A THEORETICAL STUDY ON GENERATION OF VORTICITY DUE TO CHEMICAL REACTION

by

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ABSTRACT

The possible generation of vorticity by combustion is studied, for different models of turbulent flames. Examination of the viscous, compressible vorticity equation shows that the effect of combustion might be of two kinds; viz., a "density effect," due to the change of size of the eddies by change of density, and a "pressure-density effect," due to simultaneous occurrence of non-parallel gradients of pressure and gradients of density.

For the "wrinkling laminar flame" model, an expression has been found for the change in vorticity for a particle crossing a flame front, assumed the combustion zone to be very thin, and the flame locally laminar. It is found that the change in vorticity depends strongly on the mean square pressure gradient at the flame front. Two mechanisms are considered, whether the intensity of the turbulence in the flow upstream is weak or strong, and the influence of the relevant parameters is discussed, in each case.

For the case of "volume combustion," an analysis similar to Kármán and Howarth's analysis for isotropic homogeneous turbulence has been performed, leading to a mean-square vorticity equation valid when combustion occurs. New correlations in this equation indicate the averaged effects of chemical reaction on vorticity. Examination of the term corresponding to "pressure-density effect" shows that it results from the second order interaction between the sound and entropy modes. Experimental measurements of the new correlations could determine the magnitude of combustion generated turbulence.

Interaction of sound waves with occurrence of chemical reaction as a possible mechanism of generation of vorticity is then examined. An homogeneous stagnant, chemically reacting medium, and two travelling waves are considered. Numerical resolution of the governing equations shows the influence of some of the relevant parameters, and estimates the order of magnitude of the generated vorticity.

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CHAPTER I INTRODUCTION

The phenomena occuring in turbulent combustion, though studied for many years, are still poorly understood, except in some simple cases. One way to look at the phenomena is to extend the well known decomposition in three "modes", sound, entropy and vorticity (10), established in the non-reacting case, and to see how phenomena are coupled, through the interaction terms, when combustion occurs.

The sound and entropy modes and the interaction between them have been studied theorically and experimentally (16, 17, 19). The purpose of this thesis is to investigate how vorticity could be related to the entropy and sound modes, when combustion occurs.

The generation of vorticity can be studied analytically by means of the "vorticity equation", which is a transport equation with source terms on the right hand side. The compressible vorticity equation differs from the incompressible one by two terms which take into account the specific effects of combustion. If these terms lead to an increase in vorticity , then we can consider that tubulence has been generated by combustion.

To the knowledge of the author, no such analysis has been performed in this field.

This thesis examines how vorticity could be generated in the case of "surface combustion", "volume combustion", and interaction of sound waves, showing the different processes involved, and the significant parameters of the system.

CHAPTER II . THE VORTICITY EQUATION

The vorticity equation is obtained by taking the curl of the momentum equation, and can be put under the form (1) :

$$\frac{\partial \underline{\Omega}}{\partial t} + \underline{u} \cdot \nabla \underline{\Omega} = \underline{\Omega} \cdot \nabla \underline{u} - \underline{\Omega}\, \nabla \cdot \underline{u} - \nabla\left(\frac{1}{\rho}\right) \times \nabla p + \nu \nabla^2 \underline{\Omega}$$

valid in combustion (neglecting however the effects of the variations of kinematic viscosity due to temperature change). This equation, which is remarkable for its simplicity gives valuable informations about the processes that are occurring in turbulent flows.

II.A Study of the different terms in the vorticity equation, phenomena involved.

The vorticity equation can be considered as a transport equation for the vorticity, with different source terms in the right hand side. This point of view is supported by the fact that in 2-dimension, incompressible, inviscid case, the vorticity equation becomes:

$$\frac{\partial \underline{\Omega}}{\partial t} + \underline{u} \cdot \nabla \underline{\Omega} = 0$$

which physically means that each particle in the fluid "keeps"its vorticity. The four terms composing the right hand side are each connected with a phenomenon that affects vorticity :

$\underline{\Omega} \cdot \nabla \underline{u}$ is known as representing the change in vorticity due to the stretching of the vortices (2)

$\nu\ \nabla^2 \underline{\Omega}$ is the viscous dissipation term

$-\underline{\Omega}\ \nabla\cdot\underline{u}$ corresponds to the effect of a change in density for the vortices, which rotate slowerif their size increase, by conservation of momentum.

$-\nabla\left(\frac{1}{\rho}\right)\times\nabla(p)$ is the increase in vorticity due to the existence of pressure gradients in a medium of varying density.

The two first terms and the phenomena they represent have been extensively studied in the case of incompressible turbulence, since they are related with the major features of turbulence : the decay of eddies into smaller and smaller eddies, and the viscous dissipation in a very small scale range.

It is our purpose to study the influence of the two other terms in the case of combustion, and to the knowledge of the author, little work has been done in this field.

II.B Other forms of the vorticity equation

In the case where vortex stretching and viscous dissipation could be neglected, the vorticity equation can be put under the so-called Vazsoyi equation (1) :

$$\frac{D\,\sigma\underline{\Omega}}{Dt} = -\sigma\ (\nabla\sigma \times \nabla p)$$

$$\sigma \equiv 1/\rho$$

with the help of the continuity equation. There are other forms of the vorticity equation, when the variations in density could be neglected, but we shall not use them here.

CHAPTER III GENERATION OF VORTICITY IN A SURFACE COMBUSTION MODEL

INTRODUCTION

A class of turbulent flames seems to correspond very well to the wrinkling laminar flame model (3,4), except for some discrepancies between the calculated and the measured turbulent burning velocities, discrepancies which have been explained by flame generated turbulence (5). No physical explanation or better evidence of the phenomenon has been given since, and even some recent experiments (6) have shown that the velocity fluctuations in burning jets were comparable with those of hot jets, and no increase was found in the flame brush. It is important to note, however, that the mean square velocity fluctuation is not the only measure of the turbulence, and that it is probable that the vorticity is of major importance in diffusion processes. Therefore, it has seemed important in this study to examine the possible generation of vorticity in such flames.

I Description of the model

In order to give the largest extent of validity to our theory, we shall state here the only assumptions that will be necessary further on. These assumptions are:

(a) The thickness of the combustion zones can be considered as very small compared with any other characteristic length of the model.

(b) The flame is locally laminar, and the normal velocity of the flame front relative to the unburned gas is constant, equal to the characteristic burning velocity.

Note that we do not assume the flame front to be continuous. On the other hand, assumption (b) might be restrictive in certain cases, since the laminar burning velocity is known to depend upon the velocity gradient (when the velocity gradient is too high, the flame is quenched) and on the radius of curvature of the flame front. But it seems to the author that it is not necessary to introduce corrections for these phenomena at this point of the study.

II Change in vorticity for an unburned particle crossing a flam front.

Consider a turbulent flame satisfying the assumtions of the last section. If there is generation of vorticity by combustion in the whole process, it can only occur within the flame front, since upstream and downstream the density of the particles can be assumed constant, and the usual processes of incompressible turbulence take place, stretching and viscous dissipation, no generation is expected. Note that, when no recirculation of the unburned gas occurs, the vorticity generated by the flame is unlikely to diffuse upstream, since this process of diffusion is very slow. We shall therefore restrict our study to the change in vorticity in the flame front due to combustion.

Now, since we have assumed the thickness of the flame front to be smaller than any other characteristic length of the system, the stretching and viscous effects are negligible as compared to the "density" and "pressure density" effects. With the help of the Vazsonyi equation (II-1) valid in that case, an expression for the change in vorticity through the flame front has been derived :

$$\sigma_2 \underline{\Omega_2} - \sigma_1 \underline{\Omega_1} = -\frac{\sigma_1}{S_u} (\sigma_2 - \sigma_1) \left| \frac{\partial p}{\partial \underline{\alpha}} \right| \underline{K} \qquad \text{(III-1)}$$

$\sigma_1, \sigma_2, \underline{\Omega_1}, \underline{\Omega_2}$: specific volume and vorticity upstream and downstream the flame front

S_u : characteristic burning velocity

$\frac{\partial p}{\partial \underline{\alpha}}$: component of the gradient of pressure tangent to the flame front.

$\underline{K}$: unit vector tangent to the flame front and orthogonal to $\left[\frac{\partial p}{\partial \underline{\alpha}}\right]$

The demonstration of (III-1) is given in appendix I.

This relation has several remarkable features :

(1) The increase in vorticity is independant of the flame thickness, and how density varies within the flame.

(2) It is also independant of the angle upon which the particle reach the flame front.

It has not been possible to go further and express the gradient of pressure in function of the parameters of the turbulence upstream, for reasons that will appear in the next section.

IV Discussion

Examination of equation (III-1) leads to the conclusion that the variation of vorticity for a particle through the flame front is due to two effects :
(a) A density effect, which tends to decrease the vorticity of the particle, for exothermic reactions,
(b) A "pressure density effect" , by means of the right hand side term.

Let us call "specific vorticity" the quantity $\sigma\underline{\Omega}$. Although he has no proof of it, the author thinks that the pressure density effect leads to an increase in mean square specific vorticity fluctuation : consider a great number of particles, crossing a flame zone. We shall denote by $\langle\cdot\rangle$ the average on this ensemble of experiments, and by $(\ )'$ the fluctuation relative to the average value. Equation (III-1) is equivalent, with some algebra :

$$\sigma_2^2 \langle \underline{\Omega}_2'^2 \rangle - \sigma_1^2 \langle \underline{\Omega}_1'^2 \rangle = -\frac{2\sigma_1^2}{S_u}(\sigma_2-\sigma_1)\left\langle \left|\frac{\partial p}{\partial \underline{\alpha}}\right| \underline{K}\cdot\underline{\Omega}_1' \right\rangle + \left(\frac{\sigma_1}{S_u}\right)^2(\sigma_2-\sigma_1)^2\left\langle \left|\frac{\partial p'}{\partial \underline{\alpha}}\right|^2 \right\rangle \quad \text{(III-2)}$$

Now, the pressure gradient fluctuations, and the vorticity fluctuations are both random quantities, with zero mean values. Since the local pressure gradient should not be strongly correlated with local vorticity a priori,

$$\left| \left(\frac{\sigma_1}{S_u}\right)^2 (\sigma_2-\sigma_1)^2 \left\langle \left|\frac{\partial p}{\partial \underline{\alpha}}\right|^2 \right\rangle \right| \gg \left| \frac{\sigma_1^2}{S_u} (\sigma_2-\sigma_1) \left\langle \left(\frac{\partial p}{\partial \underline{\alpha}}\right)' \underline{K} \cdot \underline{\Omega}'_1 \right\rangle \right|$$

and therefore : $\sigma_2^2 \langle \Omega_2'^2 \rangle > \sigma_1^2 \langle \Omega_1'^2 \rangle$

Thus, it is concluded, from equation (III 2), that the pressure density effect should lead to an increase in specific vorticity fluctuations.

Now, the magnitude of this effect depends much on the pressure gradient that appear in the right hand side of (III 1). Gradients of pressure in turbulent combustion, compatible with the surface combustion model, could be associated with turbulence, propagation of the flame, and pressure drop across the flame.

a) Turbulence

Rotating flows induce pressure gradients (to balance centrifugal forces). Higher pressure gradients occur in the smaller scale of the turbulence (where the radius of curvature of the trajectory of a particle is smaller), that is to say within the microscale or Kolmogorof range, according to the Reynolds number. Different expressions for the mean square pressure gradient have been derived in litterature :

$$\frac{1}{\rho^2}\overline{(\text{grad } p)^2} = 3.9\,(\varepsilon^2/\nu)^{1/2} \qquad (7)$$

$$\frac{1}{\rho^2}\overline{(\text{grad } p)^2} = \frac{\overline{u^2}}{\lambda^2}\;\frac{248}{R_\lambda} \qquad (8)$$

ε : rate of energy dissipation

ν : kinematic viscosity

λ : microscale

$\overline{u^2}$: root mean square velocity fluctuations

R_λ : $\sqrt{\overline{u^2}}\,\lambda/\nu$

But no comparison with experiments has been performed to the knowledge of the author, which is understandable since it is very difficult to measure local pressure gradients in turbulent flows, especially when they occur in the smaller scale.

b) <u>Propagation of the flame</u>

The flame front can induce pressure gradients by a modiffication of the flow upstream and downstream, due to the fact that it propagates normally. As an example, the calculations made by Landau (8) on the stability of a plane laminar flame front relates the pressure gradient with the disturbance at the flame front, but no general relation has been derived, since the amplitude of the disturbance of the flame front is expected to increase with time, and cannot be related with any characteric parameter of the flame.

We could also wonder if the pressure gradient is not relatedto the pressure drop across the flame (by dimensionnal consideration). But it seems to the author that there is no direct connection between both, according to the following reasonning : let us consider a flame front, far from boundaries. Out of the flame zone, the pressure and velocity fields are governed by the contimuity and momentum equations, and the pressure appear only under the form of a gradient. Regarding the flame front as a surface of discontinuity, the equations stating that the normal velocity to the surface is unchanged, and the pressure drop is constant all along the flame, will give a complete set of equations and boundary conditions. The point is that the pressure drop accross the flame front has no influence on the pressure gradients and on the flow field, and only the mean pressure upstream and downstream will be changed. It results that the pressure drop across the flame seems not to be related with the velocity and pressure fields ouside the flame zone, and therefore $\frac{\partial p}{\partial \underline{x}}$.

To be complete we should mention here the generation of pressure waves by turbulent flames. (12, 13, 14) This process seems to the author harly compatible with the surface combustion (Strahle (15) has recently attemted to extend the explanation of combustion noise given

given by Bragg (14) to the wrinkling laminar flame model, but his arguments are not very convincing). The study of generation of vorticity by pressure waves will be the object of the two next chapter.

Which pressure field is dominant depends certainly on the type of combustion. Both (a) and (b) seem possible. It is to be noticed that if the pressure gradient is related to turbulence, (process (a)), the mean square pressure gradient should increase with the mean square vorticity, (pressure gradients balance centrifugal forces), and therefore the variation of density through the flame front could be an increasing function of the vorticity upstream (according to (III 1)).

This raises the question of recirculation of vorticity : suppose that a particle has burned and possesses a certain vorticity. By turbulent mixing, it happens to cross a flame again, together with fresh mixture. Its vorticity will not increase through the previouly described process, since its density will not change significantly compared with unburned particles, but one might think that, before ignition occurs, the burned particle has diffused its vorticity to unburned particles. If the overall effect is an increase in vorticity, higher with higher vorticity upstream, one could forecast an acceleration process, leading to a strong increase of vorticity in turbulent flames.

However, it seems to the author that this is unlikely to occur, since a burned particle cannot transmit vorticity to an unburned particle without transmitting also heat and probably active species. As these processes are all diffusion processes, and as all the coefficients are of the same order of magnitude, it is probable that the unburned particle begins to burn before it has received vorticity from the unburned particle.

CONCLUSION

It has been shown that vorticity can be generated in a surface combustion process, and that the root mean square pressure gradient is of major importance. Further work could be done in this field, either by computer simulation of simple turbulent flames, and experiments could perhaps attempt to measure pressure gradients in turbulent flows.

CHAPTER IV GENERATION OF VORTICITY IN A VOLUME COMBUSTION MODEL

INTRODUCTION

As compared with the surface combustion processes, the volume combustion processes and the generation of vorticity are a more difficult theorical problem, since now the energy equation has to be taken into account, as well as its coupling with the momentum and continuity equations.

In this chapter, an attempt will be made to estimate the overall effects of combustion on turbulence, a new Kármán-Howarth equation will be derived, involving new termsthat take into account the specific effects of combustion. Experiments, if possible, could then determine the magnitude of these new terms, and show whether or not combustion generates turbulence.

Now, although overall effects of combustion might be known by experiments, we do not expect this theory to give us detailed information about the processes themselves. The reason is that we shall use the method of averaging , which destroys most of the information concerning the local, instantaneous processes.

Let us take an example, and consider the "ordinary vorticity equation" and the "mean square vorticity equation" derived from the Kármán-Howarth equation, both in the case of incompressible turbulence.

$$\frac{\partial \underline{\Omega}}{\partial t} + \underline{u} \cdot \nabla \underline{\Omega} = \underline{\Omega} \cdot \nabla \underline{u} + \nu \nabla^2 \underline{\Omega} \qquad \text{(a)}$$

$$\frac{d \overline{\underline{\Omega}^2}}{dt} = \frac{7}{3\sqrt{15}} \left(S - \frac{2G}{R_\lambda} \right) (\overline{\underline{\Omega}^2})^{3/2} \qquad \text{(b)}$$

$\underline{\Omega}$ vorticity

$\underline{u}$ velocity

$$S \equiv - \overline{\left(\frac{\partial u_1}{\partial x_1} \right)^3} \Big/ \left[\overline{\left(\frac{\partial u_1}{\partial x_1} \right)^2} \right]^{3/2}$$

$$G \equiv \overline{u}^2 \frac{\overline{(\partial^2 u_1 / \partial x_1^2)^2}}{[\overline{(\partial u_1 / \partial x_1)^2}]^2}$$

It is possible, by examining the different terms of the ordinary vorticity equation (a) to know what processes are involved in the generation or destruction of vorticity. For instance, it can be shown that $\Omega \cdot \nabla \underline{u}$ corresponds to the increase in vorticity due to the stretching of the vortices (2). Now, the stretching of the vortices has been shown experimentally. but it has not been possible to determine the relative magnitude of the stretching term as compared with the other terms.

On the contrary, the mean square vorticity equation (b) does not give any information about the processes themselves, but the skewness and flatness factor can be shown to represent the overall effects of the stretching and viscous terms, and by experimental determination of these correlations, it is possible to determine the relative magnitude of these effects.

Both approaches of the problem are complementary.

We shall study in this chapter the overall effects of combustion on turbulence, and some of the processes involved in the next chapter.

1) Formulation of the problem

We consider a very large enclosure, filled with an homogeneous mixture, able to be ignited by some external means, such as a mixture of hydrogen and chlorine irradiated by U.V. light. Before reaction begins to occur, the enclosure has been shaken by some means, so that turbulence inside can be considered as statistically homogeneous and isotropic, far from boundaries. Since the volume of the enclosure is constant, and reaction assumed to occur homogeneously, no mean* flow, no mean temperature gradient is expected to occur. Therefore, the turbulence can still be considered as isotropic and homogeneous during the reaction, in average.

To be still more precise, we have to consider a small volume far from boundaries, so that the radiation and acoustic fields could be considered as isotropic . The walls could reflect light and sound indifferently.

* "mean" in the sence of averaged over a great number of experiments.

2) Outline of our method.

Our analysis will follow quite closely the now classical theory of homogeneous isotropic turbulence, (7,8). We shall first summarize some results of this theory, and then show how these results can be extended in the combustion case.

