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TURBULENT CHEMICALLY REACTING FLOWS ACCORDING TO A KINETIC THEORY

by

ZUU-CHANG HONG

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TURBULENT CHEMICALLY REACTING FLOWS ACCORDING TO A KINETIC THEORY

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THESIS

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TABLE OF CONTENTS

ACKNOWLEDGEMENTS iii

TABLE OF CONTENTS iv

NOMENCLATURE v

CHAPTER I INTRODUCTION 1

I.A. General Review of the Development of Turbulent Flow Analyses 1

I.B. Review of Recent Kinetic Theories of Turbulent Flow 3

I.C. Multilength-scale Turbulent Shear Flows: Extension of the Simplified Statistical Theory 7

CHAPTER II REVIEW OF TURBULENT KINETIC THEORY DUE TO CHUNG 9

II.A. General Theory 9

II.B. Langevin Equations 11

II.C. Derivation of Kinetic Equations 14

II.D. Multiscale Kinetic Equation 19

CHAPTER III MIXING AND DECAY OF A TURBULENCE FIELD CHARACTERIZED BY TWO SIGNIFICANT LENGTH SCALES 20

III.A. Governing Equations 21

III.B. Initial Conditions 26

III.C. Generalized Moment Equations 27

III.D. Averaged Energy Equations 27

III.E. Typical Numerical Results 32

III.F. Discussion of the Results 33

CHAPTER IV GREEN'S FUNCTIONS OF THE KINETIC EQUATIONS 39

IV.A. Green's Function of the Kinetic Equations Governed by One Nonequilibrium Degree of Freedom 40

IV.B. Green's Function of the Kinetic Equation Describing the Turbulent Field Governed by Two Nonequilibrium Degrees of Freedom and the Equilibrium Degrees of Freedom 49

CHAPTER V SPECIFIC SOLUTION 61

V.A. Governing Equations 67

V.B. Properties of the Green's Functions 74

V.C. Source Conditions 75

V.D. Solutions 80

V.E. Determination of Parameters and the Similarity Solutions 88

V.F. Results of the Iteration on $\langle u \rangle$ and $\langle U_k U_k \rangle$ 92

V.G. Results 94

V.H. Discussion of the Results 94

CHAPTER VI CONCLUDING REMARKS 100

FIGURES 103

REFERENCES 118

APPENDIX I 122

APPENDIX II 125

APPENDIX III 131

VITA 141

NOMENCLATURE

A	defined in Eq. (IV-18), also of the order one
A'	defined in Eq. (II-6)
A_{ij}	defined in Eq. (IV-33)
$A_i(t), A_{a,R}, A_{b,k}$	random fast fluctuating acceleration due to smaller equilibrium eddies
B, C	defined in Eq. (IV-18), C also represents the mass concentration defined in Eq. (V-25)
B_a, B_b	defined in Eq. (IV-22)
B_c	defined in Eq. (IV-23)
a, b, c	defined in Eq. (IV-15), a, b are also constants in Eqs. (III-28b) and (III-28c)
b'	defined in Eq. (V-74)
a, b, d	numbers of moles defined in Eq. (V-1)
$a_2, b_2, c_2, d_2, e_2, g_2$	defined in Eq. (IV-30)
D	grid size defined in Eq. (IV-28b), also as a constant parameter given in Eq. (V-25)
ΔE	activation energy
E_o	$\langle U_k U_k \rangle_o$, turbulent energy given at $x = 0$
F	distribution function of chemical species z
F_α	distribution function of chemical species α
F, G, H	defined in Eq. (L-II-3)
$\bar{F}$	defined in Eq. (IV-5)
$\bar{F}_1$	function of $(\vec{T}, \vec{R}, t)$
$(F_m)_i, (F_n)_i$	chemical frozen case of F_m and F_n
$(F_{m,v})_i, (F_{n,v})_i$	defined in Eq. (V-53)
$F_{p,v}$	defined in Eq. (V-61)

$\bar{F}_{11}, \bar{F}_{12}, \bar{F}_{13}$	defined in Eq. (IV-16)
f	distribution function of fluid element
f_2	joint distribution function of fluid element affected by two families of eddies with different length scale
$f_o(u_o)$	Gaussian intensity of source at $x = 0$
G_1	single-mode Green's function
G_2	multi-mode Green's function
h, m, n	defined in Eq. (V-7)
Δh_o	heat of combustion
h_o^-	h at source for $y < 0$
h_o^+	h at source for $y > 0$
$H(u_o)$	defined in Eq. (V-30)
z_o	z at source at $x = 0$
h_p	normalized temperature due to chemical reaction
h_i	normalized temperature in a chemical frozen field
K	collection of constants in reaction rate
K_f	specific reaction rate
K_o	constant
K_j	defined in Eq. (II-5)
$K_{a,k}, K_{b,k}$	defined in Eq. (III-5)
k_j	defined in Eq. (IV-4)
$k_{a,j}, k_{b,j}$	defined in Eq. (IV-22)
ℓ_s, ℓ_s'	constants in Eq. (V-77)
M	rate of molecular dissipation of chemical species, also defined as Λ_a/Λ_b
M_r, M_s, M_p	molecular weight of fuel, oxidant and product, respectively
M_{ij}	defined in Eq. (L-III-5)
$m_1(t), m_2(t), m_3(t)$	functions of t

m_o, n_o	m, n at source at x = 0
N	defined in Eq. (V-45)
P	defined in Eq. (V-26), also defined in Eq. (L-II-1)
p	pressure
Q	general function of momentum quantity
q	defined in Eq. (III-6)
q_1	defined in Eq. (IV-4)
R	Gas constant
R_j	defined in Eq. (IV-26), also defined in Eq. (IV-9)
r	subscript representing the species r
S_o	condition of sources at x = 0
s	subscript representing the oxidant
t_o	initial time
t	time
T	$\beta_{ao} t/2$, dimensionless time used in Chapter III defined in Eq. (IV-9)
T_{jo}	$(T_j)_{t=t_o}$
$T_{a,j}, T_{b,j}$	defined in Eq. (IV-26)
$T_{ao,j}, T_{bo,j}$	$(T_{a,j})_{t=t_o}$, $(T_{b,j})_{t=t_o}$
$\vec{U}, \vec{u}$	relative and absolute velocity vector of the fluid element, also represents the relative and absolute velocity vector contributed to the fluid element from the group of eddies with a larger length scale
u	x-component of $\vec{u}$
$\vec{u}_o$	$\vec{u}$ at source at $t = t_o$
$\vec{V}, \vec{v}$	relative and absolute velocity vector of the fluid element contributed from the group of eddies with a smaller length scale
v	y-component of $\vec{u}$

$\vec{W},\vec{w}$	relative and absolute velocity vector of the fluid element in a multiscale turbulence field
w	z-component of $\vec{u}$.
$\vec{x}$	position vector
x_{ij}	spatial independent variables other than time
x_{ijo}	$(x_{ij})_{t=t_o}$
$x_{i,j}, x_{2,j}\ x_{3,j}$	vector variables in Eq. (L-III-6)
$\vec{x}_{1o},\vec{x}_{2o},\vec{x}_{3o}$	$(x_{1,j},x_{2,j},x_{3,j})_{t=t_o}$
x_1,x_2,x_3	independent variables other than time
x'	x/Λ'
Y	a function of (x_1,x_2,x_3,t)
Y_a	a function of $(\vec{x}_1,\vec{x}_2,\vec{x}_3,t)$
Y_{3a}	defined in Eq. (A-III-10)
Y_{3ao}	$(Y_{3a})_{t=t_o}$
$Y_{2o},Y_{2a1},Y_{2a2},Y_{2a3}$	defined in Eq. (A-III-17a)
y'	y/Λ'
z	chemical species concentration per unit mass
z_α	mass fraction, z, of the αth chemical species
$\langle\ \rangle$	ensemble average
$\langle\bar{\ }\rangle$	normalized ensemble average
α,β	defined in Eq. (V-8), β also defined in Eq. (IV-1)
β_1	characteristic equilibration rate of energy-containing eddies
β^ν	characteristic dissipation rate
β_a,β_b	defined in Eq. (III-2)
β_c	defined in Eq. (III-4)
ν	kinetic viscosity

