape of $\tilde{\dot{w}}$ put into evidence. The curves are less and less symmetrical as u'/u_L decreases to zero. When $u'/u_L = 1.15$ we obtain $\tilde{\dot{w}} \propto \tilde{c}(1-\tilde{c})$, given in the frame work of the Eddy Break up model. At the contrary, when u'/u_L is not very large, the curves depart from the symetrical shape of Eddy Break up formula ; it is very interesting to see that the ESCIMO model can be reduced to the formula (9), which is completely unsymetrical, and appears to be a limit curve of our simulations in the case where u'/u_L is very small.

The parameter u'/u_L influences $\tilde{\dot{w}}$ not only for its shape ; the maximum value of $\tilde{\dot{w}}$, for an intermediate value of u'/u_L is depending also on u'/u_L. In the case where $u'/u_L = 1.15$ the maximum value of $\tilde{\dot{w}}$ reaches 0.16 ; for $u'/u_L = 0.38$ it reaches 0.39.

III.4. Concluding remarks. The simple cellular automaton we have presented here has been finally able to give interesting answers for the problems, concerning turbulent flame velocity and mean combustion rate, that we mentioned §1. The classical linear law of u_T/u_L as function of u'/u_L is confirmed by our simulation, without appearance of length scale or Reynolds number dependance for very fast reactions. In addition, the simulation put into evidence that u'/u_L would be includ in $\tilde{\dot{w}}$, recovering the Eddy break up model when $u'/u_L >> 1$; the influence of u'/u_L appears to occur both on the shape of the curve $\tilde{\dot{w}}(\tilde{c})$, similarly as in the ESCIMO model (D.B. Spalding), and on the maximum value of $\tilde{\dot{w}}(\tilde{c})$ (for a certain $\tilde{c}$).

Such a cellular automaton seems to be an interesting way to study further turbulent combustion modelling. We plan now to study the influence of τ_c/τ_t.

REFERENCES

P. Clavin - Dynamic behavior of premixed flame fronts in laminar and turbulent flows - Progress in Energy and Combustion Sciences - vol. 11. pp. 1-59 - 1985.

R. Borghi - On the structure and morphology of turbulent premixed flames - In Recent advances in the aerospace sciences - Ed. Corrado Casci - pp. 117-138. Plenum Pub. Corp. - 1985.

G. Damköhler - Elecktrochemic Angewandte Phys. Chem. 46 - p. 601 - 1940.

K.I. Schelkin - Combüstion Hydrodynamics - Fizika Goreniya iVzryva - vol. 4. n° 4. pp. 455-468 - 1968.

R.G. Abdel-Gayed, K.J. Al-Khishali, D. Bradley - Turbulent Burning Velocities and flame straining in explosions - Proc. R. Soc. Lond. - A 391. pp. 393-414 - 1984.

P. Clavin, F.A. Williams - Theory of premixed flame propagation in large scale turbulence - J. Fluid. Mech. - vol. 9. part 3 - p. 589 - 1979.

W.T. Ashurst, P.K. Barr - Stochastic calculation of laminar wrinkled flame propagation via Vortex dynamics - Com. Sc. Tech. - vol. 34 - pp. 227-256 1983.

R. Borghi, B. Argueyrolles, S. Gauffié, P. Souhaité - Application of a "presumed p.d.f." model of turbulent combustion to reciprocating engines - 21th Symp. (Int.) on Combustion - Munich - 1986.

R. Borghi, E. Pourbaix. Lagrangian models for turbulent combustion - pp. 369-380-Turbulent shear flows 4-Ed : LSJ Bradbury et al. Springer Verkag(1985)

K.N.C. Bray - Turbulent flows with premixed reactants in turbulent reacting flows - Ed. P.A. Libby. F.A. Williams - Topics in Applied Physics - vol. 44 - Springer-Verlag . Heidelberg - 1980.

Bilger, R.W. - Turbulent diffusion flames - in : turbulent reacting flows - Ed. P.A. Libby, F.A. Williams - Topics in Applied Physics - vol. 44 Springer-Verlag. - 1980.

D.B. Spalding - Mixing and chemical reaction in steady confined turbulent flames - 13th Symp. on Combustion - The Combus. Inst. Pittsburg - p. 649 1971.

P.A. Libby, K.N.C. Bray - Implications of the laminar flamelet model in premixed turbulent combustion - Combustion and Flame - vol. 39, pp. 33-41 - 1980.

D.B. SPALDING - Chemical reactions in turbulent fluids Physico chemical Hydrodynamics - Ed. D.B. Spalding vol. 1. pp. 321-338. Advance Pub. - 1978.