First of all, a differential equation involving velocity correlation tensors is derived from the Navier-Stokes equation :

$$\frac{\partial}{\partial t} R_{ij}(\underline{r}) = S_{ij}(\underline{r}) + 2\nu \nabla^2 R_{ij}(\underline{r}) \qquad \text{(IV 1)}$$

with : $\overline{(\ )}$: averaged over a great number of experiments.

$$R_{ij}(\underline{r}) \equiv \overline{u_i(\underline{x})\, u_j(\underline{x}+\underline{r})}$$

$$S_{ij}(\underline{r}) \equiv \frac{\partial}{\partial r_k} \left\{ \overline{u_i(\underline{x})\, u_j(\underline{x}+\underline{r})\, u_k(\underline{x})} \right\} + \frac{\partial}{\partial r_k} \left\{ \overline{u_j(\underline{x})\, u_i(\underline{x}-\underline{r})\, u_k(\underline{x})} \right\}$$

Then, each of the tensors of (IV 1) can be expressed in function of only one scalar, by use of homogeneity, isotropy and incompressibility conditions. For instance :

$$R_{ij}(\underline{r}) = -D_r \frac{1}{2} \bar{u}_1^2 f(r)\, r_i r_j + \left(r^2 D_r + 2 \right) \frac{1}{2} \bar{u}_1^2 f(r)\, \delta_{ij}$$

$$D_r \equiv \frac{1}{r}\frac{\partial}{\partial r}$$

$$f(r) \equiv \overline{u_1(\underset{\sim}{x})\, u_1(\underset{\sim}{x}+\underset{\sim}{r})} \;/\; \overline{u_1(\underset{\sim}{x})}^2$$

$$\text{for} \quad \underset{\sim}{r} = (r, 0, 0)$$

$$r \equiv |\underset{\sim}{r}|$$

With some algebra, equation (IV 2) can be shown to be equivalent to a scalar equation, involving two velocity correlation : (Kármán-Howarth equation)

$$\frac{\partial}{\partial t}\,\overline{u^2} f(r) = \left(\frac{\partial}{\partial r} + \frac{4}{r}\right)\left[\overline{u^2}\right]^{3/2} k(r) + 2\nu\left(\frac{\partial^2}{\partial r^2} + \frac{4}{r}\frac{\partial}{\partial r}\right)\overline{u^2} f(r)$$

$$f(r) \equiv \overline{u_1(\underset{\sim}{x})\, u_1(\underset{\sim}{x}+\underset{\sim}{r})} \;/\; \overline{u_1^2(\underset{\sim}{x})}$$

$$k(r) \equiv \overline{u_1^2(\underset{\sim}{x})\, u_1(\underset{\sim}{x}+\underset{\sim}{r})} \;/\; \left[\overline{u_1^2(\underset{\sim}{x})}\right]^{3/2}$$

$$\text{For} \quad \underset{\sim}{r} = (r, 0, 0)$$

A development in power series of the different terms of this equation can be shown to lead to a "kinetic energy equation" and a "mean square vorticity equation" :

$$\frac{d\,\overline{u_1^2}}{dt} = 10\,\nu\, f_0''\, \overline{u_1^2}$$

$$\frac{d\,\overline{\Omega_1^2}}{dt} = \frac{7}{3\sqrt{15}}\left(S - \frac{2G}{R_\lambda}\right)\left[\overline{\Omega_1^2}\right]^{3/2}$$

$$f_0'' \equiv \left\{ \frac{d^2}{dr^2}\, \overline{u_1(x)\, u_1(x+r)} \;/\; \overline{u_1^2(x)} \right\}_{r=0}$$

There is no development at order one, since $f(r)$ and $k(r)$ are even functions, and the coefficients of r in the development are zero.

Now, in the case of occurence of combustion, new terms will appear in equation (IV 1) since terms involving the velocity divergence are no more zero. We shall first derive such an equation. It will be shown that each of the correlation tensors can be expressed in function of two scalars, instead of one in the incompressible case. One of the two scalars will take into account the specific effects of combustion. We shall then show that the tensorial equation (IV 1) is equivalent to two scalar equations, instead of one. By combining these two equations, a new Kármán-Howarth equation will be derived.

We shall denote by $(..)^{(0)}$ the expression of (..) when no combustion occurs, and by $(..)^{(1)}$ the part of (..) due to occurence of combustion.

3) Differential equation for the two points correlation tensor

We shall generalize here the relation :

$$\frac{\partial}{\partial t} R_{ij}(\underline{r}) = S_{ij}(\underline{r}) + 2\nu \nabla^2 R_{ij}(\underline{r})$$

to the case of combustion, using the same steps as in the incompressible case, but with new terms, since the velocity divergence is no more zero.

The complete Navier-Stokes equation is, neglecting however the effect due to change in kinematic viscosity with temperature :

$$\frac{\partial}{\partial t} u_i(\underline{x}) + u_K(\underline{x}) \frac{\partial u_i(\underline{x})}{\partial x_K} = -\frac{1}{\rho(\underline{x})} \frac{\partial p(\underline{x})}{\partial x_i} + \nu \frac{\partial^2 u_i(x)}{\partial x_K \partial x_K} + \left(\nu_v + \frac{\nu}{3}\right) \frac{\partial}{\partial x_i}\left(\frac{\partial u_K(\underline{x})}{\partial x_K}\right)$$

with : $\nu = \mu/\rho$: kinematic viscosity

$\nu_v = \mu_v/\rho$: kinematic "bulk" viscosity.

We multiply this equation by $u_j(\underline{x}+\underline{r})$ and add to the same equation at point $\underline{x}+\underline{r}$, for the component j, multiplied by $u_i(\underline{x})$, and we derive :

$$\frac{\partial}{\partial t} \overline{u_i(\underline{x}) u_j(\underline{x}+\underline{r})} + O_2\left\{\overline{u_K(\underline{x}) u_j(\underline{x}+\underline{r}) \frac{\partial u_i}{\partial x_K}(\underline{x})}\right\} = O_2\left\{\overline{-\frac{1}{\rho(x)} \frac{\partial p(\underline{x})}{\partial x_i} u_j(x+r)}\right\}$$

$$+ \nu\, O_2\left\{\overline{\frac{\partial^2 u_i(\underline{x})}{\partial x_K \partial x_K} u_j(\underline{x}+\underline{r})}\right\} + \left(\nu_v + \frac{1}{3}\nu\right) O_2\left\{\overline{\frac{\partial}{\partial x_i}\left(\frac{\partial u_K(\underline{x})}{\partial x_K}\right) u_j(\underline{x}+\underline{r})}\right\}$$

$$O_2\{c_{ij}(\underline{r})\} \equiv c_{ij}(\underline{r}) + c_{ji}(-\underline{r})$$

This equation can be simplified :

As in the incompressible case :

$$O_2 \left\{ \overline{\frac{\partial^2 u_i(\underline{x})}{\partial x_K \partial x_K} u_j(\underline{x}+\underline{r})} \right\} = 2 \nabla^2 \overline{u_i(\underline{x})\, u_j(\underline{x}+\underline{r})}$$

Also :

$$O_2 \left\{ \overline{u_K(\underline{x})\, u_j(\underline{x}+\underline{r}) \frac{\partial u_i}{\partial x_K}(\underline{x})} \right\} = -O_2 \left\{ \frac{\partial}{\partial r_K} \overline{u_K(\underline{x})\, u_j(\underline{x}+\underline{r})\, u_i(\underline{x})} \right\}$$

$$+ O_2 \left\{ \overline{\frac{\partial u_K(\underline{x})}{\partial x_K} u_j(\underline{x}+\underline{r})\, u_i(\underline{x})} \right\}$$

We set for convenience :

$$R_{ij}(\underline{r}) \equiv \overline{u_i(\underline{x})\, u_j(\underline{x}+\underline{r})}$$

$$T_{ijK}(\underline{r}) \equiv \overline{u_i(\underline{x})\, u_j(\underline{x}+\underline{r})\, u_K(\underline{x})}$$

$$W(\underline{x}) \equiv \frac{\partial u_K(\underline{x})}{\partial x_K}$$

$$S^{\alpha}_{ij}(\underline{r}) \equiv O_2 \left\{ \frac{\partial}{\partial r_K} T_{ijK}(\underline{r}) \right\}$$

$$S^{\beta}_{ij}(\underline{r}) \equiv -O_2 \left\{ \overline{W(\underline{x})\, u_j(\underline{x}+\underline{r})\, u_i(\underline{x})} \right\}$$

$$P_{ij}(\underline{r}) \equiv O_2 \left\{ \overline{-\frac{1}{\rho(\underline{x})} \frac{\partial p(\underline{x})}{\partial x_i} u_j(\underline{x}+\underline{r})} \right\}$$

$$Q_{ij}(\underline{r}) \equiv O_2 \left\{ \overline{\frac{\partial W(\underline{x})}{\partial x_i} u_j(\underline{x}+\underline{r})} \right\}$$

So that the equation for the two-points correlation tensors become :

$$\frac{\partial}{\partial t} R_{ij}(\underline{r}) = S^{\alpha}_{ij}(\underline{r}) + S^{\beta}_{ij}(\underline{r}) + P_{ij}(\underline{r}) + 2\nu \nabla^2 R_{ij}(\underline{r}) + (\nu_v + \frac{\nu}{3}) Q_{ij}(\underline{r})$$

(IV 2)

We shall now express the different tensors involved in this equation in function of measurable scalar correlations.

4) Expression of the correlation tensors $R_{ij}(\underline{r}), S^{\alpha}_{ij}(\underline{r}), S^{\beta}_{ij}(\underline{r})$ $P_{ij}(\underline{r}), Q_{ij}(r)$ in function of scalar correlations

All the tensors involved here are isotropic, since there is no preferred direction at any point in the medium, in average. It has been shown (18) that an isotropic tensor can always be expressed in function of two scalar quantities, and put under the form :

$$A_{ij}(\underline{r}) = A_1(r)\, r_i r_j + A_2(r)\, \delta_{ij}$$

$$r \equiv |\underline{r}|$$

$$r_i, r_j = \text{components of } \underline{r}$$

So, the five correlation tensors can be expressed in function of ten scalar correlations.

Now, these ten scalar correlations are not independant, but can be expressed in function of a smaller set of correlations. The reduction of the number of scalars involved will greatly simplify the the final Kármán-Howarth equation.

a) Expression of $R_{ij}(\underline{r})$

We shall express the correlation tensor $R_{ij}(\underline{r})$ in function of the ordinary correlation $f(r)$ and of a function $W_1(\underline{x})$, that will be expressed later on in function of the velocity divergence only.

Let us call $R^{(0)}_{ij}(\underline{r})$ the expression of $R_{ij}(\underline{r})$ in the incompressible case :

$$R^{(0)}_{ij}(\underline{r}) \equiv -D_r \frac{1}{2} \overline{u_1^2} f(r)\, r_i r_j + (r^2 D_r + 2) \frac{1}{2} \overline{u_1^2} f(r)\, \delta_{ij}$$

with : $\qquad D_r \equiv \frac{1}{r}\frac{\partial}{\partial r}$

And let $R^{(1)}_{ij}(\underline{r}) = R_{ij}(\underline{r}) - R^{(0)}_{ij}(\underline{r})$ to be determined.

By definition of $R_{ij}(\underline{r})$ and $f(r)$:

$$R_{11}(\underline{r}) = \overline{u_1^2} f(r) \quad \text{Where :} \quad \underline{r} = (r, 0, 0)$$

Now, by "construction" :

$$R^{(0)}_{11}(\underline{r}) = \overline{u_1^2} f(r)$$

So that $R^{(1)}_{11}(\underline{r})$ should satisfy :

$$R^{(1)}_{11}(\underline{r}) = 0 \qquad \text{for} \quad \underline{r} = (r, 0, 0) \quad \text{(IV 3)}$$

In the incompressible case,

$$\frac{\partial R_{ij}(\underline{r})}{\partial r_j} = \overline{u_i(x) \frac{\partial u_j(x+r)}{\partial x_j}} = 0 \quad \text{since} \quad \frac{\partial u_j}{\partial x_j} = 0$$

Now, in the compressible case, $\dfrac{\partial R_{ij}(\underline{r})}{\partial r_j}$ is a vector, which depends only on $\underline{r}$. By isotropy (as there is no preferred direction), $\dfrac{\partial R_{ij}(\underline{r})}{\partial r_j}$ must be parallel to $\underline{r}$. We can therefore define $W_1(r)$ by :

$$\frac{\partial R_{ij}(\underline{r})}{\partial r_j} = W_1(r)\, r_i$$

Now, by "construction",

$$\frac{\partial R^{(0)}_{ij}(\underline{r})}{\partial r_j} = 0$$

Therefore, $R^{(1)}_{ij}(\underline{r})$ should also satisfy :

$$\frac{\partial R^{(1)}_{ij}(\underline{r})}{\partial r_j} = W_1(r)\, r_i \qquad \text{(IV 4)}$$

The two conditions (IV4) and (IV5) are sufficient to determine $R^{(1)}_{ij}(\underline{r})$, and it is easily found that :

$$R^{(1)}_{ij}(\underline{r}) = \frac{W_1(r)}{2}\, r_i r_j - \frac{W_1(r)}{2}\, r^2 \delta_{ij}$$

meets all the requirements.

So, $R_{ij}(\underline{r})$ can be expressed in function of two scalars, $f(r)$ and $W_1(r)$:

$$R_{ij}(\underline{r}) = \left(-\frac{1}{2} D_r \overline{u^2} f(r) + \frac{W_1(r)}{2}\right) r_i r_j + \left(\left(r^2 D_r + 2\right) \frac{1}{2} \overline{u^2} f(r) - \frac{r^2 W_1(r)}{2}\right) \delta_{ij} \qquad \text{(IV 5)}$$

Now, $W_1(r)$ can be expressed in function of the velocity divergence only, and we shall now derive a relation between $W_1(r)$ and $W(\underline{r})$, for further purpose.

By definition of $W_1(r)$:

$$W_1(r)\, r_i = \frac{\partial}{\partial r_j} \overline{u_i(\underline{x})\, u_j(\underline{x}+\underline{r})}$$

$$= \overline{u_i(\underline{x})\, W(\underline{x}+\underline{r})}$$

$$= \overline{u_i(\underline{x}-\underline{r})\, W(\underline{x})}$$

We now take the divergence of both sides :

$$3\, W_1(r) + r\, W_1'(r) = -\overline{W(\underline{x}-\underline{r})\, W(\underline{x})} \qquad \text{(IV 6)}$$

Therefore :

$$W_1(r) = -\frac{1}{r^3}\int_0^r r^2\, \overline{W(\underline{x})W(\underline{x}+\underline{r})}\, dr + \text{const.} \qquad \text{(IV 7)}$$

The constant can be found by looking at the limits of $W_1(r)$ when r goes to zero, in equation (IV 6): assumed a development of $W_1(r)$ in power series of r :

$$W_1(r) = A + r^2 B + O(r^4)$$

it is easy to see that $r\, W_1'(r) = O(r^2)$

Therefore, the limit, when $r \to 0$ of equation (IV 6) is :

$$3\, W_1(0) = -\overline{W(\underline{x})^2}$$

Now, if we assume a development of $\overline{W(\underline{x})W(\underline{x}+\underline{r})}$ in (IV 7) and integrate, we find that :

$$W_1(r) = -\frac{1}{3}\, \overline{W[\underline{x}]^2} + \text{const} + O(r^2)$$

Therefore, the constant is zero.

b) decomposition of $S^{\alpha}_{ij}(r) = O_2\left\{ \frac{\partial}{\partial r_K} T_{ijK}(\underline{r}) \right\}$

As an isotropic tensor, $T_{ijK}(\underline{r}) = \overline{u_i(x) u_j'(x+r) u_K(x)}$ can be put under the form : (18)

$$T_{ijK}(\underline{r}) = T_1(r)\, r_i r_j r_K + T_2(r)\left[\delta_{ij} r_K + \delta_{jK} r_i \right] + T_3(r)\, \delta_{iK} r_j \quad \text{(a)}$$

$T_1(r), T_2(r), T_3(r)$ being three scalar functions of $r = |\underline{r}|$
We shall first express these functions in terms of $k(r)$, the ordinary triple correlation, and two other functions $W_2(r)$, $W_3(r)$ that will be introduced. Then we shall derive $S^{\alpha}_{ij}(\underline{r})$.

In incompressible turbulence,

$$\frac{\partial}{\partial r_j} T_{ijK}(r) = \overline{u_i(\underline{x})\, W(\underline{x}+\underline{r})\, u_K(\underline{x})}$$

is zero, since $W(\underline{x})$ is zero. In the case of occurrence of combustion, $\frac{\partial}{\partial r_j} T_{ijK}(\underline{r})$ is a second order isotropic tensor, and we have set :

$$\overline{u_i(\underline{x})\, W(\underline{x}+\underline{r})\, u_K(\underline{x})} = W_2(r)\, r_i r_K + W_3(r)\, \delta_{iK} \quad \text{(IV 8)}$$

which defines two new scalar functions $W_2(r)$ and $W_3(r)$.
By identification of the coefficients of $r_i r_K$ and δ_{iK} in $\frac{\partial}{\partial r_j} T_{ijK}(r)$ (from equation (a)) and $\overline{u_i(\underline{x})\, W(\underline{x}+\underline{r})\, u_K(\underline{x})}$ (from equation (IV 8)), one gets two differential equations involving $T_1(r)$, $T_2(r)$, $T_3(r)$:

$$\begin{cases} r\,T_1'(r) + 5\,T_1(r) + T_2'(r)/r = W_2(r) & \text{(IV 9)} \\ 2\,T_2(r) + r\,T_3'(r) + 3\,T_3(r) = W_3(r) & \text{(IV 10)} \end{cases}$$

A third equation can be obtained by writting the definition of $k(r)$:

$$k(r) = (\overline{u_1^2})^{3/2}\; T_{111}\,(r,0,0) \qquad \text{(IV 11)}$$

Equations (IV 9), (IV 10) and (IV 11) can be solved by setting the auxiliary functions $T_1^*(r)$, $T_2^*(r)$, $k^*(r)$ by :

$$\begin{cases} T_1(r) = (\overline{u_1^2})^{3/2}\,\dfrac{k^* - r k^{*\prime}}{2r^3} + T_1^* \\ T_2(r) = (\overline{u_1^2})^{3/2}\,\dfrac{2k^* + r k^{*\prime}}{4r} + T_2^* \\ T_3(r) = (\overline{u_1^2})^{3/2}\left(-\dfrac{k^*}{2r}\right) \end{cases} \qquad \text{(IV 12)}$$

Equation (IV 9) and (IV 10) reduce then to :

(k^* vanishes)

$$\begin{cases} r\,T_1^{*\prime}(r) + 5\,T_1^*(r) + T_2^{*\prime}(r)/r = W_2(r) \\ 2\,T_2^* = W_3(r) \end{cases}$$

which can be solved easily :

$$\begin{cases} T_1^*(r) = \dfrac{1}{r^5}\displaystyle\int_0^r r^4\left(W_2 - \dfrac{W_3'}{2r}\right) dr \\ T_2^*(r) = \dfrac{W_3(r)}{2} \end{cases}$$

Now,

$$T_{111}(r,0,0) = k^*(\overline{u_1^2})^{3/2} + r^3\,T_1^*(r) + 2r\,T_2^*(r)$$

$$= k\,(\overline{u_1^2})^{3/2}$$

Therefore :

$$k^{*}(r) = k(r) - \left\{ \frac{1}{r^2} \int_0^r r^4 \left(W_2 - \frac{W_3'}{2r} \right) dr + r W_3 \right\} \left(\overline{u_1^2} \right)^{-3/2} \qquad \text{(IV 13)}$$