λ	dissipation scale
Λ	integral scale
Λ'	defined in Eq. (V-76)
Λ_a	length scale of eddy family "a"
Λ_b	length scale of eddy family "b"
Λ_e	apparent length scale
$\bar{\Lambda}_b$	Λ_b/Λ_a
$\bar{\Lambda}_e$	Λ_e/Λ_a
ψ	transition probability
$\psi(t)$	a function of time
ω	chemical reaction term in Eqs. (II-8) and (II-3)
ω_α	production of α species due to chemical reation
σ	a constant
η	y/x
η_o	average mean velocities dividing line
ξ	$\sigma y/x$, also a dummy variable in Eq. (IV-18)
ξ_{ij}	auxiliary variable in integral transform
$\phi_{ij}(t)$	function of time in Eq. (IV-31)
Δ_3, Δ_{ij}	defined in Eq. (IV-31)
$\underline{\Delta}_3, \underline{\Delta}_{ij}$	defined in Eq. (L-III-4)

CHAPTER I

INTRODUCTION

I.A. General Review of the Development of Turbulent Flow Analyses

As noted by many investigators, turbulence has to be treated statistically. Continuum fluid mechanics is, of course, governed by the Navier-Stokes equation. The traditional analyses of turbulence have employed the various moment equations derived from the Navier-Stokes equation for the velocity field and associated moment equations for the scalar fields of interest. In these analyses, closure problems were immediately encountered. The classical statistical theory provides a better description of the basic characteristics of turbulence, but it is focused on certain idealized cases. These studies revealed much of the structure and dynamics of turbulence, yet they were never intended for nor capable of solving engineering problems. Because of this lack of proper modeling of engineering interest, many engineers sought solutions from phenomenological theories. The major sources[1,2,4,5] of the phenomenological theories are familiar to the reader. They are mostly modeled after some form of Prandtl's mixing length theory[1,Chapter 5] and rely heavily on empirical formulations leading to quantitative results.

Glushko[6] presented a model which is typical of the Boussinesq relationship approach. Donaldson[7] used the second order stress equations and the method of Invariant Modeling originated by himself. Again, he used various forms of the Boussinesq model in eliminating triple order moments in terms of gradients of second order moments. Another approach due to Bradshaw[8] incorporated the turbulence energy equation and a non-gradient type of modeling in which terms such as Reynolds stress are replaced by functions of the turbu-

lence energy. Basically, their approaches are more or less the same, and differ only in the particular modeling employed in the closure of the second order moment equations.

Other phenomenological theories, rather than adding turbulence energy equations or the stress equations, proposed a model equation for a total viscosity or a length scale equation. Harlow and Nakayama[9] derived a transport equation for the dissipation scale from a physical argument. Nee and Kovasznay[10] proposed a differential field theory by formulating a transport equation for the above-mentioned total viscosity, again from a physical argument in addition to that necessary for closing the turbulent momentum equation. Spalding[11,12] formed a transport equation for the integral length scale. He recognized the importance of allowing the turbulence field to determine this coupled variation throughout the flow field. His formulation also rests on physical reasoning apart from that involved in closing the lower order (moment) equations.

Another group of theories consists of those making substantial use of statistical arguments. Tchen[13] and Lin[14] are notable contributors in this area. Tchen determined the diffusing properties of small eddies by considering the pair density of a diffusive element through an analysis of the Liouville equation of the statistical mechanics. However, this diffusion is of the near-equilibrium gradient type which is known to be invalid in general since the large energy containing eddies, which are usually anisotropic, dominate the diffusion processes. Lin[14] described a fluid element as being comprised of two mass fractions, each having different dissipation characteristics, thereby taking into account both the large eddy and molecular properties of the fluid elements. His governing equations, which describe the evolution of the chemical species mass fractions comprising the fluid element,

are not easily compared with moment equations derived from the Navier-Stokes and species-conservation equations, and their consistency cannot be readily assessed. However, Lin's work gives the substance to the simplified statistical model developed by Chung[15] which is very successful in many aspects, especially in its consistency in comparison with the moment equations derived from the Navier-Stokes and species conservation equations. The primary purpose of this theory is to replace the various empirical closure schemes (which often do not reflect the true character of turbulence) by a statistical description which draws on known properties of turbulence as determined by the classical statistical theories of turbulence. It is the intent of this theory to study practical turbulent shear flows in a context allowing access to both the results of the classical statistical theories and the voluminous empirical information in the engineering theories.

The concept of the one-point averages being the appropriate moments of a probability density function which is governed by a kinetic equations, has been alien to many engineers working with turbulent flow problems. Since an average (ensemble average) simply implies a weighed moment of a probability function, one should realize the need to analyze the manner in which the averages are constructed, especially when they involve chemically reactive species. This immediately leads us to demand tools in kinetic theory which describe the probability density function. In the next section we will review several turbulent flow descriptions based on kinetic theories in recent years.

I.B. Review of Recent Kinetic Theories of Turbulent Flow

Several turbulent flow descriptions based on kinetic theories have been proposed in recent years [see Lundgren (1967), Chung (1967, 1969, 1970, 1971,

1972, 1973, 1974), Spalding (1971), Fox (1971), Yue, et al. (1974)]. The objectives of these theories, except for Chung et al., have been limited to studies of the flow fields; whereas that for Chung et al. included the analysis of chemical reactions. Starting from the formulation of statistical mechanics and employing the Navier-Stokes equations, Lundgren[16] derived an equation governing the one-point distribution function of fluid elements. There are certain direct contact points between Lundgren's and Chung's work, and these are well described in References 23 and 22.

A description of the simplified statistical theory begins by pointing out the major differences between the approach of this theory and that of the classical statistical and engineering theories. The classical studies proceed in large degree by spectral analysis yielding one of the most important conceptual results in turbulent analysis--that being the association of wave numbers or the reciprocal length scale with the eddy size. Particularly, in the analysis of the spectral energy function, a given range of turbulent energy is associated with a given range of eddy sizes. Kolmogorov's universal equilibrium hypothesis utilizes this spectral representation to describe, in the case of high turbulence Reynolds number, what is essentially a statistical separation between the low wave number, energy-containing eddies and the high wave number, viscous (near equilibrium) region. This result, which has been originally argued for the homogeneous turbulence, is known to be true also in shear flow.[1, Chapter 4] This is one of the a priori conditions that forms the basis of the simplified statistical theory. The primary difference between these two theories is that the present approach attempts no spectral analysis since it is recognized that this method leads immediately to an unsolvable formulation in the type of problems under consideration. It is known that in the high turbulence Reynolds number flows the energy-containing

region of the spectrum (eddies) accounts primarily for the observable quantities, while the high wave number region attempts to degenerate the energy containing eddies toward isotropy. In this context, the mathematical description is in terms of a probability density function (PDF) for one-nonequilibrium degree of freedom which represents the whole energy containing region and, hence, the whole turbulent field. In order to satisfy certain characteristics of high turbulence Reynolds number flows, the representative nonequilibrium degree of freedom is assumed to evolve according to generalized Brownian stochastics.[35,24] Although statistical concepts were employed in the classical theories, no substantial advances were made in dealing directly with the PDF. Hopf[25] has formulated equations for the characteristic functional of this quantity, yet progress came to an early halt with the attempt to obtain solutions. In this sense, the present theory could be looked upon as an extension of the classical statistical work to include the formulation of a solvable equation for the PDF (kinetic equation).

The essential point of comparison between the simplified statistical theory and other engineering theories is between the various moments of the Navier-Stokes and species conservation equations and the corresponding moments of the modified Fokker-Planck equation for the PDF. This is one of the main advantages of the present theory--it can be assessed by comparison with the same equation used throughout turbulent analyses of both homogeneous and shear flows. The very difference is that the closure assumption in this theory is embodied in the single assumption of Brownian stochastics. This closure assumption is free from the conventional concept of the gradient transport. It is also free from the necessity of additional often unrelated assumptions needed to eliminate triple order velocity correlations which

occur in the turbulence energy and stress equations. The most distinguished aspect of the theory is that it is not necessary to drop species correlations in chemically reacting flow problems having non-linear reaction kinetics for complete lack of any modeling method.

The simplified statistical theory has been used successfully on free shear flows, wall turbulence, inert and chemically reacting flows.[26-31,22] The most notable was the treatment of the turbulent diffusion flame indicating the dependence of the finite flame thickness on the integral scale of turbulence. At the time this result was obtained by Chung, the prevailing concept was that in the limit of fast reaction rates there exists a flame sheet similar to that predicted by laminar analyses. The many other theories utilizing mixing length models yielded flame sheet solutions simply because by the nature of the mixing length theory the governing equations became identical in structure to their laminar counterparts, and therefore naturally displayed the same limiting behavior. These equations attribute the same properties to eddy transport as they do to molecular transport, which is a serious mistake. Turbulence processes may or may not proceed at molecular rates. If the turbulence is in equilibrium, molecular or gradient transport may occur. Ascribing gradient transport to turbulence, as does the mixing length concept, prescribes that the turbulent processes are locally governed and are void of any long range nonequilibrium memory. Actually, when a fluid element crosses an interface as a result of a large eddy motion, its interior still maintains the properties existing before crossing. Therefore, in the case of chemical reaction, the reaction can proceed only as fast as the fluid element can break up through eddy breakdown and create new interfaces for reaction. The result is that the thickness of the reaction zone is of the order of the turbulence integral length scale, independent of the molecular

parameters (viscosity, diffusivity, reaction rate, etc.). More of these facts will be shown in the results of a specific solution of two-dimensional turbulent chemically reactive flow in a later chapter.

I.C. Multilength-Scale Turbulent Shear Flows: Extension of the Simplified Statistical Theory

It was through attempts to treat some of the current generation of turbulent shear flow problems that Chung's theory was found to be general enough to include multiscale analyses in the context of its original formulation. Bywater with Chung[23] extended this theory to include two non-equilibrium degrees of freedom. He solved a pair of coupled Langevin equations, each representing different degrees of freedom, and derived a Fokker-Planck type equation similar to that of one non-equilibrium degree of freedom originated by Chung. It was noted that in many flow fields of importance there are more than one predominant scale of turbulence. Turbulence fields reflect the character of the physical mechanism by which they are generated. Consequently, multiscale flows arise as a result of the simultaneous presence of more than one turbulence generating mechanism.

One example of this is the mixing of two streams, each having its own length scale. This will result in a mixing layer between the streams, where the statistical properties are governed by both length scales and the relaxation or interaction process which takes place between the two modes of turbulence. Another multiscale flow occurs at the trailing edge of a wing or plate which has a small finite thickness, in which case there is a length scale associated with the thickness and another with the boundary layer at that point. Combustors used in propulsion systems generally present a turbulence field composed of more than one scale. Swirl combustors obviously

contain two possible different length scales—one is due to the vortical flow at the wall having a length scale corresponding to the size of the inlet slits of the swirl chamber, while the other one is from the mainstream due to its generating mechanism upstream. It is recognized that the turbulent model needed must allow the variation of the scale length as determined by the flow field (similar to Spalding's approach) and must treat multiple length scales. The bimodal characteristics of velocity distribution functions are also shown in Frenkiel and Klebanoff's[33] measurements in a turbulent boundary layer.

It is the effort of this dissertation to find the general solution of the kinetic equations generated in this theory of turbulence. The bimodal method after Lee and Liu[34] as employed in references (26) through (31), has revealed many salient features of turbulent chemically reactive flow. The fundamental solutions to be constructed in a later chapter will afford more direct and accurate solutions than those obtainable from the bimodal approximation. Certain efforts are required in using the Green's function to satisfy the appropriate boundary conditions for a given physical problem.

In the next chapter, we will review Chung's theory in detail.

The structure of a homologous turbulent mixing region characterized by two significant dynamic length scales will be first studied in the third chapter. The subsequent chapters will give the fundamental solutions of the kinetic equations of the present theory. A specific solution of a plane turbuelnt shear flow with chemical reaction will also be presented as an illustrative application of the Green's function method to the solution of the present kinetic equations.

CHAPTER II

REVIEW OF TURBULENT KINETIC THEORY DUE TO CHUNG

In the analysis of later chapters, the kinetic equations developed from Chung's theory will be directly employed to solve certain physical problems. In this chapter, we shall review certain basic concepts in the formulation of the theory. For details, see references 15, 22 and 32.

II.A. General Theory

As mentioned in the beginning of the first chapter, turbulence must be treated statistically. Yet, the objective of classical statistical turbulence theories has been limited to providing a certain basic understanding of the dynamic structure of the homogeneous turbulence field. These theories are not intended for nor capable of providing quantities of engineering interest such as the distribution function for the inhomogeneous flow problems. On the other hand, the mixing-length type theories were not concerned with the study of the dynamic turbulence structure, but rather they were concerned with the solution of the one-point averaged quantities of engineering interest for the inhomogeneous flow problems. As it was pointed out earlier [Chung, 1972 reference (29)], Prandtl's approach could face difficulty when a chemical reaction is involved. In Prandtl's closure technique, the second order moments are first modeled in terms of the gradients of the first order moments via suitable eddy diffusivities. It can be shown that such a model is equivalent to assuming that the probability distribution functions of the fluid elements and chemical species are in near statistical equilibrium. This is often incorrect, especially in reactive flows [see Chung, 1967, reference (15)].

Since it is the energy-containing eddies that account for the observable properties of turbulence, a logical approach to a statistical formulation is to model the turbulence dynamics around the energy-containing eddies according to the known statistical behavior of the energy-containing eddies from the classical statistical theories.

Let us first make a conceptual distinction between the fluid elements and the eddies. On the physical plane of a turbulence field, all size eddies are intermingled together (these eddies can be discerned only on a spectral plane). A fluid element physically belongs to all size eddies affecting that fluid element. Thus, the behavior of a fluid element at a physical point $(\vec{x})$ is correlated to all other fluid elements comprising the eddies of which this fluid element, at $(\vec{x})$, is also a constituent. The maximum size of the eddies that affect a fluid element substantially is of the order of the integral length scale of turbulence. Because of the transport of momentum and the chemical species (as well as the thermal energy), which are contained in and carried by the fluid elements, the description of the movement of the fluid element becomes the central point in the present modeling of turbulent flow. This description will be carried out statistically as it is done with the movement of the molecules in the molecular kinetic theory.

There is a basic difference between the molecular kinetic theory and the present description of the fluid elements. In the former, the collision of a molecule with its neighboring molecules changes the momentum of the molecule and, finally, randomizes its movement, while in the latter, the fluid element is always in direct interaction with all fluid elements comprising the eddies of which our fluid element is a part. That is, the fluid element interacts continually and directly with all fluid elements within the distance of the integral scale.

It is the movement of the fluid element at a physical point $(\vec{x})$ which we wish to describe, but it is the behavior of all size eddies surrounding the given point $(\vec{x})$ which determines the behavior of this fluid element. If the eddies are in nonequilibrium such that they have memories and preferred directions, then the movement of the fluid element at point $(\vec{x})$ will have preferred directions, and its behavior will be statistically in nonequilibrium. Hence, the present kinetic equations would contain the terms which impart the overall effect of the eddies on the movement of the fluid elements in place of the collision integral found in the molecular kinetic equations.

II.B. Langevin Equations

As described in the previous paragraph, the behavior of a fluid element at a given position $(\vec{x})$ is governed by all size eddies of which the fluid element is a constituent. These effects of the intermingled eddies on the movement of the fluid element are well established in the classical statistical theories,[2] for turbulence fields with sufficiently high turbulence Reynolds numbers. These properties, to be discussed below, have been originally established for homogeneous fields. However, their validity for inhomogeneous fields has been strongly suggested by Batchelor[2] and by subsequent researchers [see also Monin and Yaglom, reference (4)].