The calculation of $S_{ij}^{\alpha}(\underline{r})$ is straightforward now, and it is found :

$$S_{ij}^{\alpha}(\underline{r}) = \left(-\frac{1}{2} D_r K^{*}(r) + 2 W_2 \right) r_i r_j$$

$$+ \left(\frac{1}{2} (r^2 D_r + 2) K^{*}(r) + 4 W_3 + r W_3' \right) \delta_{ij}$$

with : $$K^{*}(r) = \left(\frac{\partial}{\partial r} + \frac{4}{r} \right) \left(\overline{u_1^2} \right)^{3/2} k^{*}(r) \qquad \text{(IV 14)}$$

c) Decomposition of $S^{\beta}_{ij}(\underline{r}) \equiv - O_2 \{ \overline{w(x)\, u_j(x+r)\, u_i(x)} \}$

$$\overline{w(\underline{x})\, u_j(\underline{x}+\underline{r})\, u_i(\underline{x})} \quad \ldots$$

cannot be connected with :

$$\overline{u_i(x)\, w(x+r)\, u_j(x)} = W_2\, r_i r_j + W_3\, \delta_{ij}$$

and therefore, we have to introduce two new correlation functions, by the defining relation :

$$\overline{w(x)\, u_j(x+r)\, u_i(x)} = W_6\, r_i r_j + W_7\, \delta_{ij}$$

It follows :

$$S^{\beta}_{ij}(r) = - O_2 \{ W_6\, r_i r_j + W_7\, \delta_{ij} \}$$

$$= - 2\, W_6\, r_i r_j - 2\, W_7\, \delta_{ij} \qquad \text{(IV 15)}$$

d) Decomposition of $P_{ij}(\underline{r})$

We have set : $P_{ij}(\underline{r}) = O_2 \{ W_4(r)\, r_i r_j + W_5(r)\, \delta_{ij} \}$

$$P_{ij}(r) = 2\, W_4\, r_i r_j + 2\, W_5\, \delta_{ij} \qquad \text{(IV 16)}$$

e) decomposition of $\nabla^2 R_{ij}(\underline{r})$

From the expression of $R_{ij}(\underline{r})$, already found, we derive :

$$\nabla^2 R_{ij}(\underline{r}) = \nabla^2 R^{(0)}_{ij}(\underline{r}) + \left(\frac{W_1''}{2} + \frac{3W_1'}{r} \right) r_i r_j + \left(- \frac{W_1''}{2} r^2 - 3r W_1' - 2 W_1 \right) \delta_{ij}$$

(IV 17)

where : $$\nabla^2 R^{\circ}_{ij}(\underline{r}) = -\frac{1}{2} D_r \, F(r)\, r_i r_j + \frac{1}{2}\left(r^2 D_r + 2\right) F(r)\, \delta_{ij} \qquad \text{(IV 17')}$$

with : $$F(r) \equiv \left(\frac{\partial^2}{\partial r^2} + \frac{4}{r}\frac{\partial}{\partial r} \right) \overline{u_1^2}\, f(r) \qquad \text{(IV 18)}$$

as in the incompressible case.

f) <u>Decomposition of $Q_{ij}(r) \equiv O_2 \left\{ \overline{\frac{\partial w}{\partial x_i}(\underline{x})\, u_j(\underline{x}+\underline{r})} \right\}$</u>

We shall now show that $Q_{ij}(r)$ can be expressed in function of $W_1(r)$ only.

$$Q_{ij}(\underline{r}) = O_2 \left\{ \overline{\frac{\partial w}{\partial x_j}(\underline{x})\, u_i(\underline{x}-\underline{r})} \right\}$$

since : $O_2 \{ C_{ij}(\underline{r}) \} = O_2 \{ C_{ji}(-\underline{r}) \}$

$$Q_{ij}(\underline{r}) = O_2 \left\{ \overline{\frac{\partial w}{\partial x_j}(x+r)\, u_i(x)} \right\} = O_2 \left\{ \frac{\partial}{\partial r_j} \overline{w(x+r)\, u_i(x)} \right\}$$

$$= O_2 \left\{ \frac{\partial}{\partial r_j} W_1(r)\, r_i \right\}$$

by definition of $W_1(r)$ (IV 4)

Hence : $$Q_{ij}(\underline{r}) = O_2 \left\{ W_1' \frac{r_i r_j}{r} + W_1\, \delta_{ij} \right\} \qquad \text{(IV 19)}$$

The decomposition of all the tensors involved in (IV 2) is now complete. All the coefficients of $r_i r_j$ and δ_{ij} for each tensor are given in table (I), columns 1 and 2.

5) Kármán-Howarth equation

Equation (IV 2) can be put under the form :

$$A(r)\, r_i r_j + B(r)\, \delta_{ij} = C(r)\, r_i r_j + D(r)\, \delta_{ij}$$

and is equivalent to the two scalar equations :

$$A(r) = C(r)$$
$$B(r) = D(r)$$

Therefore :

$$r^2 A(r) + B(r) = r^2 C(r) + D(r)$$

which is a new Kármán-Howarth equation. The terms corresponding to the different correlations are given in column (3). For instance, the terms corresponding to $\frac{\partial}{\partial t} R_{ij}(r)$ are :

$\frac{\partial}{\partial t} \left\{ - D_r \frac{1}{2} \overline{u_1^2} f(r) + \frac{W_1}{2} \right\}$ coefficient of $r_i r_j$

$\frac{\partial}{\partial t} \left\{ (r^2 D_r + 2) \frac{1}{2} \overline{u_1^2} f(r) - \frac{W_1 r^2}{2} \right\}$ coefficient of δ_{ij}

$\frac{\partial}{\partial t} \overline{u_1^2} f(r)$ in the Kármán-Howarth equation.

Note that the term corresponding to P_{ij} in the Kármán Howarth equation is $2 r^2 W_4(r) + 2 W_5(r)$ according to columns (1) and (2). Now,

$$2 r^2 W_4 + 2 W_5 = - \frac{2}{\rho(\underline{x})} \overline{\frac{\partial p(\underline{x})}{\partial x_i} u_1(\underline{x}+\underline{r})}$$

for $\underline{r} = (r,0,0)$

by an appropriate choice of i, j and $\underline{r}$ in (IV 16)

We shall denote this correlation function by :

$-\overline{\frac{2}{\rho}\frac{\partial p}{\partial x_1} u_1(r)}$ for convenience.

The same remark applies to the term corresponding to S^{β}_{ij}, which is $-2W_6(r)\,r^2 - 2W_7(r)$, which can be written :

$$-2\,\overline{u_1(\underline{x})W(\underline{y})u_1(\underline{x}+\underline{r})} = -2\,\overline{u_1 W u_1(r)} \qquad \text{with } \underline{r} = (r,0,0)$$

The other terms involved come directly from the decomposition of the correlation tensors, in section 4.

The new Kármán-Howarth equation is :

$$\frac{\partial}{\partial t}\,\overline{u_1^2} f(r) = \left(\frac{\partial}{\partial r} + \frac{4}{r}\right)\left(\overline{u_1^2}\right)^{3/2} k^*(r) + 2r^2 W_2 + 4W_3 + rW_3'$$

$$-2\,\overline{u_1 W u_1(r)} + 2\;\overline{-\frac{1}{\rho}\frac{\partial p}{\partial x_1} u_1(r)}$$

$$+2\nu\left[\left(\frac{\partial^2}{\partial r^2} + \frac{4}{r}\frac{\partial}{\partial r}\right)\overline{u_1^2} f(r) - 2W_1\right]$$

$$+\left(\mathcal{N}_\nu + \frac{1}{3}\nu\right)\left[rW_1' + W_1\right] \qquad \text{(IV 20)}$$

with :

$$\begin{cases} k^*(r) \equiv k(r) - \left\{\dfrac{1}{r^2}\displaystyle\int_0^r r^4\left(W_2 - \dfrac{W_3'}{2r}\right)dr + rW_3\right\}\left(\overline{u_1^2}\right)^{-3/2} & \text{(IV 13)} \\ \overline{u_i(\underline{x})u_j(\underline{x})W(x+r)} \equiv W_2\, r_i r_j + W_3\,\delta_{ij} & \text{(IV 18)} \\ W_1(r) \equiv -\dfrac{1}{r^3}\displaystyle\int_0^r r^2\,\overline{W(\underline{x})W(\underline{x}+\underline{r})}\,dr & \text{(IV 7)} \end{cases}$$

6) Development in power series of r of the Kármán-Howarth equation, derivation of the mean square velocity equation and of a mean square vorticity equation.

We shall first expand $W_1(r), W_2(r), W_3(r)$ in power series of r, then develop the whole Kármán-Howarth equation.

Since : $$W_1(r) \equiv -\frac{1}{r^3}\int_0^r \overline{W(\underline{x})W(\underline{x}+\underline{r})}\, r^2\, dr$$

(IV 7)

and : $$\overline{W(\underline{x})W(\underline{x}+\underline{r})} = \overline{[W(\underline{x})]^2} + \frac{r^2}{2}\ \overline{W[\underline{x}]\frac{d^2W}{dx_1^2}[\underline{x}]} + O(r^4)$$

$$= \overline{W^2} - \frac{r^2}{2}\ \overline{W'^2} + O(r^4)$$

with the notation :

$$\overline{W^2} = \overline{W(\underline{x})^2}$$

$$\overline{W'^2} = \overline{\left(\frac{dW}{dx_1}\right)^2}$$

Then :

$$W_1(r) = -\frac{1}{3}\overline{W^2} + \frac{r^2}{10}\overline{W'^2} + O(r^4)$$

Now, from the definition of W_2 and W_3 (IV 8) :

$$r^2 W_2 + W_3 = \overline{u_1^2 W(r)}$$

$$W_3 = \overline{u_2^2 W(r)}$$

with the notations :

$$\overline{u_1^2 W(r)} \equiv \overline{u_1(\underline{x})\, u_1(\underline{x})\, W(\underline{x}+\underline{r})}$$
$$\overline{u_2^2 W(r)} \equiv \overline{u_2(\underline{x})\, u_2(\underline{x})\, W(\underline{x}+\underline{r})}$$

for $\underline{r} = (r,0,0)$

Therefore :

$$W_2(r) = \frac{1}{2}\left(\overline{u_1^2 W''} - \overline{u_2^2 W''}\right) + O(r^2) \qquad \text{(IV 21)}$$

$$W_3(r) = \overline{u_2^2 W} + \frac{r^2}{2}\,\overline{u_2^2 W''} + O(r^4) \qquad \text{(IV 22)}$$

Note that $\overline{u_1^2 W} = \overline{u_2^2 W}$ by isotropy

but $\overline{u_1^2 W''} \neq \overline{u_2^2 W''}$ in general

Now, all the coefficients of the Kármán-Howarth equation can be expanded easily (see columns 4 and 5 of the table)

As an example, consider the term corresponding to $S_{\cdot j}^{\alpha}$ in the Kármán Howarth equation :

$$K^*(r) + 2r^2 W_2 + 4 W_3 + r W_3'$$

$$= \left(\frac{\partial}{\partial r} + \frac{4}{r}\right)\left\{ (\overline{u_1^2})^{3/2} k(r) - \frac{1}{r^2}\int_0^r r^4\left(W_2 - \frac{W_3'}{2r}\right)dr - r W_3 \right\}$$

$$+ 2r^2 W_2 + 4 W_3 + r W_3'$$

by definition of K^*(IV 14) and k^* (IV 12)

$$= \left(\frac{\partial}{\partial r} + \frac{4}{r}\right)\left\{ (\overline{u_1^2})^{3/2} k_0''' \frac{r^3}{6} - \frac{r^3}{5}\left(\frac{\overline{u_1^2 W''}}{2} - \overline{u_2^2 W''}\right) - r\,\overline{u_2^2 W} - \frac{r^3}{2}\overline{u_2^2 W''}\right\}$$

$$+ 4\,\overline{u_1^2 W} + r^2\left[\overline{u_1^2 W''} + 2\,\overline{u_2^2 W''}\right] + O(r^4)$$

by use of relations (IV 21) , (IV 22) and

$$k(r) = \frac{r^3}{12} k_0''' + O(r^5)$$

(as in the incompressible case (7))

So, the term corresponding to S^{α}_{ij} in the Kármán-howarth equation is :

$$- \overline{u_1^2 w} + r^2 \left\{ \frac{7}{6} (\overline{u^2})^{3/2} k'''_0 + \frac{3}{10} \overline{u_1^2 W''} - \frac{1}{10} \overline{u_2^2 W''} \right\}$$

which is found in column 4 and 5 of the table.

The development of the Kármán-Howarth equation at the order zero gives the "mean square velocity equation"

$$\frac{d}{dt} \overline{u_1^2} = - \overline{u_1^2 W} - \overline{\frac{2}{\rho} \frac{\partial p}{\partial x_1} u_1} + 10 \nu f''_0 \overline{u_1^2} + \frac{4}{3} \nu \overline{W^2} + (\nu_v + \frac{\nu}{3})(-\frac{2}{3} \overline{W^2})$$

Now, since the mean square vorticity is related to the mean square velocity by :

$$\overline{\Omega_1^2} = - 5 f''_0 \overline{u_1^2}$$

(as in the incompressible case (7))

the development at order two of the Kármán-Howarth equation, multiplied by -10, will give the "mean square vorticity equation" :

$$\frac{d \overline{\Omega_1^2}}{dt} = - \frac{35}{3} k'''_0 (\overline{u^2})^{3/2} - \frac{70}{3} \nu f^{IV}_0 \overline{u^2} + \overline{u_2^2 W''} - 3 \overline{u_1^2 W''}$$

$$+ 10 \overline{u_1 W u_1''} + 10 (- \overline{\frac{1}{\rho} \frac{\partial p}{\partial x_1} u_1''}) + 4 \nu \overline{W'^2} - (\nu_v + \frac{\nu}{3}) 6 \overline{W'^2}$$

7) Estimation of $W(\chi)$ in the case of combustion

Until now, we have not made any assumption with respect to the physical process of combustion. We shall now show that with a reasonable hypothesis, the divergence of the velocity can be connected to the local heat release.

The density fluctuations are either due to acoustic travelling waves or fluctuations of reaction rate. In the first case, the relative fluctuations of pressure are usually very small compared to one (for a sound of 80 dB, $\left|\frac{p'}{\bar{p}}\right| \sim 2 . 10^{-6}$). It is then a good assumtion, when the combustion is not too weak, to neglect the effect of the sound waves as compared to the effects of combustion, on the density fluctuations. With this assumption, an estimation of W_1 can be made.

From the continuity equation :

$$\frac{1}{\sigma}\frac{D\sigma}{Dt} = \nabla \cdot \underline{u} = W$$

$$\sigma \equiv 1/\rho$$

Now, the energy equation can be written : (10)

$$\frac{p}{R}\frac{D\varepsilon}{Dt} = Q \quad \text{or} \quad \frac{1}{p}\frac{Dp}{Dt} + \gamma\frac{1}{\sigma}\frac{D\sigma}{Dt} = (\gamma-1)\frac{Q}{p} \qquad \text{(IV 23)}$$

$$\begin{cases} Q : \text{ rate of heat release, per unit volume.} \\ \varepsilon \equiv c_v \log\left\{\frac{p}{p_{ref}}\left(\frac{\sigma}{\sigma_{ref}}\right)^{\gamma}\right\} \end{cases}$$

At constant volume, the mean pressure decreases during the combustion, but the mean density is constant. Therefore :

$$\left| \overline{\frac{1}{\sigma} \frac{D\sigma}{Dt}} \right| \ll \left| \overline{\frac{1}{p} \frac{Dp}{Dt}} \right|$$

And :

$$\frac{\gamma}{\sigma} \frac{D\sigma}{Dt} = (\gamma - 1) \left(\frac{Q}{p}\right)' - \left(\frac{1}{p} \frac{Dp}{Dt}\right)'$$

(..)' : absolute fluctuations, relative to the mean value.

Therefore :

$$W(\underline{x}) = \frac{\gamma - 1}{\gamma} \left(\frac{Q}{p}\right)'(x) - \frac{1}{\gamma} \left(\frac{1}{p} \frac{Dp}{Dt}\right)'(\underline{x})$$

With our assumption that the density fluctuations are related with the heat released, and not with the acoustic fluctuations, the second term of the right hand side is negligeable as compared to the first, so we can write :

$$W(\underline{x}) = \frac{\gamma - 1}{\gamma} \left(\frac{Q}{p}\right)'(\underline{x}) \qquad \text{(IV 24)}$$

8) Discussion

The Kármán-Howarth equation generalized to the case of combustion can be considered as a relation between correlation functions, which is exact as far as the Navier-Stokes equations are available, and the influence of the kinematic viscosity variations negligible. New terms in this equation take into account the specific effects of combustion on turbulence.

Now, orders of magnitude of these phenomena can only be given by experimental measurements of the new correlations, and we do not expect to deduce orders of magnitude from the theory itself for several reasons. First, we have used an averaging method which loses information necessarily. Also, in the case of combustion, a strong coupling between the flow and the chemical reaction is expected, and it is not possible to obtain orders of magnitude by considering only one of the three governing equations, as we have done. In other words, we have not introduced enough information about the processes to get quantitative results.

Important conclusions may however be drawn by examination of some of the correlation functions.

In the Kármán-Howarth equation, the correlation taking into account the "pressure density" effect is :

$$-2\,\overline{\sigma\frac{\partial p}{\partial x_1}\,u_1(r)}$$

as it comes from the term $-\sigma\nabla p$ of the Navier-Stokes equation.

It is remarkable that this correlation is a function of a component of the pressure gradient : $\frac{\partial p}{\partial x_1}$ and a component of the velocity u_1 that are parallel : in the terminilogy of Chu and Kovasnay (10), the pressure gradient and velocity associated with the sound mode are parallel, whereas they are orthogonal in the vorticity mode (pressure gradients balance centrifugal forces). Therefore, it seems that the information concerning the velocity mode is eliminated in this product, and that the pressure density effect involves essentially the pressure and entropy modes.

We now examine the qualitative influence of the "pressure density effect" on the mean square velocity. The correlation appearing in the mean square velocity equation is: $-2\,\overline{\sigma\frac{\partial p}{\partial x_1}u_1}$

Now :

$$-2\,\overline{\sigma\frac{\partial p}{\partial x_1}u_1} = -\frac{2}{3}\lim_{r\to 0}\left\{\overline{\sigma(\underline{x})\frac{\partial p}{\partial x_i}(\underline{x}+\underline{r})\,u_i(\underline{x})}\right\}$$

$$= -\frac{2}{3}\lim_{r\to 0}\left\{\frac{\partial}{\partial r_i}\overline{\sigma(\underline{x})\;\;p(\underline{x}+\underline{r})\,u_i(\underline{x})}\right\}$$

$$= -\frac{2}{3}\lim_{r\to 0}\left\{\frac{\partial}{\partial r_i}\overline{\sigma(\underline{x}-\underline{r})\,p(\underline{x})\,u_i(\underline{x}-\underline{r})}\right\}$$

Hence : $$2\left(-\overline{\frac{1}{\rho}\frac{\partial p}{\partial x_1}u_1}\right) = \frac{2}{3}\left(\overline{p\sigma W} + \overline{p u_i \frac{\partial \sigma}{\partial x_i}}\right)$$

Lets examine first the correlation $\overline{p\sigma W}$. Assuming perfect gas,

$$\overline{p\sigma W} = \mathcal{R}\ \overline{TW}$$

$$= \mathcal{R}\ \overline{T'W} \qquad \text{since : } \overline{W} = 0$$

Now, according to section 7,

$$W = \frac{\gamma-1}{\gamma}\left(\frac{Q}{p}\right)'$$

$$= \frac{\gamma-1}{\gamma}\left(\frac{\bar{Q}}{\bar{p}}\right)\left[\frac{Q'}{\bar{Q}} - \frac{p'}{\bar{p}}\right]$$

The relative fluctuations of pressure are usually very small compared to one*, and it is a good assumption to set :

$$\left|\frac{Q'}{\bar{Q}}\right| \gg \left|\frac{p'}{\bar{p}}\right|$$

Therefore :

$$W = \frac{\gamma-1}{\gamma}\frac{Q'}{\bar{p}}$$

and :

$$\overline{p\sigma W} = \frac{\gamma-1}{\gamma}\frac{\mathcal{R}}{\bar{p}}\overline{Q'T'}$$

Consider now two point in our medium, with temperature $\bar{T}_1 + \Delta T_1$, $\bar{T} - \Delta T_2$. For exothermic reaction and positive activation energy, the local heat released will be $\bar{Q} + \Delta Q_1$ and $\bar{Q} - \Delta Q_2$ an instant later. In both cases, $(\Delta T_1)(\Delta Q_1) > 0$ and $(-\Delta T_2)(-\Delta Q_2) > 0$. Therefore, $\overline{Q'T'} > 0$ and $\overline{p\sigma W} > 0$. This correlation is expected to be important , since

* For a noise of 80 dB, $\left|\frac{p'}{p}\right| \sim 2 . 10^{-6}$

regions of higher heat released should also be regions of higher temperature.

We now examine the other correlation $\overline{p\, u_K \frac{\partial \sigma}{\partial x_K}}$ appearing in $\overline{-\frac{1}{\rho} \frac{\partial p}{\partial x_1} u_1}$.

From the continuity equation,

$$\frac{\partial \sigma}{\partial t} + u_K \frac{\partial \sigma}{\partial x_K} = \sigma W$$

we derive :

$$\overline{p \frac{\partial \sigma}{\partial t}} + \overline{p\, u_K \frac{\partial \sigma}{\partial x_K}} = \overline{p\, \sigma W}$$

which is equivalent to : (since $\bar{\sigma}$ = const.)

$$\overline{p' \frac{\partial \sigma'}{\partial t}} + \bar{p}\, \overline{u_K \frac{\partial \sigma}{\partial x_K}} + \overline{p'\, u_K \frac{\partial \sigma}{\partial x_K}} = \bar{p}\, \overline{\sigma W} + \overline{p' \sigma W}$$

We shall assume $\left| \frac{p'}{\bar{p}} \right|$ very small compared to one. The leading terms $\bar{p}\, \overline{\sigma W}$ for the right hand side, and $\bar{p}\, \overline{u_K \frac{\partial \sigma}{\partial x_K}}$ for the left hand side. These two terms are however equal, by average of the continuity equation. It is therefore concluded that :

$$\overline{p\, u_K \frac{\partial \sigma}{\partial x_K}} \simeq \overline{p\, \sigma W}$$

and that the correlation $\overline{-\frac{2}{\rho} \frac{\partial p}{\partial x_1} u_1}$ is equal to $\frac{4}{3}\, \overline{p \sigma W}$

It follows as $\overline{p \sigma W} > 0$, that the "pressure density effect" leads to an increase in mean square velocity fluctuations.

An increase in mean square velocity fluctuation could related either to an increase in turbulent kinetic energy, or generation of sound waves.

Now, in the mean square vorticity equation, the correlation corresponding to the "pressure-density effect" is : $-\overline{\frac{2}{\rho}\frac{\partial p}{\partial x_1}\frac{\partial^2 u_1}{\partial x_1^2}}$. It has not been possible to determine the sign of this quantity by physical considerations. If the correlation function $-\overline{\frac{1}{\rho}\frac{\partial p}{\partial x_1}u_1(r)}$ can be measured experimentally, the sign of the correlation $-\overline{\frac{2}{\rho}\frac{\partial p}{\partial x_1}\frac{\partial^2 u_1}{\partial x_1^2}}$ can be deduced from the curvature of the former function near the point $r = 0$. If the correlation decreases, then $-\overline{\frac{2}{\rho}\frac{\partial p}{\partial x_1}\frac{\partial^2 u_1}{\partial x_1^2}}$ is negative and, according to the mean square vorticity equation, this would mean that combustion generate vorticity by the "pressure density " effect. Inverse conclusions may be drawn if the correlation function $-\overline{\frac{1}{\rho}\frac{\partial p}{\partial x_1}u_1(r)}$ decreased near $r = 0$.

It has not been possible unfortunately to make such deductions for the other new terms appearing in the Karman-Howarth equation. Experiments should determine whether or not these new terms balance the pressure-density terms that we have just studied.

Conclusion

A Kármán Howarth equation valid in the case of homogeneous isotropic turbulence with occurence of combustion has been derived. New terms in the zeroth and second order expansion in r show the influence of the chemical reaction on the mean square velocity and vorticity. It is found that exothermic reactions should generate turbulent velocity fluctuations or pressure waves, and that additionnal vorticity might be generated, by interaction of sound waves. The corresponding terms have been expressed in function of theorically measurable quantities, and, though difficult, an order of magnitude might be given by experiments.

CHAPTER V GENERATION OF VORTICITY BY INTERACTION OF SOUND WAVES

INTRODUCTION

In the last chapter, it has been shown that in the case of homogeneous isotropic turbulence, with occurence of combustion, additionnal turbulence might be generated. The source term in the statistical averaged vorticity equation is a correlation, which represents the mean effect of the phenomenon associated with $\nabla\sigma \times \nabla p$ of the vorticity equation. This term involves only the sound wave and entropy modes, in the terminology of Chu and Kovasnay (10), not the vorticity mode, hence suggesting that the mechanism of generation of vorticity in combustion involves essentially chemical reaction and sound waves. This is the purpose of the present chapter to study how interaction of sound waves, with occurence of chemical reaction can generate vorticity, and what are the significant parameters. A model is developed, and numerical computations give orders of magnitude.

ANALYSIS

A) The process of generation of vorticity by sound waves

If a gradient of pressure is applied to particles of different densities, those of lower density will acquire, in the same conditions, higher velocity than the heavier ones. Now, if the gradient of pressure is applied to a medium of varying density in the direction orthogonal to the pressure gradient, a shear wave will be induced, and therefore, vorticity. In the vorticity equation, this process is taken into account by the term : $\nabla p \times \nabla \sigma$

Now, it has been shown experimentally and theorically (16, 17), that a sound wave propagating in a reacting medium induces local fluctuations of reaction rate, and therefore, extra-variations in density. So, we have simultaneously gradients of pressure and gradients of density. Now, as the effect of one sound wave is essentially one dimensionnal, the gradient of pressure and the gradient of density induced by the process mentionned before are always parallel, therefore the cross product $\nabla p \times \nabla \sigma$ is zero everywhere, and no vorticity is generated. So, two sound waves, at least, are necessary to have vorticity : the pressure gradient of one sound wave interacting with the density gradient of the other and vice versa.

When no reaction occurs, however, the two interaction terms cancel out, and no vorticity is generated :

$$\frac{p_1'}{\bar{p}} + \gamma \frac{\sigma_1'}{\bar{\sigma}} = 0 \qquad \frac{p_2'}{\bar{p}} + \gamma \frac{\sigma_2'}{\bar{\sigma}} = 0$$

$p_1', p_2', \sigma_1', \sigma_2'$: pressure and specific volume fluctuations

imply : $$\nabla\sigma \times \nabla p = \underline{K_1} \times \underline{K_2} \left(\frac{\partial p_1'}{\partial x} \cdot \frac{\partial \sigma_2'}{\partial y} - \frac{\partial p_2'}{\partial y} \cdot \frac{\partial \sigma_1'}{\partial x} \right)$$

$\underline{K_1}, \underline{K_2}$: wave number of the sound waves

When reaction occurs, the relation :

$$\gamma \frac{\sigma'}{\bar{\sigma}} + \frac{p'}{\bar{p}} = 0$$

do not hold any more, but, as it will be shown in the next paragraph, the density fluctuation at a point depends among other parameters, on the frequency of the sound waves. In other words, two sound waves, for the same chemical reaction, will induce fluctuations of density that are not similar to each other. Therefore, the two interaction terms do not cancel out generally, and vorticity is generated.

This quick approach shows that the physics of the problem is not simple, and the development of a model, as a computed solution, will give more insight and orders of magnitude.

B) Our model

We shall consider an homogeneous stagnant medium, in a very large enclosure, filled with a mixture of gas able to react homogeneously by external means, such as hydrogen and chlorine when irradiated by U.V. light.

Before reaction begins to occur, two sound waves are travelling in the medium, and meet in a sufficiently small volume, so that interaction sound - sound could be neglected. The angle between the two sound waves is θ .

C) Governing equations

We shall call "mean" the average in space, at a given time. Mean quantities will depend on time, except for the density, since we assume constant volume reaction. The fluctuations relative to the mean quantities will be funtions of time and space.

Since our medium is initially at rest, and the relative pressure fluctuations small compared to one, the governing equations are the linearized Navier-Stokes equations, exact to a good approximation. We shall neglect the molecular effects, conductivity, viscosity, diffusion of species. With a little of algebra : (see appendix II)

$$
(\text{V } 1) \qquad \begin{cases} \dfrac{\partial^2 P^{(1)}}{\partial t^2} - a^2(t)\, \nabla^2 P^{(1)} = \dfrac{\partial}{\partial t} \left(\dfrac{Q}{\varrho C_p T} \right)^{(1)} \\[2ex] \qquad\qquad\qquad \dfrac{\partial S^{(1)}}{\partial t} = \left(\dfrac{Q}{\varrho C_p T} \right)^{(1)} \end{cases}
$$

$$
\text{with :} \qquad P^{(1)} \equiv \frac{p^{(1)}}{\gamma\, \bar{p}(t)} \qquad S^{(1)} \equiv P^{(1)} - \frac{\varrho^{(1)}}{\bar{\varrho}} \qquad a^2(t) \equiv \gamma \mathcal{R} T
$$

Q : heat released per unit volume and time.

It is to be noticed that the relative fluctuations of pressure are with respect to the mean pressure, which is here a function of time.

D) Chemical kinetics assumptions, expression of $\left(\frac{Q}{\rho C_p T}\right)^{(1)}$

Since our main purpose is to show the processes involved in the generation of vorticity, and to give orders of magnitude, simple chemical assumptions have been chosen : we shall consider the reaction : A + B → C + D, and we shall assume :

1) first order reaction rate in component A
2) the reaction rate dependance on temperature to be of an Arrhenius form.

In fact, little is known about the kinetics of chemical reaction when temperature, pressure, and species concentration fluctuate. In this direction, efforts have to be done.

The mean temperature and concentration of component A are governed by :

$$\begin{cases} \rho C_v \dfrac{DT}{Dt} = -\Delta U \, W_A - p \, \nabla \cdot \underline{u} \\ \rho \dfrac{DY_A}{Dt} = W_A \end{cases}$$

with : $W_A = -K \, Y_A \exp\left(-\frac{E}{RT}\right)$

Y_A : mass fraction of component A

W_A : mass rate of production of component A per unit volume

ΔU : heat of reaction, per unit mass of component A

K : kinetic constant

E : activation energy.

Taking the average, and neglecting the second order terms $\overline{\underline{u} \cdot \nabla \rho^{(1)}}$, $\overline{\underline{u} \cdot \nabla Y_A^{(1)}}$, $\overline{\rho^{(1)} \nabla \cdot \underline{u}}$ as compared with the mean time derivatives :

$$\left\{ \begin{aligned} \bar{\rho}\, C_v \frac{d\bar{T}}{dt} &= -\Delta U\, \overline{W_A} \\ \bar{\rho}\, \frac{d\bar{Y}_A}{dt} &= \overline{W_A} \end{aligned} \right.$$

Hence :

$$\frac{d}{dt}\left(C_v \bar{T} + \Delta U\, Y_A \right) = 0$$

$$\bar{Y}_A = Y_{A,0} + \frac{C_v}{\Delta U}\left[T_0 - \bar{T} \right]$$

Changing $\bar{Y}_A$ for its expression in function of $\bar{T}$ in the energy equation, we obtain a differential equation involving only $\bar{T}$:

$$\text{(V 2)} \qquad \bar{\rho}\, C_v \frac{d\bar{T}}{dt} = \Delta U\, K \left[Y_{A,0} + \frac{C_v}{\Delta U}\left[T_0 - \bar{T} \right] \right] \exp\left(-\frac{E}{R\bar{T}}\right)$$

which gives $\bar{T}$ in function of time by integration.

We now wish to express $\left(\frac{Q}{\rho\, c_p T}\right)^{(1)}$ in function of $S^{(1)}$ and $P^{(1)}$.

According to (V 2) :

$$\bar{Q} = \Delta U \cdot K \left[Y_{A,0} + \frac{C_v}{\Delta U} \left[T_0 - \bar{T} \right] \right] \exp\left(-\frac{E}{R\bar{T}}\right) \qquad (V\ 3)$$

valid for all times.

$\bar{Q}$ can be considered as a function of $\bar{T}$. Now, for small fluctuations of temperature, we shall assume :

$$Q^{(1)} = \left(\frac{d\bar{Q}}{d\bar{T}}\right) T^{(1)} \qquad (V\ 4)$$

Note that this expression does not take into account the difference of phase between $Q^{(1)}$ and $T^{(1)}$ due to chemical induction times, and we do not assume any dependance of $Q^{(1)}$ on $P^{(1)}$. However, this expression seems realistic to the author, as far as the induction times are small compared with the characteristic acoustic times, and that the pressure has no direct effect on chemical reaction.

From relations (V 3) and (V 4), an expression for $\left(\frac{Q}{\rho C_p T}\right)^{(1)}$ in function of $S^{(1)}$ and $P^{(1)}$ can be found :

$$\left(\frac{Q}{\rho C_p T}\right)^{(1)} = \frac{1}{\bar{\rho} C_p \bar{T}} Q^{(1)} + \bar{Q} \left(\frac{1}{\rho C_p T}\right)^{(1)}$$

$$= \frac{1}{\bar{\rho} C_p} \frac{d\bar{Q}}{d\bar{T}} \left(S^{(1)} + (\gamma - 1) P^{(1)} \right) - (\gamma - 1) \frac{\bar{Q}}{\bar{p}} \cdot \frac{p^{(1)}}{\gamma \bar{p}}$$

$$= \frac{1}{\bar{\rho} C_p} \frac{d\bar{Q}}{d\bar{T}} S^{(1)} + \frac{1}{\bar{\rho} C_p} \left[(\gamma - 1) \frac{d\bar{Q}}{d\bar{T}} - \gamma \frac{\bar{Q}}{\bar{T}} \right]$$

We set for convenience :

$$W_1 \equiv \frac{1}{\bar{\rho} C_p} \frac{d\bar{Q}}{d\bar{T}}$$

$$= \frac{K \Delta U}{\bar{\rho} C_p} \exp\left(-\frac{E}{R\bar{T}}\right) \left\{ \left(Y_{A,0} - C_v \frac{(\bar{T} - T_0)}{\Delta U} \right) \frac{E}{R\bar{T}^2} - \frac{C_v}{\Delta U} \right\}$$

$$W_2 \equiv \frac{1}{\bar{\rho} C_p} \left[(\gamma - 1) \frac{d\bar{Q}}{d\bar{T}} - \gamma \frac{\bar{Q}}{\bar{T}} \right]$$

$$= \frac{K \Delta U}{\bar{\rho} C_p} \exp\left(-\frac{E}{R\bar{T}}\right) \left\{ (\gamma - 1) \left(Y_{A,0} - C_v \frac{(\bar{T} - T_0)}{\Delta U} \right) \frac{E}{R\bar{T}^2} - (\gamma - 1) \frac{C_v}{\Delta U} - \gamma \frac{Y_{A,0} - C_v \frac{(\bar{T} - T_0)}{\Delta U}}{\bar{T}} \right\}$$

So that :

$$\left(\frac{Q}{\rho C_p T} \right)^{(1)} = W_1 S^{(1)} + W_2 P^{(1)}$$

Our equations become

$$\bar{\rho} C_v \frac{d\bar{T}}{dt} = K \Delta U \left[Y_{A,0} - \frac{\bar{T} - T_0}{\Delta U} C_v \right] \exp\left(-\frac{E}{R\bar{T}}\right)$$

(V 5) $$\frac{\partial^2 P^{(1)}}{\partial t^2} - a^2(t) \nabla^2 P^{(1)} = \frac{\partial}{\partial t} \left(W_1 S^{(1)} + W_2 P^{(1)} \right)$$

$$\frac{\partial S^{(1)}}{\partial t} = W_1 S^{(1)} + W_2 P^{(1)}.$$

E) Constant wave number hypothesis and transformation of the system of partial differential equations into ordinary differential equations

Consider a one-dimensionnal travelling wave, periodic in space,(wave number $\underline{k}$), and we suppose that the speed of sound changes, due to chemical reaction. Let's A,B two consecutive nodes ($AB = 2\pi / \underline{k}$ at time $t = 0$), A and B travelling at the speed of sound. Now, if the speed of sound is uniformely varying, the distance AB will remain constant. That is to say the wave number will remain constant.

When the sound wave is produced by a loudspeaker emitting at constant frequency, the wave number of the sound near the source will change, due to change in temperature, but the disturbance will not be felt at a distance superior to :

$$\int_0^t a(\eta)\, d\eta$$

$a(\eta)$: speed of sound at time η

t : duration of the chemical reaction

If we are far enough from the loudspeaker, the wave number should remain constant, equal to its value before reaction begins to occur.

With this remark, the governing partial differential equations can be transformed into ordinary diffrential equations.

If $P^{(1)}(\underline{x},t)$ is periodic in space, then $S^{(1)}(\underline{x},t)$ is periodic too, according to the linearity of the equations. So, we can set :

$$\begin{cases} P^{(1)}(\underline{x},t) = \sum P_n^{(1)}(t) \exp(in\,\underline{k}\cdot\underline{x}) \\ S^{(1)}(\underline{x},t) = \sum S_n^{(1)}(t) \exp(in\,\underline{k}\cdot\underline{x}) \end{cases}$$

The partial differential equations are tranformed into a set of ordinary differential equations, with time-varying coefficients :

$$\begin{cases} \dfrac{d^2 P_n^{(1)}}{dt^2} + n^2 a^2(t)\, k^2\, P_n^{(1)} = \dfrac{d}{dt}\left[W_1 S_n^{(1)} + W_2 P_n^{(1)}\right] \\ \dfrac{dS_n^{(1)}}{dt} = W_1 S_n^{(1)} + W_2 P_n^{(1)} \end{cases}$$

Now, if $P_n^{(1)}=0$ at time $t=0$, as well as all its derivatives, it results that $P_n^{(1)}=0$ for all times. It is therefore concluded that no new wave number will be generated in this process.