[1] Turbulence properties of fluid elements are mainly due to the eddies whose sizes are of the order of the integral scale. These eddies are called the "energy-containing" eddies.

[2] Behavior of the energy-containing eddies is statistically separated from that of the smaller eddies which are in statistical equilibrium.

[3] Turbulence properties continuously cascade from the larger to the smaller eddies across the eddy spectrum and they finally dissipate.

The above collective properties of the eddies implies that the movements of the fluid elements are mainly governed by the larger, energy-containing eddies which may be in nonequilibrium, and by the smaller, equilibrium eddies. Shear and other turbulence generating mechanisms supply the energy-containing eddies and, therefore, these eddies may be in nonequilibrium; that is, these eddies may be non-isotropic and contain preferred memories imparted to them by the generating mechanisms. Through interactions between the eddies, these larger eddies become isotropic or random. For the usual situations wherein the eddies are continuously generated, the energy-containing eddies are in nonequilibrium.

The sum total effect of the eddies on the movement of the fluid elements must contain both the nonequilibrium influence of the larger, energy-containing eddies, and the completely random influence of the smaller, equilibrium eddies. With the known eddy properties [1] - [3], the equation to be used to describe the effect of the dynamics of interaction on the movement of the fluid elements is the stochastic Langevin equation,

$$\frac{du_i}{dt} = -\beta_1(u_i - \langle u\rangle_i) + A_i(t) + K_i \qquad \text{(II-1)}$$

In the above equation, the first term on the right side represents the influence on the fluid element of the energy-containing eddies, which may be in nonequilibrium and contain preferred memories. The second term, $A_i(t)$, represents the randomizing influence of the smaller, equilibrium eddies on the movement of the fluid element. K_i represents the dissipation rate of

the fluid momentum caused by the smaller equilibrium eddies, and the effect of the mean pressure gradient and other body forces on the acceleration of the fluid element. β_1 is the characteristic equilibration rate of the larger, energy-containing eddies, and is known[2] to be

$$\beta_1 = A \frac{\langle U_k U_k \rangle^{1/2}}{2\Lambda} \qquad \text{(II-2)}$$

where A is of the order of unity.

The description of the eddy influence on the fluid element by the Langevin equation which separates the influence of the nonequilibrium degrees, $\beta_1(u_i - \langle u \rangle_i)$, from that of the equilibrium degrees, $A_i(t)$, is possible because of the eddy property [2].

The generalized Brownian stochastics describe a process which is governed by a few nonequilibrium degrees of freedom and a sea of equilibrium degrees of freedom wherein the former are statistically separated from the latter, and the characteristic times of the former are sufficiently longer than those of the latter. In the present problem, the eddies represent the degrees of freedom. The energy-containing eddies represent the nonequilibrium degrees and the smaller equilibrium eddies represent the equilibrium degrees. It is very clear that the known properties [1] - [3] satisfy the basic conditions required for the use of the Brownian stochastics. Detailed discussion of the Langevin equation is given in references (15) and (24).

We note that Eq. (II-1) is simply an equation which imparts certain collective properties of the eddies into the description of the behavior of a fluid element. The collective properties of the eddies we use are those found from the turbulence structure studies carried out in the classical statistical theories by use of the Navier-Stokes equation. The present Langevin

equation, Eq. (II-1), is used to describe an entirely different physical phenomenon from the well known problem of large molecules moving through a sea of small molecules described by Chandrasekhar.[24] This difference between the present turbulent flow problems and the molecular problems has been explained in the previous section.

II.C. Derivation of Kinetic Equations

We recognize the fact that, in the present continuum turbulence, the chemical species move as they are being transported by the fluid elements. Therefore, the transport velocity of the chemical species is the fluid element velocity $\vec{U}$ governed by Eq. (II-1).

Let us consider the probability density function (henceforth, it will be called the distribution function after the molecular kinetic-theory terminology) of a chemical species, $F(t,\vec{x},\vec{u})$. This quantity is defined such that $F(t,\vec{x},\vec{u})d\vec{u}$ denotes the mass fraction of the chemical species with velocities between $\vec{u}$ and $\vec{u} + d\vec{u}$ at t and $\vec{x}$. Then these distribution functions at two different phase points are related by the integral relationship,

$$F(t + \Delta t,\vec{x},\vec{u}) = \int [F(t,\vec{x} - \vec{u}\Delta t,\vec{u} - \Delta\vec{u}) + \omega^*(t,\vec{x} - \vec{u}\Delta t,\vec{u} - \Delta\vec{u})\Delta t + Mf(t,\vec{x} - \vec{u}\Delta t,\vec{u} - \Delta\vec{u})\Delta t] \times \psi(\vec{x} - \vec{u}\Delta t,\vec{u} - \Delta\vec{u};\Delta\vec{u})d(\Delta\vec{u}) \qquad \text{(II-3)}$$

The function ψ is the transition probability of the fluid elements between the two phase points. ψ is obtained from the stochastic solution

*All symbols used are defined in the nomenclature.

of the Langevin equation, Eq. (II-1), to satisfy the boundary condition that in the limit of time much longer than the characteristic equilibration time, $1/\beta_1$, and in the absence of dissipation, the mean pressure gradient, and the other body forces ($K_i \to 0$), the velocity distribution function, f, should be Maxwellian about the local mean turbulence energy, $\langle U_k U_k \rangle$. M denotes the rate of molecular dissipation of the chemical species which will be defined presently.

With the use of the solution of the Langevin equation for ψ, Eq. (II-3) can be manipulated to give the kinetic equation of the chemical species [see references (15), (26-28) for details].

$$\frac{\partial}{\partial t} + u_j \frac{\partial F}{\partial x_j} + \frac{\partial}{\partial u_j}(FK_j)$$

$$= \beta_1 \left\{ \frac{\partial}{\partial u_j}\left[(u_j - \langle u \rangle_j)F\right] + \frac{\langle U_k U_k \rangle}{3} \frac{\partial^2 F}{\partial u_j \partial u_j} \right\} + \omega f + M \qquad \text{(II-4)}$$

Commensurate with the form of the first term on the right of Eq. (II-1), we express for the free shear layers[22] with no body forces

$$K_j = -\beta^{\nu}(u_j - \langle u_j \rangle) - \frac{1}{\rho}\frac{\partial \langle p \rangle}{\partial x_j}$$

(II-5)

$$M = -\beta^{\nu}(F - \langle z \rangle f)$$

where z is the species concentration, and the characteristic dissipation rate, β^{ν}, is known to be[1]

$$\beta^{\nu} = A' \frac{\nu}{\lambda^2} \tag{II-6}$$

β^{ν} can be related to β through a turbulence Reynolds number. This will be given in detail in a later chapter. ω is the chemical reaction term, and the detail of this term is given in references (26) - (28).

In a turbulent flow field consisting of n-chemical species, we would have n-equations of the type of Eq. (II-4). That is, we would have Eq. (II-4) for F_1, F_2, . . . F_n. The sum of these equations then becomes the kinetic equation of the fluid elements

$$\frac{\partial f}{\partial t} + u_j \frac{\partial f}{\partial x_j} + \frac{\partial}{\partial u_j}(\omega K_j)$$

$$= \beta_1 \left\{ \frac{\partial}{\partial u_j} [(u_j - \langle u_j \rangle) f] + \frac{\langle U_k U_k \rangle}{3} \frac{\partial^2 f}{\partial u_j \partial u_j} \right\} \tag{II-7}$$

Derivation of the kinetic equation is now essentially complete.