This remark allows us to consider the effect of one single harmonic wave, without loss of generality. We shall now use the complex notation $\hat{P}$, $\hat{S}$, with the following meaning :

$$P = \mathrm{Re}\ (\ \hat{P}^{(1)}\ )$$

$$S = \mathrm{Re}\ (\ \hat{S}^{(1)}\ )$$

$$\mathrm{Re}\ (\,)\ :\ \text{real part of}\ (\,)$$

Since the wave number $\underline{k}$ is constant, we can set:

$$\hat{P}^{(1)} = \tilde{P}^{(1)}(t)\ \exp\ (\ i\ \underline{k}.\underline{x}\ )$$

$$\hat{S}^{(1)} = \tilde{S}^{(1)}(t)\ \exp\ (\ i\ \underline{k}.\underline{x}\ )$$

where $\tilde{P}^{(1)}(t)$ and $\tilde{S}^{(1)}(t)$ are the complex amplitudes of the fluctuation of pressure and entropy in space.

The equations for $\tilde{P}^{(1)}(t)$ and $\tilde{S}^{(1)}(t)$ are, for each sound wave :

$$\frac{d^2\tilde{P}_j^{(1)}}{dt^2} + a^2 k_j\ \tilde{P}_j^{(1)} = \frac{d}{dt}\ (\ W_1 \tilde{S}_j^{(1)} + W_2 \tilde{P}_j^{(1)})$$

$$\frac{d\tilde{S}_j^{(1)}}{dt} = W_1 \tilde{S}_j^{(1)} + W_2 \tilde{P}_j^{(1)}$$

$$(\ j = 1,\ 2\ )$$

which gives a system of four ordinary differential equations.

On these equations, two remarks can be made :

1) We have included any phase difference between $\hat{P}^{(1)}$ and $\hat{S}^{(1)}$ in $\tilde{P}^{(1)}$ and $\tilde{S}^{(1)}$, so that there is generally a phase

difference, in our system, between entropy and pressure.

2) We have taken into account the fluctuations of concentrations of species A, which corresponds, in the previous work by Pariseanu (16) to the case he studied when $m = 1$.

F) Expression of the vorticity generated in function of $S^{(1)}$ and $P^{(1)}$.

The complete vorticity equation is, neglecting the viscous terms :

$$\frac{D\underline{\Omega}}{Dt} = \underline{\Omega}.\nabla\underline{u} - \underline{\Omega}\,\nabla.\underline{u} - \nabla\sigma\times\nabla p$$

or :

$$\frac{D\underline{\Omega}}{Dt} = \underline{\Omega}\cdot\nabla\underline{u} - \underline{\Omega}\,\nabla.\underline{u} - \nabla\sigma^{(1)}\times\nabla p^{(1)}$$

since $\bar{p}$ and $\bar{\sigma}$ are not functions of space.

Assumed some initial vorticity $\underline{\Omega}_o$, $\underline{\Omega}$ can be decomposed into :

$$\underline{\Omega} = \underline{\Omega}^{\alpha} + \underline{\Omega}^{\beta}$$

$\underline{\Omega}^{\alpha}$ and $\underline{\Omega}^{\beta}$ satisfying :

$$\begin{cases} \dfrac{D\underline{\Omega}^{\alpha}}{Dt} = \underline{\Omega}^{\alpha}.\nabla\underline{u} - \underline{\Omega}^{\alpha}\,\nabla.\underline{u} \\ (\underline{\Omega}^{\alpha})_o = \underline{\Omega}_o \end{cases} \qquad \begin{cases} \dfrac{D\underline{\Omega}^{\beta}}{Dt} = \underline{\Omega}^{\beta}.\nabla\underline{u} - \underline{\Omega}^{\beta}\,\nabla.\underline{u} - \nabla\sigma^{(1)}\times\nabla p^{(1)} \\ (\underline{\Omega}^{\beta})_o = 0 \end{cases}$$

$\underline{\Omega}^{\beta}$ represents the part of the vorticity which has been generated by the pressure-density effect, whereas $\underline{\Omega}^{\alpha}$ is due to presence of initial vorticity in the medium.

Now, in the terminology of Chu and Kovasnay, (10), the density and pressure could be further decomposed into their components for the sound and vorticity modes :

$$\begin{cases} \sigma^{(1)} = \sigma_{\Omega}^{(1)} + \sigma_{p}^{(1)} \\ p^{(1)} = p_{\Omega}^{(1)} + p_{p}^{(1)} \end{cases}$$

Now, when sound is present in the medium, it is generally admitted that :

$$|p_{\Omega}^{(1)}| \ll |p_{p}^{(1)}| \quad \text{and} \quad |\sigma_{\Omega}^{(1)}| \ll |\sigma_{p}^{(1)}|$$

The reason is that the velocity associated with the sound mode satisfies :

$$\frac{\partial \underline{u}_p}{\partial t} = -\frac{1}{\rho} \nabla p_p$$

and therefore :

$$\left|\frac{p_p}{\bar{p}}\right| = O\left(\frac{u_p}{a}\right)$$

where a is the speed of sound.

For the velocity associated with the vorticity mode :

$$u_{\Omega} \cdot \nabla u_{\Omega} = -\frac{1}{\rho} \nabla p_{\Omega}$$

hence : $\left|\frac{p_{\Omega}}{\bar{p}}\right| = O\left(\left(\frac{u_{\Omega}}{a}\right)^2\right)$

since $\left(\frac{u_{\Omega}}{a}\right)^2 \ll \frac{u_p}{a}$ when sound is present in most cases, it follows that :

$$|p_{\Omega}| \ll |p_p| \quad \text{and} \quad |\sigma_{\Omega}| \ll |\sigma_p|$$

and : $$\nabla \sigma^{(1)} \times \nabla p^{(1)} = \nabla \sigma_p \times \nabla p_p$$

The generation of vorticity by the pressure-density effect depends only on the sound mode, and not the vorticity mode. There is no influence of $\underline{\Omega}^{\alpha}$ and $\underline{\Omega}^{\beta}$ on $\nabla\sigma^{(1)} \times \nabla p^{(1)}$, and we can assume $\underline{\Omega}_0 = 0$ without loss of generality.

The vorticity reduces to :

$$\frac{\partial \underline{\Omega}}{\partial t} = - \nabla\sigma^{(1)} \times \nabla p^{(1)}$$

or :

$$\frac{\partial \underline{\Omega}}{\partial t} = a^2 \, \nabla P^{(1)} \times \nabla S^{(1)}$$

since :

$$S^{(1)} \equiv P^{(1)} + \frac{\sigma^{(1)}}{\overline{\sigma}}$$

In our model involving two sound waves, the vorticity is always orthogonal to the two sound waves. Since its direction is well defined, we shall now consider $\underline{\Omega}$ as an algebric quantity.

If the subscript $(..)_k$ indicates the value of $(..)$ associated with the k-th sound wave,

$$\nabla P^{(1)} \times \nabla S^{(1)} = \nabla P_1^{(1)} \times \nabla S_2^{(1)} + \nabla P_2^{(1)} \times \nabla S_1^{(1)}$$

and :

$$\frac{\partial \Omega}{\partial t} = a^2 k_1 k_2 \sin\theta \left\{ Re\left(\left(\tilde{P}_2^{(1)} \tilde{S}_1^{(1)} - \tilde{P}_1^{(1)} S_2^{(1)}\right) \exp\left(i(\underline{k}_1 + \underline{k}_2)\cdot\underline{x}\right)\right) - Re\left(\left(\left(\tilde{P}_2^{(1)}\right)^c \tilde{S}_1^{(1)} - \tilde{P}_1^{(1)}\left(\tilde{S}_2^{(1)}\right)^c\right) \exp\left(i(\underline{k}_1 - \underline{k}_2)\cdot\underline{x}\right)\right) \right\} \qquad \text{(V 6)}$$

θ : angle between the two sound waves.

G) Pattern of $\Omega\,(x,t)$ in space, at a given time.

If we wish to give orders of magnitude of the vorticity at the end and during the reaction, it is necessary to know how $\Omega\,(\underline{x},t)$ varies in space, at a given time.

We shall now take the complex notations for $\Omega\,(\underline{x},t)$, $\hat{\Omega}(x,t)$. By integration of (V 6), with respect to t, $\hat{\Omega}\,(\underline{x},t)$ can be put under the form :

$$\hat{\Omega}\,(\underline{x},t) = C_1(t)\,\exp(\,i\,\underline{I}.\underline{x}\,) + C_2(t)\,\exp\,(\,i\,\underline{J}.\underline{x}\,)$$

with :

$$\underline{I} = \underline{k}_1 + \underline{k}_2$$
$$\underline{J} = \underline{k}_1 - \underline{k}_2$$

First, we shall show that it is possible to change our axis, at any given time, so that the new functions $C_1(t)$ and $C_2(t)$ are real :

Let's $\quad \underline{x} = \underline{x}' - \underline{c}$

$\underline{x}'$: new coordinates,

$\underline{c}$: a vector to be determined.

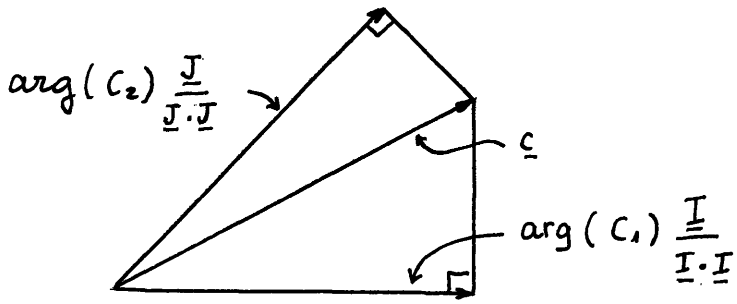
Then :

$$\hat{\Omega}\,(\underline{x},t) = C_1(t)\,\exp\,(-i\,\underline{I}.\underline{c}\,)\,\exp\,(\,i\,\underline{I}.\underline{x}'\,) + \ldots$$

We can chose $\underline{c}$ so that :

$$\underline{I}.\underline{c} = \arg\,(\,C_1(t))$$
$$\underline{J}.\underline{c} = \arg\,(\,C_2(t))$$

It can be easily verified that the vector $\underline{c}$ shown by the figure fulfils all the requirements :



We shall now consider that such a transformation has been done, and consider C_1 and C_2 as real quantities.

It is easy to verify that $\Omega(\underline{x})$ has two spatial periods* :

$$\frac{2\pi\ \underline{I}'}{\underline{J}.\underline{I}'} \quad \text{and} \quad \frac{2\pi\ \underline{J}'}{\underline{I}.\underline{J}'}$$

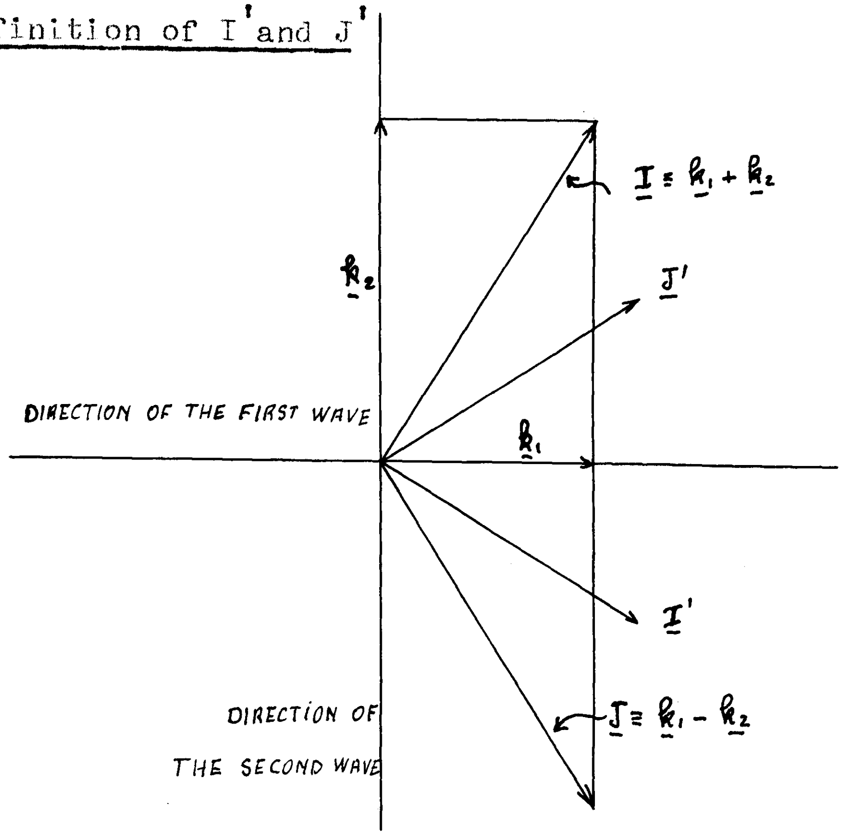
$\underline{I}'$: a vector orthogonal to $\underline{I}$

$\underline{J}'$: a vector orthogonal to $\underline{J}$

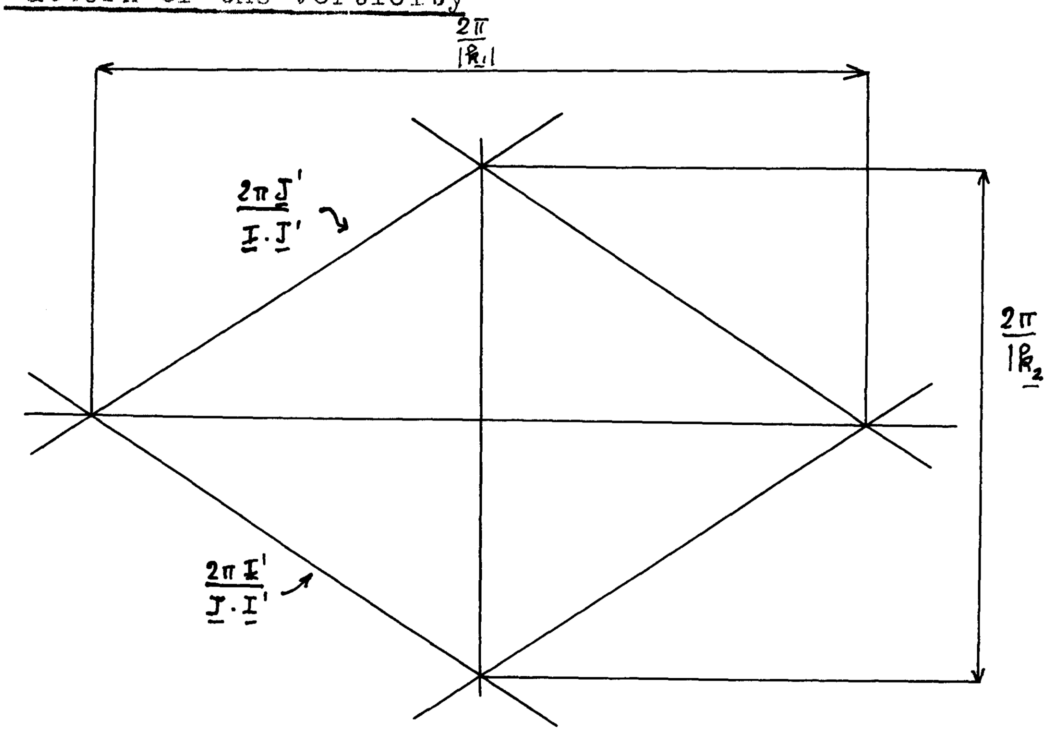
The sense and length of the vectors $\underline{I}'$ and $\underline{J}'$ have no influence on the periods. The pattern of vorticity is shown by the figure :

* A period for a function $f(\underline{x})$ of space is a vector $\underline{v}$ which satisfies : $f(\underline{x}) = f(\underline{x} + n\underline{v})$, for all $\underline{x}$ and all integer n.

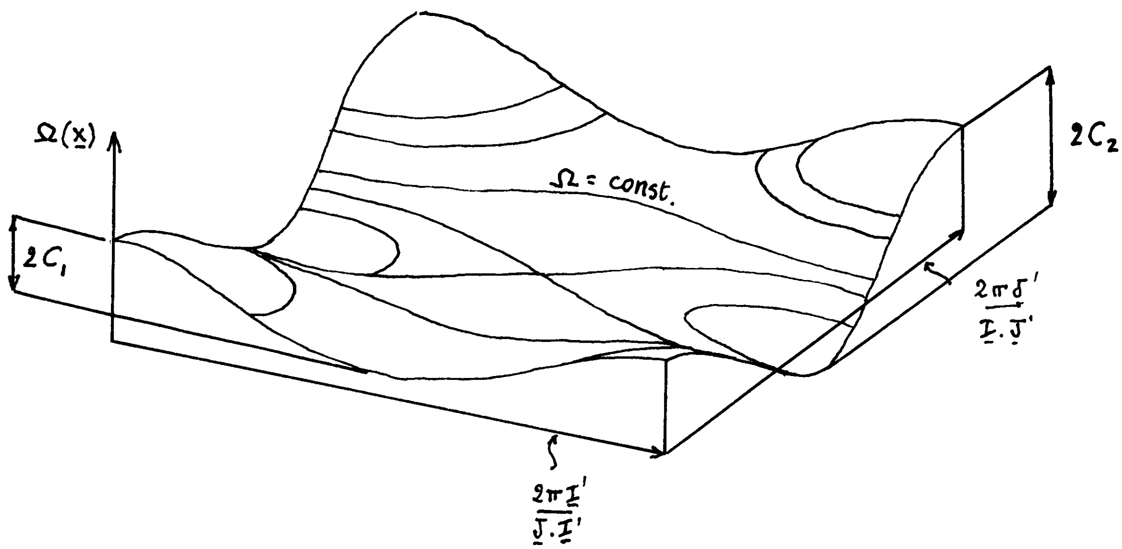
Definition of I' and J'



Pattern of the vorticity



Vorticity variations in space



H) Non dimensionnalization and numerical computations

Let' introduce :

non dimensionnal parameters :

$$\alpha = \frac{\Delta U \, Y_{A,0}}{C_v T_0} + 1$$

$$\beta = \frac{E}{RT_0}$$

$$\omega_1^* = a_0 \, k_1 \frac{\gamma \bar{\rho}}{K}$$

$$\omega_2^* = a_0 \, k_2 \frac{\gamma \bar{\rho}}{K}$$

ratios $\dfrac{\text{chemical time}}{\text{acoustic time}}$ for each of the sound waves.

non dimensionnal variables :

$$t^* = t \frac{K}{\gamma \bar{\rho}} \qquad T^* = \frac{T}{T_0} \qquad Q^* = \frac{Q}{K \, C_v \, T_0}$$

$$W_1^* = W_1 \frac{\gamma \bar{\rho}}{K} \qquad W_2^* = W_2 \frac{\gamma \bar{\rho}}{K} \qquad \Omega^* = \Omega \frac{\gamma \bar{\rho}}{K}$$

Our equations become :

$$\frac{d^2 \tilde{P}^{(1)}}{dt^{*2}} + (\omega^*)^2 \, T^* \, \tilde{P}^{(1)} = \frac{d}{dt^*} (W_1^* \tilde{S}^{(1)} + W_2^* \tilde{P}^{(1)})$$

$$\frac{d\tilde{S}^{(1)}}{dt^*} = W_1^* \tilde{S}^{(1)} + W_2^* \tilde{P}^{(1)})$$

(for each of the two sound waves)

$$\frac{dT^*}{dt^*} = (\alpha - T^*) \exp\left(-\frac{\beta}{T^*}\right)$$

$$\frac{d\Omega^*}{dt^*} = \omega_1^* \omega_2^* \frac{T^*}{2} \left(\mathrm{Re}((\tilde{P}_2^{(1)}\tilde{S}_1^{(1)} - \tilde{P}_1^{(1)}\tilde{S}_2^{(1)}) \exp(i\,\underline{I}.\underline{x})) - \mathrm{Re}(((\tilde{P}_2^{(1)})^c\tilde{S}_1^{(1)} - \tilde{P}_1^{(1)}(\tilde{S}_2^{(1)})^c) \exp(i\,\underline{J}.\underline{x})) \right)$$

An order of magnitude of has been obtained by numerical computation.

As we have seen, $\hat{\Omega}^*$ is a periodic function of space, and varies with the real amplitude : (at the end of the reaction)

$$\int_0^\infty \omega_1^* \omega_2^* \frac{T^*}{2} \mathrm{Re}(\tilde{P}_2^{(1)}\tilde{S}_1^{(1)} - \tilde{P}_1^{(1)}\tilde{S}_2^{(1)})\, dt^*$$

in the direction orthogonal to $\underline{J} = \underline{k}_1 - \underline{k}_2$, and with the amplitude :

$$\int_0^\infty \omega_1^* \omega_2^* \frac{T^*}{2} \mathrm{Re}((\tilde{P}_2^{(1)})^c\tilde{S}_1^{(1)} - \tilde{P}_1^{(1)}(\tilde{S}_2^{(1)})^c)\, dt^*$$

in the direction orthogonal to $\underline{I} = \underline{k}_1 + \underline{k}_2$. By symetry considerations, we do not expect one of these amplitudes to be much higher than the other in any configuration. Therefore, an order of magnitude can be obtained by computing the integral :

$$\int_0^\infty \omega_1^* \, \omega_2^* \, T^* \left(\operatorname{Re}(\tilde{P}_2^{(1)}) \operatorname{Re}(\tilde{S}_1^{(1)}) - \operatorname{Re}(\tilde{P}_1^{(1)}) \operatorname{Re}(\tilde{S}_2^{(1)}) \right) dt^*$$

which is a linear combination of the two amplitudes previously mentionned. $\tilde{P}_1^{(1)}, \tilde{S}_1^{(1)}, \tilde{P}_2^{(1)}, \tilde{S}_2^{(1)}$, have been chosen real by the appropriate set of initial conditions :

$$\tilde{P}_1^{(1)} = 1 \qquad \tilde{P}_2^{(1)} = 0$$

$$\frac{d\tilde{P}_1^{(1)}}{dt^*} = 0 \qquad \frac{d\tilde{P}_2^{(1)}}{dt^*} = \omega_2^*$$

$$\tilde{S}_1^{(1)} = 0 \qquad \tilde{S}_2^{(1)} = 0$$

We have chosen, as numerical values for $\alpha, \beta, \omega_1^*, \omega_2^*$:

$$\alpha = 3.0 \qquad \beta = 6.0$$

$$\omega_1^* : \text{variable} \qquad \omega_2^* = 2.0$$

The choice of ω_2^* relies on the curve $T^*(t)$, as it corresponds to a ratio : $\dfrac{\text{"Characteristic chemical time"}}{\text{acoustic time}}$ near to one, the "Characteristic chemical time" being defined as the time at the inflection point of the curve $T^*(t)$

The results will be given and analysed in the next paragraph.

I) Results and discussion

1) Interaction of the two sound waves and the chemical reaction

a) Effects on the sound wave (Figures 1,2,3,4)

The curves obtained by computer of the pressure versus time show two important features, for any configuration.

* As time goes on, the pseudo-period of the pressure fluctuation decreases, which is easily explained by the effect of temperature on frequency, at constant wave number.
* The amplitude of the sound wave apparenly increases before the inflection point of the curve $T^{*}(t)$, and decreases afterwards. This is compatible with the explanations of previous theories (1) where the reaction rate was approximated by a polynomial expression : $w = w_o \left(\frac{T}{T_o} \right)^n$. It was shown that the sound wave should be amplified when $n > 0$ and damped when $n < 0$. Now, the inflection point of the curve $T^{*}(t)$ occurs when $w(T)$ reaches a maximum :

$$\bar{\rho}\, C_v \frac{d\bar{T}}{dt} = \Delta V\, \dot{w}(\bar{T})$$

imply : $$\bar{\rho}\, C_v \frac{d^2\bar{T}}{dt^2} = \frac{dw(\bar{T})}{d\bar{T}} \frac{d\bar{T}}{dt}$$

since $\frac{d\bar{T}}{dt} \neq 0$, $\frac{d^2\bar{T}}{dt^2} = 0$ when $\frac{dw(\bar{T})}{dt} = 0$

When $w(\bar{T})$ reaches a maximum, the polynomial approximation is $w = w_o$ (or $n=0$) and it follows that $n > 0$ before the inflection point and $n < 0$ afterwards.

So, the results obtained by computer perfectly agree with the previous theories.

b) Effect on the entropy fluctuations (Figures 1,2,3,4)

The results obtained by computer show that the entropy fluctuation versus time is a wavy curve which depends upon the frequency of the sound wave. In other words, for two different initial frequencies of the sound wave are not similar to each other. And this explains mathematically why the terms in the cross product $\nabla P \times \nabla S$ do not cancel out.

Now, the influence of the chemical reaction is not simple, although some insight into the physical process can be obtained by looking at the equations: provided $\tilde{P}^{(1)}$ (complex amplitude of the fluctuations of pressure in space) is a known function of time, the variations of entropy can be expressed exactly in function of the pressure fluctuations :

$$\begin{cases} \dfrac{d\tilde{S}^{(1)*}}{dt^*} = W_1^* \tilde{S}^{(1)} + W_2^* \tilde{P}^{(1)} \\ \tilde{S}^{(1)}(0) = 0 \end{cases}$$

is equivalent to :

$$\tilde{S}^{(1)}(t^*) = \left[\exp\left(\int_0^{t^*} W_1^*(\eta)\,d\eta \right) \right] \cdot \left[\int_0^{t^*} W_2^*(\mu)\, P(\eta) \exp\left(- \int_0^{\eta} W_1^*(\eta)\,d\eta \right) d\mu \right]$$

The "weighting function" : $\exp \left(\int_0^{t} W_1^*(\eta)\,d\eta \right)$ can be be expressed in function of $T^*(t)$, which will show the influence of the chemical reaction on the entropy fluctuations:

$$\int_0^{t^*} W_1^*(\eta)\,d\eta = \int_0^{t^*} \frac{dQ^*}{dT^*}\,d\eta$$

$$= \int_0^{t^*} \left(\frac{d^2T^*}{dt^{*2}} \Big/ \frac{dT^*}{dt^*} \right) d\eta \quad \text{since } Q^* = \frac{dT^*}{dt^*}$$

$$= \int_0^{t^*} \frac{d}{d\eta} \left(\log_e \frac{dT^*}{dt}(\eta) \right) d\eta$$

$$\text{so,} \quad \exp\left(\int_0^{t^*} W_1(\eta)\,d\eta \right) = \frac{dT^*}{dt} \cdot \text{const.}$$

In the expression of $\tilde{S}^{(1)}(t)$, the constant drops, and

$$\tilde{S}^{(1)}(t) = \frac{dT^*}{dt} \cdot \int_0^{t^*} W_2(\eta)\,P\ (\eta) \left(\frac{dT^*}{dt}\right)^{-1} d\eta$$

We see that S (t) can be expressed in function of a "memory integral", depending on how the pressure, the temperature, and the coefficient W_2 vary from the beginning of the reaction, to the point considered.

2) Generation of vorticity (Figures 1,2,3,4,5)

The results obtained by numerical resolution of our equations show that, indeed, vorticity is generated. However, for the choice of parameters we have made , the amplitude is very small : for

$$P_1^{(1)} = P_2^{(1)} = 2.\ 10^{-6}$$

which corresponds to a sound intensity of 80 dB, and for a chemical time of 1 sec., the vorticity at the end of the reaction is of the order of $40.\ 10^{-12}\ \sec^{-1}$, which is very small.

The vorticity has also been computed for different frequencies of the first sound wave (with the frequency of the second sound wave fixed), and it results that the effect is maximum when the two sound waves have frequencies near to each other. However, when they are very near ($0.9 < \frac{\omega_1^*}{\omega_2^*} < 1.1$) the vorticity decreases, which can be explained by the fact that the the two entropy waves are nearly similar, and the two interaction terms $\nabla P_1^{(1)} \times \nabla S_2^{(1)}$ and $\nabla P_2^{(1)} \times \nabla S_1^{(1)}$ cancel out, though each is important. Besides this range, for $0.5 < \frac{\omega_1^*}{\omega_2^*} < 0.9$ and $1.1 < \frac{\omega_1^*}{\omega_2^*} < 2.$, the largest amplitudes are found. They rapidly decrease for low and large frequencies.

3) Flow field at the end of the reaction

In complex notations, the vorticity at the end of the reaction can be written :

$$\hat{\Omega}(\underline{x}) = C_1 \exp(i\ \underline{I}.\underline{x}) + C_2 \exp(i.\ \underline{J}.\underline{x})$$

where C_1 and C_2 are complex constants.

It has already been shown that it is always possible to change of axis, so that the new constants are real. It is easy to see that by the same process, the sign of C_1 and C_2 can also be chosen. For convenience, we now suppose that C_1 and C_2 are real negative.

Due to incompressibility, there exists a stream function $\psi(\underline{x})$, which satisfies :

$$u_x(\underline{x}) = \frac{\partial \psi}{\partial y}$$

$$u_y(\underline{x}) = -\frac{\partial \psi}{\partial x}$$

Hence :

$$\nabla^2 \psi(\underline{x}) = C_1 \exp(i\ \underline{I}.\underline{x}) + C_2 \exp(i\ \underline{J}.\underline{x})$$

By integration :

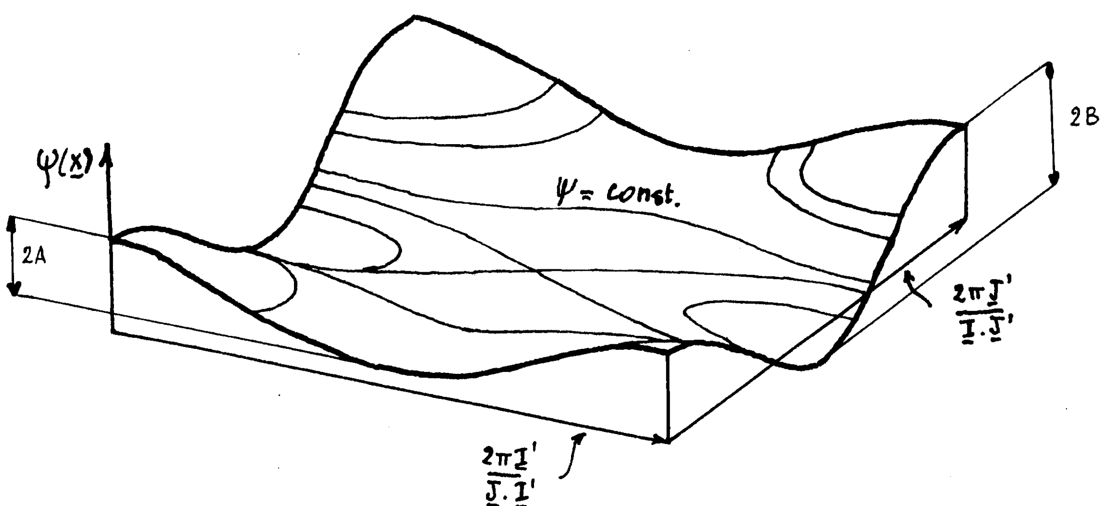
$$\psi(\underline{x}) = -\frac{C_1}{\underline{I}^2}\exp(i\,\underline{I}.\underline{x}) - \frac{C_2}{\underline{J}^2}\exp(i\,\underline{J}.\underline{x})$$

Let :

$$A = -\frac{C_1}{\underline{I}^2} \qquad B = -\frac{C_2}{\underline{J}^2}$$

A and B are real positives.

The variations of $\psi(\underline{x})$ in space are similar to the variations of $\Omega(\underline{x})$:



Concluding remarks to the Vth Chapter

It has been shown that the interaction of sound waves in a chemically reacting medium generated vorticity. The effect, for the numerical example we have chosen, was the highest when both of the characteristic acoustic times were near the characteristic chemical time, and decreases rapidly when one of the two sound waves had a lower or a higher frequency. The flow field at the end of the reaction has been shown to be formed of regularely spaced eddies, which scale are of the order of magnitude of the wave length of the two sound waves.

The order of magnitude of the vorticity generated at the end of the reaction is indeed very small, as expected, since this is a second order phenomenon. It seems to the author however, that it is not possible to extrapolate our results to the case of turbulent flames, since more involved mechanism have to be considered.

A method has also been developed for the calculation of the interaction of a travelling sound wave and chemical reaction, assumed that the reaction rate can be expressed in function of the temperature, even for small fluctuations.

The computed results for a first order reaction rate expression correlate the conclusion of a recent theoretical study (16). More elaborate reaction rate expression should lead to a good agreement with experimental results.

CONCLUSION

Generation of vorticity in both "surface" and "volume" combustion is possible through the "pressure-density" effect corresponding to the term $\nabla(-\frac{1}{\rho}) \times \nabla p$ of the vorticity equation.

In the case of surface combustion, the mean square gradient of pressure seems to be the significant parameter. It can be associated either with turbulence or propagation of the flame front, depending on which type of flame is considered. In the first case, the generation of vorticity should increase with vorticity in the unburned gas. The scale of the vorticity generated should be of the order of magnitude of the tangential disturbances of the flame front, and no increase in turbulent transport in the flame brush is expected, due to this process.

In the case of volume combustion, the term corresponding to the average effect of $\nabla(-\frac{1}{\rho}) \times \nabla p$ in a modified Kármán-Howarth equation shows that generation of vorticity involves essentially the sound and entropy modes, not the vorticity mode. Consequently, the generation of vorticity does not depend on the vorticity in the medium, but is due to interaction of sound waves in the reacting medium, or interaction of "expanding bubbles" according to the picture of turbulent volume combustion suggested by recent studies in combustion noise (14).The interaction of sound waves with occurence of chemical reaction might generate vorticity, when the periodsof the sound waves and the duration of the reaction are of the same order of magnitude. The vorticity generated should be negligible when one of these times is very different from the others, and also when the periods of the sound waves are very near to each other. The scale of the vorticity generated is of the order of magnitude of the wavelengths of the sound waves. The generation of vorticity by interaction of"expanding bubbles" has not been studied, but a measurable correlation has been found, which could give an order of magnitude of the generation of vorticity by combustion, with the help of experiments.

Surface and volume combustion represent two extremes, and it is presumable that real turbulent flames involve features belonging to both models.

	Coefficient of $r_i r_j$ (1)	coefficient of δ_{ij} (2)	Karman-Howarth equation (3)	Development at order 0 (4)	Development at order 2 (5)
$\frac{\partial}{\partial t} R_{ij}(\underline{r})$	$\frac{\partial}{\partial t}\left\{-\frac{1}{2} D_r \overline{u_1^2} f(r) + \frac{W_1(r)}{2}\right\}$	$\frac{\partial}{\partial t}\left\{\left(\frac{1}{2}(r^2 D_r + 2)\overline{u_1^2} f(r) - \frac{W_1(r) r^2}{2}\right\}$	$\frac{\partial}{\partial t} \overline{u_1^2} f(r)$	$\frac{d}{dt} \overline{u_1^2}$	$\frac{1}{2} \frac{d}{dt}\left(f_0'' \overline{u_1^2}\right)$
$S_{ij}^{\alpha}(\underline{r})$	$-\frac{1}{2} D_r K^*(r) + 2 W_2(r)$	$\frac{1}{2}(r^2 D_r + 2) K^*(r) + 4 W_3(r) + r W_3'(r)$	$K^*(r) + 2 r^2 W_2(r) + 4 W_3(r) + r W_3'(r)$	$-\overline{u_1^2 W}$	$\frac{7}{6} k_0'''(\overline{u^2})^{3/2} + \frac{3}{10}\overline{u_1^2 W''} - \frac{1}{10}\overline{u_2^2 W''}$
$S_{ij}^{\beta}(\underline{r})$	$-2 W_6(r)$	$-2 W_7(r)$	$-2 \overline{u_1 W u_1(r)}$	$-2 \overline{u_1^2 W}$	$-\overline{u_1 W u_1''}$
$P_{ij}(\underline{r})$	$2 W_4(r)$	$2 W_5(r)$	$-\overline{\frac{2}{\rho}\frac{\partial p}{\partial x_1} u_1(r)}$	$-\overline{\frac{2}{\rho}\frac{\partial p}{\partial x_1} u_1}$	$-\overline{\frac{1}{\rho}\frac{\partial p}{\partial x_1} u_1''}$
$\nabla^2 R_{ij}^{(0)}(\underline{r})$	$-\frac{1}{2} D_r F(r)$	$\frac{1}{2}(r^2 D_r + 2) F(r)$	$F(r)$	$5 f_0'' \overline{u_1^2}$	$\frac{7}{6} f_0^{IV} \overline{u_1^2}$
$\nabla^2 R_{ij}^{(1)}(\underline{r})$	$\frac{W_1''(r)}{2} + \frac{3 W_1'(r)}{r}$	$-\frac{W_1''(r)}{2} r^2 - 3 r W_1'(r) - 2 W(r)$	$-2 W_1(r)$	$\frac{2}{3} \overline{W^2}$	$-\frac{1}{5} \overline{W'^2}$
$Q_{ij}(\underline{r})$	$\frac{W_1'(r)}{r}$	$W_1(r)$	$r W_1'(r) + W_1(r)$	$-\frac{2}{3} \overline{W^2}$	$\frac{3}{5} \overline{W'^2}$