More specifically, an equation for the free shear layers can be derived for the distribution function for a scalar quantity z (such as temperature or chemical species) and is given as [the reader is referred to references (15),(32) and (26-29) for details]

$$\frac{\partial(fz)}{\partial t} + u_j \frac{\partial(fz)}{\partial x_j}$$

$$= \beta_1 \left\{ \frac{\partial}{\partial u_j} \left[(u_j - \langle u_j \rangle) fz\right] + \frac{\langle U_k U_k \rangle}{3} \frac{\partial^2 fz}{\partial u_j \partial u_j} \right\}$$

$$+ \beta^{\nu} \left\{ \frac{\partial}{\partial u_j} \left[(u_j - \langle u_j \rangle) fz\right] - f(z - \langle z \rangle) \right\} + \omega f \qquad \text{(II-8)}$$

The moment equations constructed from the present kinetic equations are termwise comparable to the one-point averaged equations derived from the Navier-Stokes and species conservation equations. Details of this comparison are well presented in previous references.[15,26-28] Some of the salient features will be explained herein.

The starting point of testing the consistency of the present theory and the conventional one-point averaged equations derived from the Navier-Stokes and species concentration equations is the kinetic equations given in Chung[22] which are the generalized version of Eq. (II-8) including the effects of the mean pressure gradient and wall. We first multiply the kinetic equation through by an undetermined tensor function $Q(\vec{U})$ and integrate it termwise with respect to the velocity space. This results in the generalized moment equation of the present theory. We can then generate from this equation various particular moment equations by assigning particular functions for Q.

First, we set $z = 1$. Then, when we also set $Q = 1$, there results the standard averaged continuity equation. With $Q = U_i$, we obtain the averaged momentum equation, Eq. (II-3). With $Q = U_i U_j$, we obtain the averaged Reynolds equation, except it does not contain the diffusion term of the pressure energy.

Now, we restore z and then set $Q = 1$. The generalized moment equation

then gives the averaged species conservation equation. With $Q = W_i$, we obtain the second order averaged equation, obtainable by multiplying the standard species conservation equation by W_i and averaging it. The higher order moment equations are found to be termwise comparable to the corresponding order one-point averaged equations obtainable from the Navier-Stokes and standard species conservation equations except for the terms resulting from the pressure-energy diffusion term. For many flow problems of our interest, the pressure energy diffusion is not too large. It is felt that the order of inaccuracy involved with this term may be within the order of the other approximations of this theory.

The above shows that the present kinetic theory basically satisfies the conservation of the averaged quantities as dictated by the Navier-Stokes and species conservation equations. Therefore, the present theory is as consistent in describing turbulent flow as those theories which begin from the one-point averaged equations.

Further support for the consistency of Chung's theory can be obtained from the work of Lundgren.[16-18] Starting from the formalism of statistical mechanics and employing the Navier-Stokes equation, Lundgren[16] derived an equation governing the distribution function of the fluid element. An equation similar to Lundgren's equation can be derived for fz using the Navier-Stokes and species conservation equations [see references (22) and (32)]. Again, if we express the eddy interaction effects in Fokker-Planck form, we derive the present kinetic equation for fz. Details of these derivations are well presented in reference (32) and (15) and will not be repeated here.

In the above derivations, the present analysis, based on the Langevin equation, supplies a detailed rationale for the Fokker-Planck form based on

the known dynamics of the eddies and the physical arguments for the turbulent movements of the chemical species.

II.D. Multiscale Kinetic Equation

Based on Chung's theory, Bywater[23] with Chung solved two coupled Langevin equations and derived a kinetic equation for two nonequilibrium degrees of freedom governing the one-point joint distribution function of the fluid elements. These two Langevin equations are given as

$$\frac{d\vec{U}_k}{dt} = -\beta_a[u_k - \langle u_k \rangle] + A_{a,k}(t) + K_{a,k} + \beta_c[U_k - V_k]$$

$$\frac{d\vec{V}_k}{dt} = -\beta_b[v_k - \langle v_k \rangle] + A_{b,k}(t) + K_{b,k} + \beta_c[V_k - U_k] \qquad \text{(II-9)}$$

This time the flow field is assumed to be characterized by two nonequilibrium families of eddies in addition to the equilibrium eddies. The above two equations each represent the contribution from each mode of nonequilibrium families of eddies and many equilibrium eddies on the movement of the fluid element. These two coupled Langevin equations are formed based on the same physical reasoning as Chung's theory, except that the interaction terms $\pm\,\beta_c[U_j - V_j]$ are added to take in account the interaction between two nonequilibrium eddies. The resulting kinetic equation for two nonequilibrium degrees of freedom governing the distribution function of the fluid element will be presented in the next chapter. The reader is referred to reference (23) for details of this derivation.

CHAPTER III

MIXING AND DECAY OF A TURBULENCE FIELD CHARACTERIZED BY TWO SIGNIFICANT LENGTH SCALES

The need to describe length scales in the modeling of a turbulent flow has been noted by many investigators (Spalding, Chung, Yen, Bywater, et al.). Many of the important turbulent flow fields are actually characterized by more than one significant dynamic length scale as mentioned in the previous chapter. Although Spalding[12] has proposed an equation governing the length scale of turbulent flow, its approach is rather traditional and is similar to that of other equations governing the transferrable physical quantities of the flow. His formulation is based on the physical reasoning similar to those employed in the closure of the other moment (averaged) equations. Instead of closing the moment equation, a more basic and general--in the sense of generating moments--kinetic theory of turbulence due to Chung[15] has been developed as described in the previous chapter. Although the original model lumped the turbulent flow field into one nonequilibrium degree of freedom, Chung's theory is found to be general enough to include the multiscale features of the flow field in its original formulation. Bywater with Chung[23] extended the theory to include two nonequilibrium degrees of freedom.

In this chapter, the kinetic equation of two nonequilibrium degrees of freedom will be employed to study some of the mixing behavior of a multiscale turbulence field. The physical problem of interest is the mixing and decay of an initially uniform and homogeneous turbulence field which is characterized by two different length scales. The generation and subsequent behavior of the apparent length scale will also be analyzed.

III.A. Governing Equations

The starting point of this analysis is the kinetic equation of two nonequilibrium degrees of freedom given in reference (23), which is,

$$\frac{\partial f_2}{\partial t} - \left[\frac{\partial \langle u\rangle_k}{\partial t}\frac{\partial f_2}{\partial U_k} + \frac{\partial \langle v\rangle_k}{\partial t}\frac{\partial f_2}{\partial V_k}\right] + (U_k + V_k + \langle w\rangle_k)$$

$$\times \left[\frac{\partial f_2}{\partial x_k} - \frac{\partial \langle u\rangle_m}{\partial x_k}\frac{\partial f_2}{\partial U_m} - \frac{\partial \langle v\rangle_m}{\partial x_k}\frac{\partial f_2}{\partial V_m}\right]$$

$$= \frac{\partial}{\partial U_k}\left\{[\beta_a U_k + \beta_c(U_k - V_k) - K_{a,k}]f_2\right\}$$

$$+ \frac{\partial}{\partial V_k}\left\{[\beta_b V_k + \beta_c(V_k - U_k) - K_{b,k}]f_2\right\}$$

$$+ q\left\{\frac{\partial^2}{\partial U_k \partial U_k} + 2\frac{\partial^2}{\partial U_k \partial V_k} + \frac{\partial^2}{\partial V_k \partial V_k}\right\}f_2 \qquad \text{(III-1)}$$

where $f_2(t,\vec{x},\vec{U},\vec{V})$ is the one-point joint distribution function of the fluid elements affected by two families of nonequilibrium degrees of freedom as well as the equilibrium degrees of freedom. U_k, u_k and $\langle u\rangle_k$, and V_k, v_k and $\langle v\rangle_k$ are the relative, absolute, and mean velocity contributions to the same fluid element of the two different nonequilibrium degrees of freedom, respectively. β_a and β_b are the characteristic relaxation rates of the two nonequilibrium degrees of freedom, respectively. As in the previous analysis, β_a and β_b are given as

$$\beta_a = \frac{\langle W_k W_k \rangle^{1/2}}{2\Lambda_a}$$

$$\beta_b = \frac{\langle W_k W_k \rangle^{1/2}}{2\Lambda_b} \qquad \text{(III-2)}$$

where $\langle W_k W_k \rangle$ is the total turbulence energy, and Λ_a and Λ_b are, respectively, the characteristic lengths of the two nonequilibrium degrees of freedom representing the two families of the nonequilibrium eddies. W_k and w_k are, respectively, the relative and absolute velocities of the fluid element, and these are the vector sums of the contributions from the two nonequilibrium degrees of freedom (see Figure 1)