Notations

$$D_r \equiv \frac{1}{r}\frac{\partial}{\partial r}$$

$$\left.\begin{aligned} f(r) &\equiv \overline{u_1(\underline{x}) u_1(\underline{x}+\underline{r})} / \overline{u_1^2(\underline{x})} \\ k(r) &\equiv \overline{u_1^2(\underline{x}) u_1(\underline{x}+\underline{r})} / [\overline{u_1^2(\underline{x})}]^{3/2} \end{aligned}\right\} \underline{r} = (r, 0, 0)$$

$$W(\underline{x}) \equiv \frac{\partial u_k(\underline{x})}{\partial x_k}$$

$$W_1(r) \equiv -\frac{1}{r^3}\int_0^r r^2\, \overline{W(\underline{x}) W(\underline{x}+\underline{r})}\, dr$$

$$W_2(r) r_i r_j + W_3(r)\delta_{ij} = \overline{u_i(\underline{x}) W(\underline{x}+\underline{r}) u_j(\underline{x})}$$

$$W_4(r) r_i r_j + W_5(r)\delta_{ij} = -\overline{\frac{1}{\rho(\underline{x})}\frac{\partial p(\underline{x})}{\partial x_i} u_j(\underline{x}+\underline{r})}$$

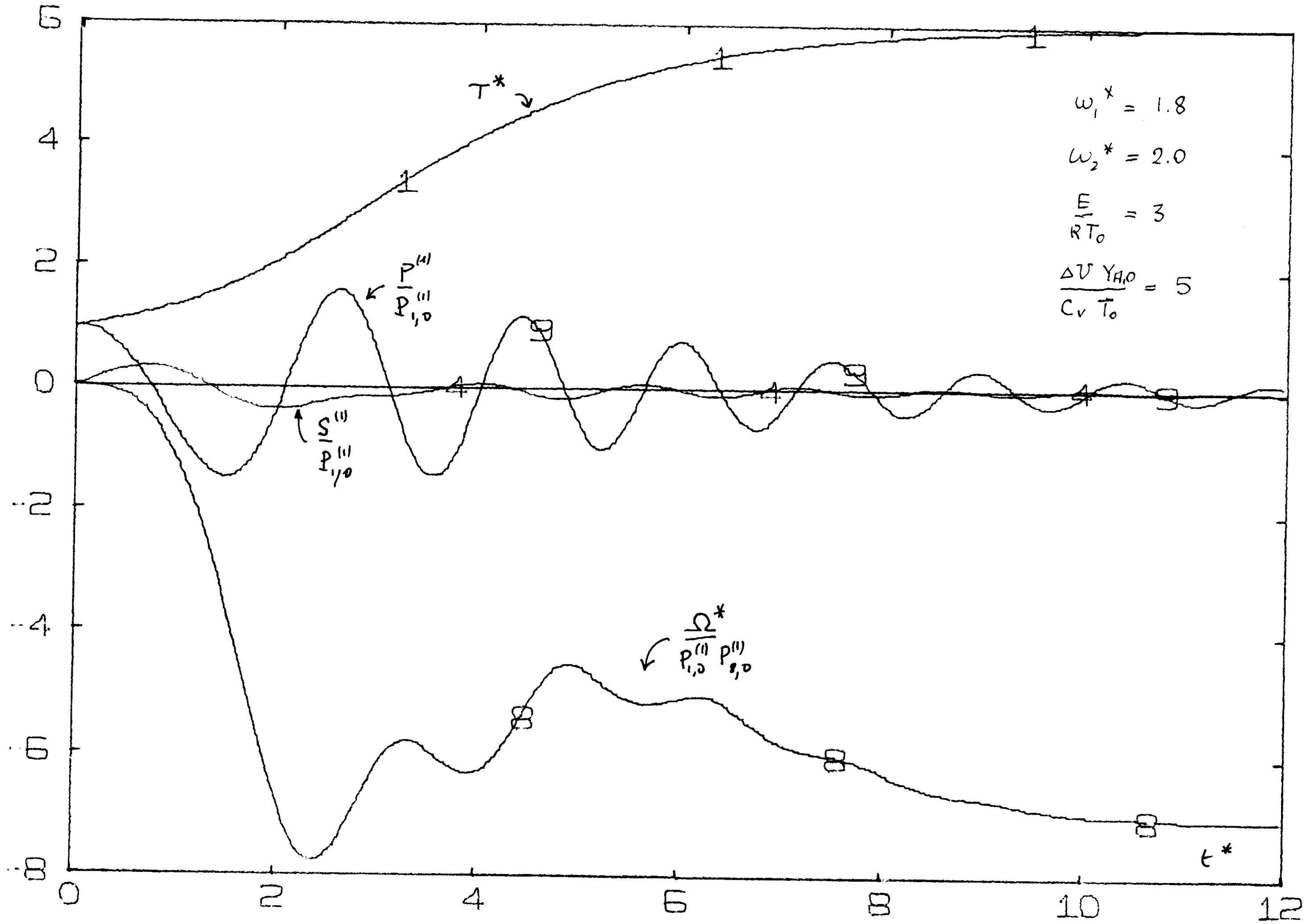
$$W_5(r) r_i r_j + W_7(r)\delta_{ij} = \overline{W(\underline{x}) u_j(\underline{x}+\underline{r}) u_i(\underline{x})}$$

$$k^*(r) \equiv k(r) - (\overline{u_1^2})^{-3/2}\left\{\frac{1}{r^5}\int_0^r r^4\left[W_2(r) - \frac{W_3'(r)}{2r}\right] dr + r W_3(r)\right\}$$

$$K^*(r) \equiv \left(\frac{\partial}{\partial r} + \frac{4}{r}\right)(\overline{u_1^2})^{3/2} k^*(r)$$

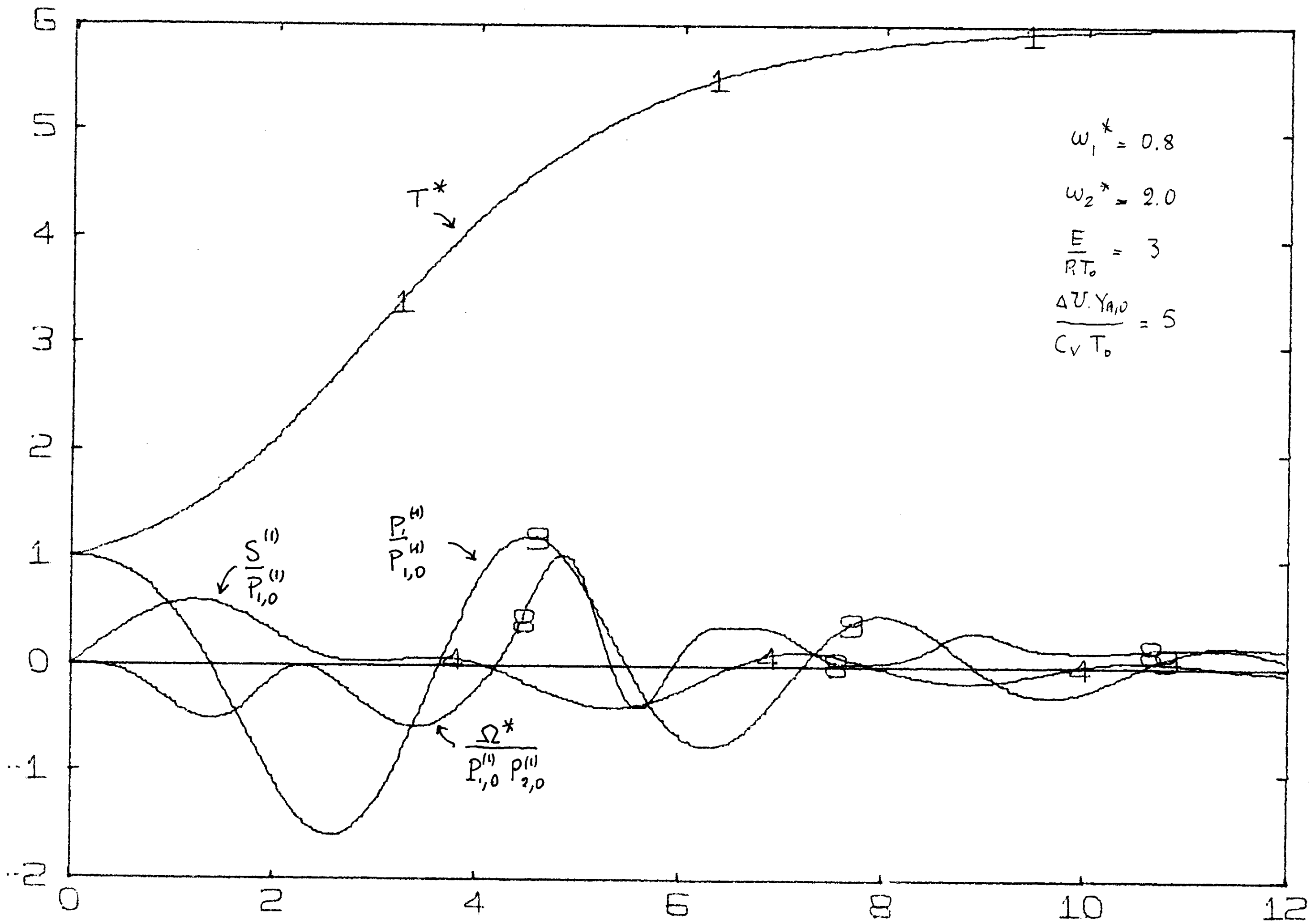
$$F(r) \equiv \left(\frac{\partial^2}{\partial r^2} + \frac{4}{r}\frac{\partial}{\partial r}\right)\overline{u_1^2} f(r)$$

Figure 1



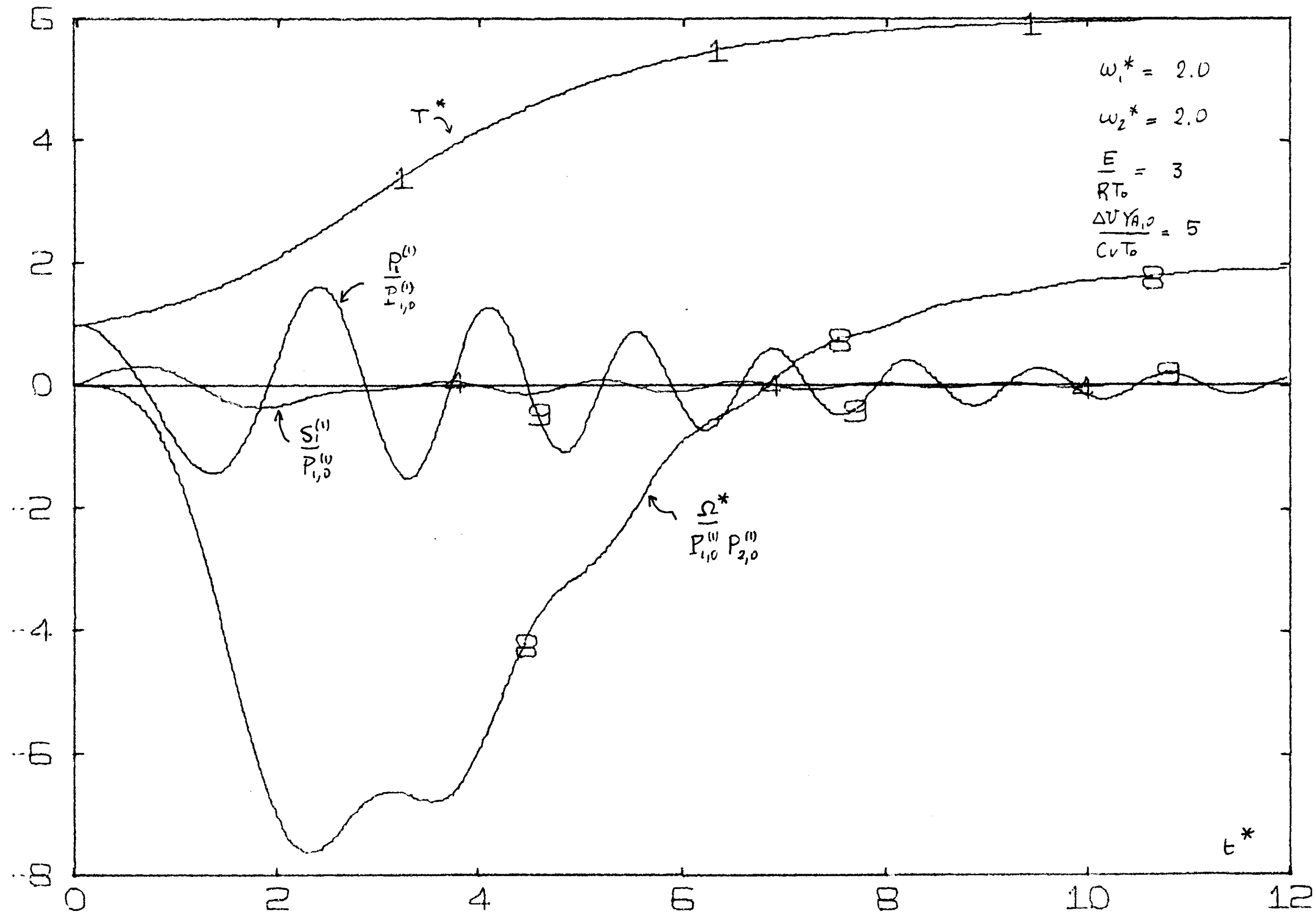
6
4
2
0
-2
-4
-6
-8
0
2
4
6
8
10
12
T^*
$\frac{P^{(1)}}{P^{(1)}_{1,0}}$
$\frac{S^{(1)}}{P^{(1)}_{1,0}}$
$\frac{\Omega^*}{P^{(1)}_{1,0}\,P^{(1)}_{2,0}}$
t^*
$\omega_1^* = 1.8$
$\omega_2^* = 2.0$
$\frac{E}{RT_0} = 3$
$\frac{\Delta U\ Y_{A,0}}{C_v\ T_0} = 5$

Figure 2



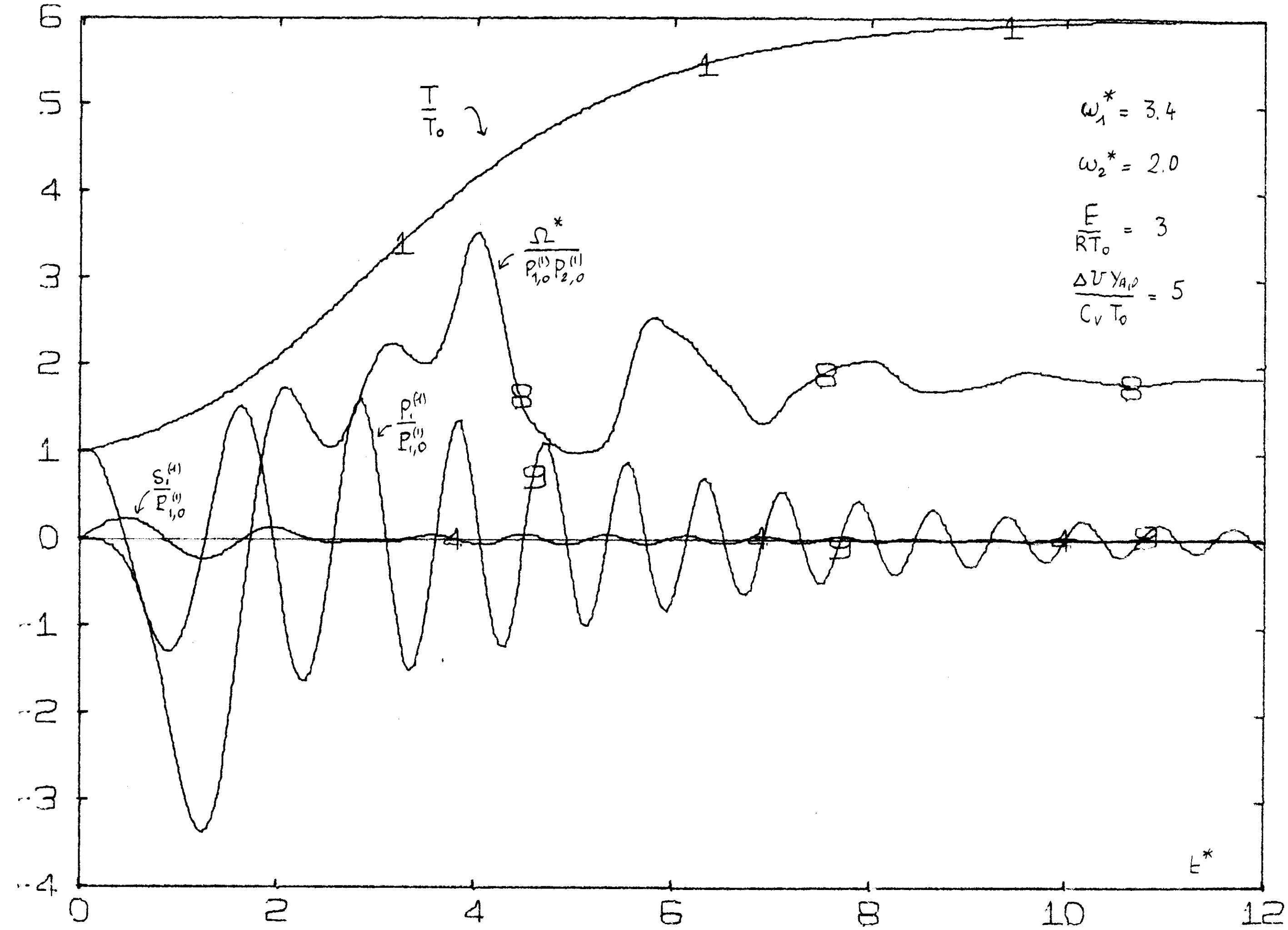
6
5
4
3
2
1
0
-1
-2
0
2
4
6
8
10
12
T*
$\omega_1^* = 0.8$
$\omega_2^* = 2.0$
$\frac{E}{RT_0} = 3$
$\frac{\Delta U . Y_{A,0}}{C_V T_0} = 5$
$\frac{S^{(1)}}{P_{1,0}^{(1)}}$
$\frac{P_1^{(4)}}{P_{1,0}^{(4)}}$
$\frac{\Omega^*}{P_{1,0}^{(1)} P_{2,0}^{(1)}}$