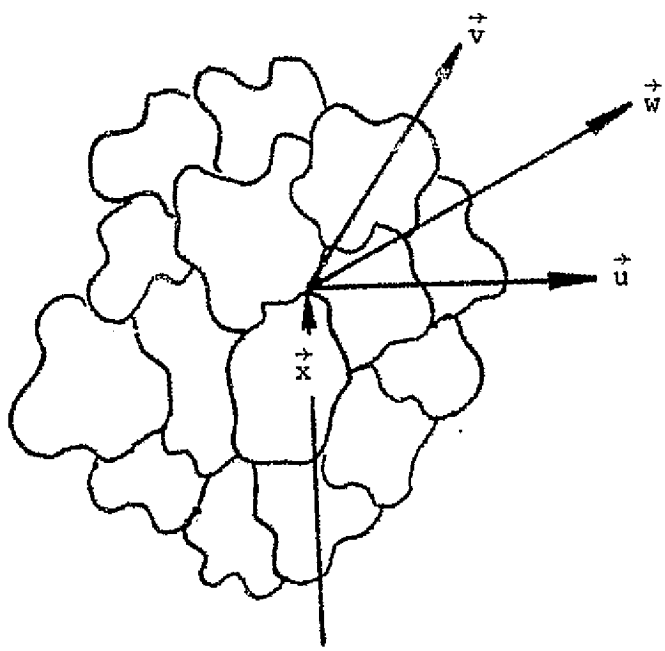


Figure 1 Contribution of two nonequilibrium degrees of freedom to the velocity of a fluid element

Thus, W_k and w_k are given as

$$W_k = U_k + V_k$$

$$w_k = \langle w \rangle_k + W_k \qquad \text{(III-3)}$$

or

$$w_k = u_k + v_k$$

β_c is the characteristic rate of interaction between the two nonequilibrium degrees of freedom which, according to Chung and Bywater, is

$$\beta_c = \begin{cases} \beta_a & \text{if } \Lambda_a > \Lambda_b \\ \beta_b & \text{if } \Lambda_a < \Lambda_b \end{cases} \qquad \text{(III-4)}$$

Equation (III-4) is based on the premise that the larger (therefore, the lower wave number) fluctuating eddies control the rate of momentum exchange between the two families of eddies.

For the flows with no mean pressure gradient and laminar sublayer, the molecular dissipation rates $K_{a,k}$ and $K_{b,k}$ are given, analogous to references (26-29), as,

$$K_{a,k} = -\beta_a U_k$$

$$K_{b,k} = -\beta_b V_k \qquad \text{(III-5)}$$

The right hand side of Eq. (III-1) describes three major aspects of the eddy interactions consisting of (1) the relaxation of the nonequilibrium eddies toward equilibrium, (2) the exchange of momentum between the two nonequilibrium degrees, and (3) the dissipation. The first two aspects pertain only to the internal redistribution of the properties, whereas the dissipation constitutes a sink for the turbulence properties. If a turbulence-energy conservation equation is constructed by taking an appropriate moment of Eq. (III-1), all terms except those containing $K_{a,k}$ and $K_{b,k}$ should vanish independently of any particular f_2. q is thus defined by Bywater as,

$$q = \frac{\beta_a \langle U_k U_k \rangle + (\beta_a + \beta_b) \langle U_k V_k \rangle + \beta_b \langle V_k V_k \rangle}{12} \qquad \text{(III-6)}$$

The physical phenomena of present interest are the mixing and decay of a turbulence field characterized by two nonequilibrium degrees of freedom representing two families of nonequilibrium eddies. We assume that initially (t = 0) these two families of eddies are uniformly distributed throughout the field. We consider that there exists no mean velocity. The solution would be the same if the mean velocity were non-zero but uniform. We specify, initially, the contributions of the two families of eddies to the turbulence energy* of the field as $\langle U_k U_k \rangle$ and $\langle V_k V_k \rangle$. The characteristic length scales Λ_a and Λ_b are also specified. We then seek the solution of Eq. (III-1), for $t > 0$, for $\langle U_k U_k \rangle$, $\langle V_k V_k \rangle$, $\langle U_k V_k \rangle$, and Λ_e. The apparent length scale, Λ_e, represents the length scale of a hypothetical turbulence field characterized by one family of nonequilibrium eddies wherein the behavior of $\langle W_k W_k \rangle$ is

*Note that since the field is spacially isotropic, the only nontrivial components of $\langle w_i w_j \rangle$ is the turbulence energy $\langle W_k W_k \rangle$.

the same as that in the actual field governed by the two nonequilibrium families of eddies. Λ_e is defined subsequently in Eq. (III-20). Note that

$$\langle W_k W_k \rangle = \langle U_k U_k \rangle + 2\langle U_k V_k \rangle + \langle V_k V_k \rangle \tag{III-7}$$

where $\langle U_k V_k \rangle$ evolves for $t > 0$ through the interaction of the two nonequilibrium degrees of freedom.

Thus, for the present problem,

$$\frac{\partial \langle u \rangle_m}{\partial x_k} = 0 \quad , \qquad \frac{\partial \langle u \rangle_m}{\partial t} = 0$$

$$\frac{\partial \langle v \rangle_m}{\partial x_k} = 0 \quad , \qquad \frac{\partial \langle v \rangle_m}{\partial t} = 0 \tag{III-8}$$

$$\langle w \rangle_i = 0$$

for all t.

Our governing equation, Eq. (III-1), then simplifies to,

$$\begin{aligned} \frac{\partial f_2}{\partial t} = & \frac{\partial}{\partial U_k} \left\{ [\beta_a U_k + \beta_c (U_k - V_k) - K_{a,k}] f_2 \right\} \\ & + \frac{\partial}{\partial V_k} \left\{ [\beta_b V_k + \beta_c (V_k - U_k) - K_{b,k}] f_2 \right\} \\ & + q \left\{ \frac{\partial^2}{\partial U_k \partial U_k} + 2 \frac{\partial^2}{\partial U_k \partial V_k} + \frac{\partial^2}{\partial V_k \partial V_k} \right\} f_2 \end{aligned} \tag{III-9}$$

III.B. Initial Conditions

For the present physical problem, we have the following initial conditions:

At $t = 0$

The contribution to the turbulence energy of the family of eddies denoted by "a":

$$\langle U_k U_k \rangle = \langle U_k U_k \rangle_o , \quad \text{length scale } \Lambda_a \tag{III-9a}$$

The contribution to the turbulence energy of the family of eddies denoted by "b":

$$\langle V_k V_k \rangle = \langle V_k V_k \rangle_o , \quad \text{length scale } \Lambda_b \tag{III-9b}$$

No interaction between the two nonequilibrium degrees of freedom, i.e., $\langle U_k V_k \rangle = \langle U_k V_k \rangle_o = 0$.

And the turbulence energy:

$$\langle W_k W_k \rangle = \langle W_k W_k \rangle_o \tag{III-9c}$$

Obviously, we have

$$\langle W_k W_k \rangle_o = \langle U_k U_k \rangle_o + \langle V_k V_k \rangle_o \tag{III-9d}$$

In the subsequent analysis we will let "a" represent the family of eddies with the larger length scale, ($\Lambda_a > \Lambda_b$), and $\langle U_k V_k \rangle$ will be called the "interaction turbulence energy."

III.C. Generalized Moment Equations

We multiply each term of Eq. (III-9) by a general function, $Q(\vec{V},\vec{U})$. Then, the term-wise integration with respect to $\vec{U}$ and $\vec{V}$ and the subsequent manipulation result in the following generalized moment equation,

$$\frac{\partial}{\partial t}\iint f_2 Q d\vec{U}d\vec{V} - \iint f_2 \frac{\partial Q}{\partial t} d\vec{U}d\vec{V}$$

$$= -\iint [2\beta_a U_k + \beta_c(U_k - V_k)] f_2 \frac{\partial Q}{\partial U_k} d\vec{U}d\vec{V}$$

$$- \iint [2\beta_b V_k + \beta_c(V_k - U_k)] f_2 \frac{\partial Q}{\partial V_k} d\vec{U}d\vec{V}$$

$$+ q\iint f_2 \left[\frac{\partial^2 Q}{\partial U_k \partial U_k} + 2\frac{\partial^2 Q}{\partial U_k \partial V_k} + \frac{\partial^2 Q}{\partial V_k \partial V_k}\right] d\vec{U}d\vec{V} \qquad \text{(III-10)}$$

III.D. Averaged Energy Equations

As it has been mentioned, the only nontrivial component of $\langle W_i W_j \rangle$ is the turbulence energy, $\langle W_k W_k \rangle$, which consists of the three constituents shown in Eq. (III-7). We can directly deduce the governing moment equations for the turbulence energy and its constituents by substituting the following particular values for Q in Eq. (III-10) as,

$\underline{Q = U_k U_k}$

$$\frac{\partial \langle U_k U_k \rangle}{\partial t} = -6\beta_a \langle U_k U_k \rangle + 2\beta_a \langle U_k V_k \rangle + 6q \qquad \text{(III-10)}$$

$\underline{Q = V_k V_k}$

$$\frac{\partial \langle V_k V_k \rangle}{\partial t} = -(4\beta_b + 2\beta_a)\langle V_k V_k \rangle + 2\beta_a \langle U_k V_k \rangle + 6q \qquad \text{(III-12)}$$

$\underline{Q = U_k V_k}$

$$\frac{\partial \langle U_k V_k \rangle}{\partial t} = \beta_a \langle U_k U_k \rangle + \beta_a \langle V_k V_k \rangle - (4\beta_a + 2\beta_b)\langle U_k V_k \rangle + 6q \qquad \text{(III-13)}$$

$\underline{Q = W_k W_k}$

$$\frac{\partial \langle W_k W_k \rangle}{\partial t} = -4\beta_a \langle U_k U_k \rangle - 4\beta_b \langle V_k V_k \rangle - 4(\beta_a + \beta_b)\langle U_k U_k \rangle + 24q \qquad \text{(III-14)}$$

Substituting Eq. (III-6) into Eq. (III-14), we obtain

$$\frac{\partial \langle W_k W_k \rangle}{\partial t} = -2[\beta_a \langle U_k U_k \rangle + (\beta_a + \beta_b)\langle U_k V_k \rangle + \beta_b \langle V_k V_k \rangle] \qquad \text{(III-15)}$$

We let β_e represent the apparent characteristic relaxation rate and Λ_e represent the apparent length scale for a hypothetical turbulence field characterized by one nonequilibrium family of eddies wherein the behavior of $\langle W_k W_k \rangle$ will be the same as that in the actual field characterized by two nonequilibrium degrees of freedom. The kinetic equation for one nonequilibrium degree of freedom, Eq. (II-7), can be employed to describe this hypothetical turbulence field characterized by one nonequilibrium family of

eddies. Under the same assumptions as cited in section III.A.--i.e., that there is no mean velocity, no mean pressure gradient, no laminar sublayer, and the turbulence is initially isotropic throughout the field--the governing equation of this hypothetical turbulence field characterized by one nonequilibrium family of eddies can be obtained, from Eq. (II-7) as,

$$\frac{\partial f}{\partial t} = 2\beta_e \frac{\partial f W_j}{\partial W_j} + \beta_e \frac{\langle W_j W_j \rangle}{3} \frac{\partial^2 f}{\partial W_k \partial W_k} \tag{III-16}$$

We multiply the above equation by $W_k W_k$ and term-wise integrate with respect to $\vec{W}$, as,

$$\frac{\partial \langle W_k W_k \rangle}{\partial t} = -2\beta_e \langle W_k W_k \rangle \tag{III-17}$$

Analogous to Eq. (II-2), β_e can be written as

$$\beta_e = \frac{\langle W_k W_k \rangle^{1/2}}{2\Lambda_e} \tag{III-18}$$

Now, by equating the right sides of Eqs. (III-15) and (III-17), the apparent relaxation rate, β_e, can be written as

$$\beta_e = \beta_a \frac{\langle U_k U_k \rangle + \langle U_k V_k \rangle}{\langle W_k W_k \rangle} + \beta_b \frac{\langle V_k V_k \rangle + \langle U_k V_k \rangle}{\langle W_k W_k \rangle} \tag{III-19}$$

One of our main interests is the equation explicitly governing the apparent length scale of the flow field. This is readily obtained from Eqs. (III-2),

(III-18) and (III-19), and can be written as

$$\Lambda_e = \left[\frac{1}{\Lambda_a} \frac{\langle U_k U_k \rangle + \langle U_k V_k \rangle}{\langle W_k W_k \rangle} + \frac{1}{\Lambda_b} \frac{\langle U_k V_k \rangle + \langle V_k V_k \rangle}{\langle W_k W_k \rangle} \right]^{-1} \qquad \text{(III-20)}$$

Equation (III-20) describes the apparent characteristic length Λ_e in terms of the two constant dynamic scales Λ_a and Λ_b, and the energies associated with these scales. The energies in Eq. (III-20) are dependent upon the solution of the governing equation, Eq. (III-8). The apparent length scale, Λ_e, and its variation depend on the solution of the governing equation itself. This is in basic agreement with the concept proposed by Spalding[11,12] that the length scale depends on a given problem, and that it should have a governing equation which must be solved simultaneously with the governing equations of the other turbulence properties.

Equations (III-11) through (III-15) and Eq. (III-20) are manipulated and nondimensionalized as,

$$\frac{d\langle \overline{U_k U_k} \rangle}{dT} = \langle \overline{W_k W_k} \rangle^{1/2} \left[-11 \langle \overline{U_k U_k} \rangle + M \langle \overline{V_k V_k} \rangle + (5 + M) \langle \overline{U_k V_k} \rangle \right] \qquad \text{(III-21a)}$$

$$\frac{d\langle \overline{V_k V_k} \rangle}{dT} = \langle \overline{W_k W_k} \rangle^{1/2} \left[\langle \overline{U_k U_k} \rangle - (7M + 4) \langle \overline{V_k V_k} \rangle + (5 + M) \langle \overline{U_k V_k} \rangle \right]$$

(III-21b)

$$\frac{d\langle\overline{U_k V_k}\rangle}{dT} = \langle\overline{W_k W_k}\rangle^{1/2} \left[3\langle\overline{U_k V_k}\rangle + (2 + M)\langle\overline{V_k V_k}\rangle - (7 + 3M)\langle\overline{U_k V_k}\rangle\right] \tag{III-21c}$$

$$\frac{d\langle\overline{W_k W_k}\rangle}{dT} = \langle\overline{W_k W_k}\rangle^{1/2} \left[- 4\langle\overline{U_k U_k}\rangle - 4M\langle\overline{V_k V_k}\rangle - (4 + 4M)\langle\overline{U_k V_k}\rangle\right] \tag{III-21d}$$

and

$$\overline{\Lambda_e} = \left[\frac{\langle\overline{U_k U_k}\rangle + \langle\overline{U_k V_k}\rangle}{\langle\overline{W_k W_k}\rangle} + M \frac{\langle\overline{V_k V_k}\rangle + \langle\overline{U_k V_k}\rangle}{\langle\overline{W_k W_k}\rangle}\right]^{-1} \tag{III-22}$$

where < > is normalized by $\langle W_k W_k\rangle_o$

$$\langle\overline{\ }\rangle = \frac{\langle\ \rangle}{\langle W_k W_k\rangle_o} \tag{III-23}$$

and M is the length scale ratio,

$$M = \frac{\Lambda_a}{\Lambda_b} \tag{III-24}$$

The limit t, is nondimensionalized by $\beta_{ao}/2$, as

$$T = \frac{t\beta_{ao}}{2} \tag{III-25}$$

where

$$\beta_{ao} = \frac{\langle W_k W_k \rangle_o^{1/2}}{2\Lambda_a} \tag{III-26}$$

and

$$\overline{\Lambda_e} = \frac{\Lambda_e}{\Lambda_a} \tag{III-27}$$

Equations (III-21a) through (III-21d) and (III-22) are now self-contained and are closed.