Figure 3



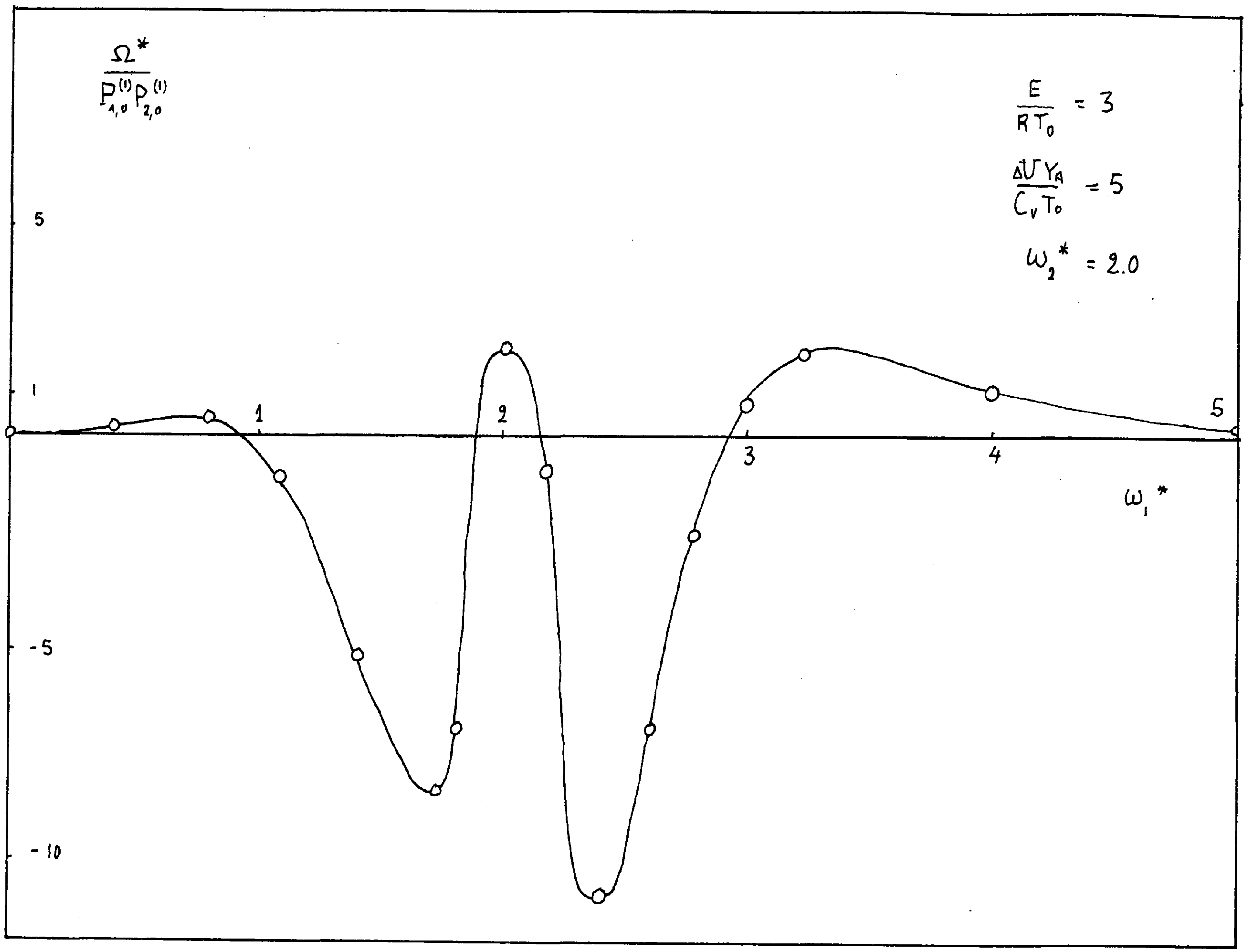
6
4
2
0
-2
-4
-6
-8
0
2
4
6
8
10
12
T^*
$\frac{P_1^{(1)}}{P_{1,0}^{(1)}}$
$\frac{S_1^{(1)}}{P_{1,0}^{(1)}}$
$\frac{\Omega^*}{P_{1,0}^{(1)} P_{2,0}^{(1)}}$
$\omega_1^* = 2.0$
$\omega_2^* = 2.0$
$\frac{E}{RT_0} = 3$
$\frac{\Delta U Y_{A,0}}{C_v T_0} = 5$
t^*

Figure 4



6
5
4
3
2
1
0
-1
-2
-3
-4
0
2
4
6
8
10
12
t^*
$\frac{T}{T_0}$
$\frac{\Omega^*}{P_{1,0}^{(1)} P_{2,0}^{(1)}}$
$\frac{P_1^{(1)}}{P_{1,0}^{(1)}}$
$\frac{S_1^{(1)}}{P_{1,0}^{(1)}}$
$\omega_1^* = 3.4$
$\omega_2^* = 2.0$
$\frac{E}{RT_0} = 3$
$\frac{\Delta U\, y_{A,0}}{C_V T_0} = 5$

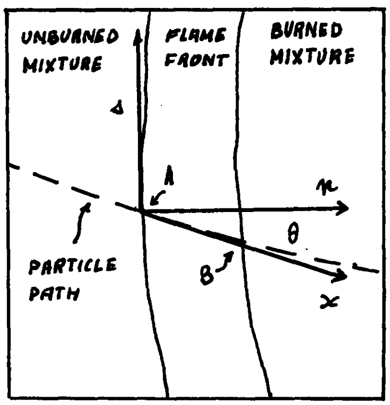
Figure 5



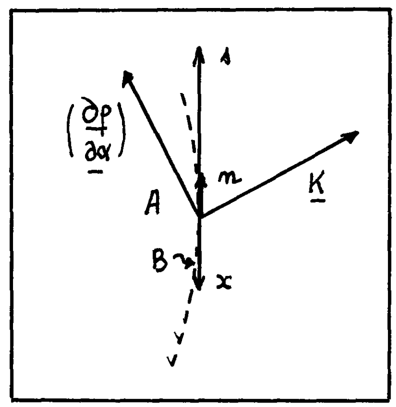
$\frac{\Omega^*}{P^{(1)}_{1,0}P^{(1)}_{2,0}}$
$\frac{E}{RT_0} = 3$
$\frac{\Delta U Y_A}{C_v T_0} = 5$
$\omega_2^* = 2.0$
5
1
-5
-10
1
2
3
4
5
ω_1^*

APPENDIX I

Change in vorticity for an unburned particle crossing a flame front



side view



front view

We shall consider a particle crossing a flame front from A to B. Let :

AB the particle path across the flame front

Ax axis tangent to AB in A

An the normal to the flame front in A

As the tangent to the flame front, in the same plan as Ax

$\left(\frac{\partial p}{\partial \underline{\alpha}}\right)$ the component of the pressure gradient tangent to the flame front

$\underline{K}$ unit vector orthogonal to $\frac{\partial p}{\partial \underline{\alpha}}$ and An

θ the angle between Ax and An

ε the thickness of the flame front

x the abscissa of the particle on the axis Ax

$\Omega(x)$ its vorticity

$\sigma(x)$ its specific volume

$v(x)$ its velocity in the axis An, As

Since the gradient of density along AB is parallel to An, the only component of the gradient of pressure that has to be taken into account in the cross product $\nabla\sigma \times \nabla p$ is : $\left(\frac{\partial p}{\partial \underline{\alpha}}\right)$. Now, the pressure gradient in the flame front is expected to vary in the An direction, but not in any direction tangent to the flame front. Therefore, we shall assume $\left(\frac{\partial p}{\partial \underline{\alpha}}\right)$ to ce constant from A to B :

$$\nabla\sigma \times \nabla p = \left(\frac{\partial \sigma(x)}{\partial n}\right) \cdot \left|\frac{\partial p}{\partial \underline{\alpha}}\right| \underline{K}$$

The thickness of the flame front is very small, so the stretching and viscous effects are negligeable as compared with the"density" and "pressure density" effects in the flame zone, and we can use the vorticity under the form (I 2) (Vazsoyi equation) :

$$\frac{D(\sigma \underline{\Omega}(x))}{Dt} = -\sigma(x)\left(\frac{\partial \sigma(x)}{\partial n}\right)\left|\frac{\partial p}{\partial \underline{\alpha}}\right| \underline{K}$$

Now, the material derivative can be expressed in any axis since if represents the derivative with respect to time of a quantity associated with the particles. Therefore :

$$\frac{\partial \sigma \underline{\Omega}}{\partial t} + |\underline{v}(x)| \frac{\partial \sigma \underline{\Omega}}{\partial x} = -\sigma(x) \frac{\partial \sigma(x)}{\partial n} \left| \frac{\partial p}{\partial \underline{\alpha}} \right| \underline{K}$$

We can now introduce two functions f and g to take into account the variations of $\sigma\Omega$ and σ in the flame front :

$$f(\xi) \equiv \left(\sigma \underline{\Omega}(x) - \sigma_1 \underline{\Omega}_1 \right) / \left(\sigma_2 \underline{\Omega}_2 - \sigma_1 \underline{\Omega}_1 \right)$$

$$g(\xi) \equiv \left(\sigma(x) - \sigma_1 \right) / \left(\sigma_2 - \sigma_1 \right)$$

$$\xi \equiv \frac{x}{\varepsilon \cos \theta}$$

The vorticity equation becomes :

$$\frac{\varepsilon}{\sigma(x)} \frac{\partial \sigma \underline{\Omega}}{\partial t} + \frac{|\underline{v}(x)|}{\sigma(x) \cos \theta} \left(\sigma_2 \underline{\Omega}_2 - \sigma_1 \underline{\Omega}_1 \right) f'(\xi) = - \left| \frac{\partial p}{\partial \underline{\alpha}} \right| (\sigma_2 - \sigma_1) \, g'(\xi) \, \underline{K}$$

The continuity equation leads to :

$$\frac{|v(x)|}{\sigma(x) \cos \theta} = \frac{S_u}{\sigma_1}$$ (independant of x and θ)

Therefore :

$$\frac{\varepsilon}{\sigma(x)} \frac{\partial \sigma \underline{\Omega}}{\partial t} + \frac{S_u}{\sigma_1} \left(\sigma_2 \underline{\Omega}_2 - \sigma_1 \underline{\Omega}_1 \right) f'(\xi) = - \left| \frac{\partial p}{\partial \underline{\alpha}} \right| (\sigma_2 - \sigma_1) \, g'(\xi) \, \underline{K}$$

If we now integrate from $\xi = 0$ to $\xi = 1$, we get :

$$\varepsilon \int_0^1 \frac{1}{\sigma} \frac{\partial \sigma \Omega}{\partial t} d\xi + \frac{S_u}{\sigma_1} \left(\sigma_2 \underline{\Omega}_2 - \sigma_1 \underline{\Omega}_1 \right) = - \left| \frac{\partial \rho}{\partial \underline{\alpha}} \right| (\sigma_2 - \sigma_1) \underline{K}$$

When $\varepsilon \rightarrow 0$, the first term vanishes. The two functions $f(\xi)$ and $g(\xi)$ have now disappeared, and θ too, which was not expected.

The final result is :

$$\sigma_2 \underline{\Omega}_2 - \sigma_1 \underline{\Omega}_1 = - \frac{\sigma_1}{S_u} (\sigma_2 - \sigma_1) \left| \frac{\partial \rho}{\partial \underline{\alpha}} \right| \underline{K}$$

APPENDIX II

Derivation of equations (V 1)

The complete "entropy equation" is :

$$\rho \frac{DE}{Dt} = - \frac{\Sigma h_K w_K}{T}$$

with :

$$E \equiv E_{ref} + c_v \log \left\{ \frac{p}{p_{ref}} \cdot \left(\frac{\rho_{ref}}{\rho}\right)^{\gamma} \right\}$$

Hence :

$$\frac{1}{C_p} \frac{DE}{Dt} = \frac{Q}{\rho C_p T} \qquad Q \equiv - \Sigma h_K w_K$$

and :

$$\frac{1}{C_p} \frac{DE^{(1)}}{Dt} = \left(\frac{Q}{\rho C_p T}\right)^{(1)} \quad \text{with :} \quad (\ )^{(1)} \equiv (\ ) - \overline{(\ )}$$

We set :

$$S^{(1)} \equiv \frac{E^{(1)}}{C_p} = \frac{C_v}{C_p} \left\{ \frac{p^{(1)}}{\bar{p}} - \gamma \frac{\rho^{(1)}}{\bar{\rho}} \right\} + 0 \left\{ \left[\frac{p^{(1)}}{\bar{p}}\right]^2 \right\}$$

$$= \frac{p^{(1)}}{\gamma \bar{p}} - \frac{\rho^{(1)}}{\bar{\rho}}$$

Then :

$$\frac{DS^{(1)}}{Dt} = \left(\frac{Q}{\rho C_p T}\right)^{(1)}$$

Now, as we consider a stagnant medium, the convective term is negligeagle as compared to the time derivative, and :

$$\frac{\partial S^{(1)}}{\partial t} = \left(\frac{Q}{\rho C_p T}\right)^{(1)}$$

We shall now derive the "sound equation". From the momentum and continuity equations :

$$\begin{cases} \dfrac{\partial \rho^{(1)}}{\partial t} + \bar{\rho}\ \nabla \cdot \underline{u}^{(1)} = 0 \\ \nabla p^{(1)} + \bar{\rho}\ \dfrac{\partial \underline{u}^{(1)}}{\partial t} = 0 \end{cases}$$

we get : $$\nabla^2 p^{(1)} = \frac{\partial^2 \rho^{(1)}}{\partial t^2}$$

Another relation between $\rho^{(1)}$ and $p^{(1)}$ can be derived, by elimination of $S^{(1)}$ between :

$$\frac{\partial S^{(1)}}{\partial t} = \left(\frac{Q}{\rho c_p T}\right)^{(1)}$$

$$S^{(1)} = \frac{p^{(1)}}{\gamma \bar{p}} - \frac{\rho^{(1)}}{\bar{\rho}}$$

which gives :

$$\frac{\partial}{\partial t}\left[\frac{p^{(1)}}{\gamma \bar{p}}\right] - \frac{\partial}{\partial t}\left[\frac{\rho^{(1)}}{\bar{\rho}}\right] = \left(\frac{Q}{\rho c_p T}\right)^{(1)}$$

or : $$\frac{\partial^2}{\partial t^2}\left[\frac{p^{(1)}}{\gamma \bar{p}}\right] - \frac{1}{\bar{\rho}}\frac{\partial^2 \rho^{(1)}}{\partial t^2} = \frac{\partial}{\partial t}\left(\frac{Q}{\rho c_p T}\right)^{(1)}$$

since $\bar{\rho}$ is not a function of time.

Now, $$\frac{1}{\bar{\rho}}\frac{\partial^2 \rho^{(1)}}{\partial t^2} = \frac{1}{\bar{\rho}}\nabla^2 p^{(1)}$$ as we have seen

$$= \frac{\gamma \bar{p}}{\bar{\rho}}\nabla^2\left[\frac{p^{(1)}}{\gamma \bar{p}}\right]$$

$$= \bar{a}^2 \nabla^2 P^{(1)}$$

since $\bar{p}$ is not a function of space.

So, the "sound equation" becomes :

$$\frac{\partial^2 P^{(1)}}{\partial t^2} - \bar{a}^2 \nabla^2 P^{(1)} = \frac{\partial}{\partial t}\left(\frac{Q}{\rho c_p T}\right)^{(1)}$$

Notations for chapters I,II,III

$\underline{v}$ velocity

$\underline{\Omega}$ vorticity

ν kinematic viscosity

ε rate of energy dissipation

λ Taylor microscale

$\underline{n}$ unit vector, normal to the flame front

$\frac{\partial p}{\partial \underline{\alpha}}$ component of the gradient of pressure, tangent to the flame front.

$\underline{K}$ unit vector, orthogonal to $\underline{n}$ and $\frac{\partial p}{\partial \underline{\alpha}}$

S_u laminar burning velocity.

ρ density

σ specific volume

θ angle between the path of a particle and the normal to the flame front.

$\langle .. \rangle$ average over a great number of particles

Notations for chapter IV

Subscripts and superscripts

$(\overline{\;..\;})$ average over space of $(\;)$

$(\;)^{(1)}$ fluctuating quantity : $(\;)^{(1)} \equiv (\;) - (\overline{\;})$

$(\underline{\;})$ denotes a vector

Thermodynamic properties of the mixture

ρ density

σ specific volume

p pressure

Q heat release per unit volume of the mixture

$\mathcal{E}$ entropy for a perfect gas

C_v, C_p specfic heats

γ ratio of specific heats

Kinematic notations

$\underline{u}$ velocity

$\underline{\Omega}$ vorticity

$r \equiv |\underline{r}|$

$D_r \equiv \frac{1}{r}\frac{\partial}{\partial r}$

S Skewness factor

G flatness factor

$f(r)$ double velocity correlation function

$k(r)$ triple velocity correlation function

$R_{ij}(\underline{r})$ double velocity correlation tensor

$T_{ijk}(\underline{r})$ triple velocity correlation tensor

$S_{ij}(\underline{r})$ see equation IV 1

:

$W(\underline{x})$ divergence of the velocity

$S^{\alpha}_{ij}(\underline{r}), S^{\beta}_{ij}(\underline{r}), P_{ij}(\underline{r}), Q_{ij}(\underline{r})$ see section 3

$W_1(r)$ see equation IV 4

$W_2(r), W_3(r)$ see equation IV 8

$W_4(r), W_5(r)$ see equation IV 16

$W_6(r), W_7(r)$ see equation IV 15

$k^*(r)$ see equation IV 13

$K^*(r)$ see equation IV 14

$F(r)$ see equation IV 18

$\overline{u_1^2 W(r)} = \overline{u_1^2(\underline{x}) W(\underline{x}+\underline{r})}$ for $\underline{r} = (r,0,0)$

$\overline{u_1 W u_1(r)} = \overline{u_1(\underline{x}) W(\underline{x}) u_1(\underline{x}+\underline{r})}$ for $\underline{r} = (r,0,0)$

$\overline{W^2} = \overline{W(\underline{x})^2}$

$\overline{W'^2} = \overline{\left[\frac{\partial W}{\partial x_1}(\underline{x})\right]^2}$

Notations for chapter V

Subscripts and superscripts

$(\bar{\ })$ average over space of $(\ )$

$(\ )^{(1)}$ fluctuating quantities $\quad (\ )^{(1)} \equiv (\ ) - (\bar{\ })$

$Re(..)$ real part of $(..)$

$(..)^c$ complex conjugate of $(..)$

$arg(..)$ argument of $(..)$

$(\ )_0$ refers to initial values

$(\ )_1$ refers to the first sound wave

$(\ )_2$ refers to the second sound wave

dimensional quantities

p pressure

ρ density

σ specific volume $\quad \sigma = 1/\rho$

T temperature

C_p, C_v specific heats

Q heat release per unit volume of the mixture

ΔU heat of the reaction, per unit mass of component A

W_A mass rate of production of component A, per unit volume

K kinetic constant

E activation energy

$\underline{k}_k$ wave number of the k-th sound wave

a speed of sound

θ angle of the two sound waves

$\underline{u}$ velocity

$\underline{\Omega}$ vorticity

non-dimensional quantities

$P^{(1)}$ pressure (real) $P^{(1)} \equiv \frac{p^{(1)}}{\gamma \bar{p}}$

$S^{(1)}$ entropy (real) $S^{(1)} \equiv P^{(1)} - \frac{\rho^{(1)}}{\bar{\rho}}$

$\hat{P}^{(1)}$ pressure (complex)

$\hat{S}^{(1)}$ entropy (complex)

$\tilde{P}^{(1)}$ complex amplitude of the pressure

$\tilde{S}^{(1)}$ complex amplitude of the entropy

Ω^* vorticity (real)

$\hat{\Omega}^*$ vorticity (complex)

ω_k^* frequency of the k-th sound wave

γ ratio of specific heats

$\alpha \equiv \frac{\Delta U \cdot Y_{A,0}}{C_v T_0} + 1$

$\beta \equiv \frac{E}{R T_0}$

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