III.E. Typical Numerical Results

Equations (III-21a) through (III-21d) constitute a system of nonlinear first order ordinary differential equations. This system is numerically integrated to satisfy the initial conditions, Eqs. (III-9a) through (III-9d).

Typical results for three different length-scale ratios are presented in Figures 2 through 7. These three length-scale ratios are chosen in such a way that they may represent small, intermediate and large length-scale ratios. Two sets of initial conditions are chosen for each set of calculations for a given length-scale ratio--one is for $\langle U_k U_k \rangle_o$ relatively larger than $\langle V_k V_k \rangle_o$, and the other one is for $\langle U_k U_k \rangle_o$ relatively smaller than $\langle V_k V_k \rangle_o$.

Figures 2 and 3 give the solution of the decay of $\langle \overline{W_k W_k} \rangle$ for different length-scale ratios and initial conditions. Figures 4 and 5 present the variation of $\langle \overline{U_k U_k} \rangle$--the turbulence energy contributed by the group of eddies with a larger length scale--under various given conditions. Figures 4 and 5 also show the changes of $\langle \overline{V_k V_k} \rangle$--the turbulence energy contributed by the group of

eddies with a smaller length-scale--for different length-scale ratios and given initial conditions. Figures 6 and 7 indicate the emergence and decay of the interacting turbulence energy, $\langle\overline{U_k V_k}\rangle$, under various given conditions.

III.F. Discussion of the Results

Figure 2 shows the decay of $\langle\overline{W_k W_k}\rangle$ and the variation of the normalized apparent length-scale, Λ_e/Λ_a, for different values of the length-scale ratio M. The curves in Figure 2 are under the initial conditions of $\langle\overline{U_k U_k}\rangle_o = 0.8$ and $\langle\overline{V_k V_k}\rangle_o = 0.2$, which indicates that the initial turbulence energy, $\langle W_k W_k\rangle_o$, is mainly contributed by the family of eddies with a larger length scale (Λ_a).

In Figure 2, $\langle\overline{W_k W_k}\rangle$ decays approximately in proportion to the inverse of T, i.e.,

$$\langle\overline{W_k W_k}\rangle \propto (T - T_o)^{-1} \qquad \text{(III-28)}$$

where T_o is zero. Equation (III-28) shows the simple power law of the decay of turbulence energy as studied in the grid-generated homogeneous turbulence.[2] If the turbulence field has a uniform mean velocity $\langle w\rangle_\infty$, Eq. (III-28) may be written as

$$\langle W_k W_k\rangle \propto (x - x_o)^{-1} \qquad \text{(III-28a)}$$

where $(x - x_o)$ is the down stream distance from the grid. From experimental evidence,[2] Eq. (III-28a) is further given as[2]

$$\frac{\langle W_k W_k \rangle}{\langle w \rangle_\infty^2} = \left[\frac{a}{D} (x - x_o) \right]^{-1} \tag{III-28b}$$

where D is the grid size and a is a function of the shape of the grid and the grid Reynolds number, $\langle W_k W_k \rangle^{1/2} D/\nu$. Our Figure 2 shows that $\langle \overline{W_k W_k} \rangle$ decays faster or slower according to whether its corresponding normalized apparent length scale is smaller or larger. If we would put an equal sign in Eq. (III-28), the proportionality constant would be a function of the normalized apparent length scale. Thus, Eq. (III-28) may be written as,

$$\langle \overline{W_k W_k} \rangle \sim \frac{b}{\overline{\Lambda_e}} (T - T_o)^{-1} \tag{III-28c}$$

Since the grid size D is approximately the integral length scale of the grid-generated turbulence, the meaning of the proportionality constants of Eq. (III-28b) is equivalent to that of Eq. (III-28c).

If the apparent length scale is larger, one would expect that it would take a longer time for the energy-containing eddies to relax toward equilibrium, or that the turbulence energy would decay more slowly. These properties are shown in Figure 2 for the decay of $\langle \overline{W_k W_k} \rangle$.

The variation of the normalized apparent length scale $\overline{\Lambda_e}$ is given by Eq. (III-22). For a given length-scale ratio M, the initial value of $\overline{\Lambda_e}$ is determined by the initial values of $\langle \overline{U_k U_k} \rangle_o$ and $\langle \overline{V_k V_k} \rangle_o$, which is easily seen from Eq. (III-22), and can be written as

$$\overline{\Lambda_e} \Big|_{t=0} = [\langle \overline{U_k U_k} \rangle_o + M \langle \overline{V_k V_k} \rangle_o]^{-1} \tag{III-29}$$

Equation (III-29) gives the starting point of the curve for $\overline{\Lambda_e}$ for a given M and the initial values of $\langle\overline{U_k U_k}\rangle_o$ and $\langle\overline{V_k V_k}\rangle_o$. When mixing of the two families of nonequilibrium eddies begins, T > 0, the normalized apparent length scale $\overline{\Lambda_e}$ varies according to the redistribution of the varying turbulence energies which appeared in Eq. (III-22). Since we do not have a closed form solution for each turbulence energy and the normalized apparent length-scale $\overline{\Lambda_e}$, it is difficult to see the variation of $\overline{\Lambda_e}$ in the initial period, 0 < T < 2.5, of mixing and decay. However, after T > 2.5, the normalized apparent length-scales, $\overline{\Lambda_e}$'s, tend to reach a steady value which is slightly less than the value of (1/2)(1 + 1/M) as shown in Figures 2 and 3. Since our turbulence field is characterized by two length scales, the apparent length scale of a hypothetical turbulence field characterized by one length scale, Λ_e, would have a value between Λ_a and Λ_b. It seems logical to estimate that Λ_e has a value which is close to the average value of Λ_a and Λ_b. This gives us the normalized length scale $\overline{\Lambda_e}$ as approximately equal to (1/2)(1 + 1/M).

Figure 3 shows the decay of $\langle\overline{W_k W_k}\rangle$ and the variation of Λ_e/Λ_a with the initial conditions $\langle\overline{U_k U_k}\rangle_o = 0.2$ and $\langle\overline{V_k V_k}\rangle_o = 0.8$. The decay of $\langle\overline{W_k W_k}\rangle_o$ in Figure 3 is similar to that in Figure 2, and the curves of Figure 2 are discussed in the previous paragraph. This time, the initial turbulence energy is mainly contributed by the turbulence energy of the group of eddies with a smaller length scale. From Eq. (III-29), for each M, we can see that the initial value of the normalized apparent length scale $\overline{\Lambda_e}\Big|_{t=0}$ in Figure 3 is relatively smaller than those in Figure 2. Before $\overline{\Lambda_e}$ reaches its steady value, 0 < T < 2.5, for any given M, $\langle\overline{W_k W_k}\rangle$ of Figure 3 decays faster than that in Figure 2. This again reflects the same property that when the corresponding normalized apparent length scale is smaller, the turbulence energy will decay faster.

Figure 4 presents the decay of $<\overline{U_k U_k}>$ with the initial conditions of $<\overline{U_k U_k}>_o = 0.8$ and $<\overline{V_k V_k}>_o = 0.2$. Figure 4 shows that the decay of $<\overline{U_k U_k}>$ is relatively insensitive to the length scale ratio, M. Since the initial turbulence energy of the field is mainly contained in the family of eddies with a large length scale ($<U_k U_k>$), which has a domineering role in the decay of the turbulence field, the behavior of the family of eddies with a smaller initial value ($<V_k V_k>_o$) and a smaller length scale (Λ_b) would have very little effect on the behavior of the other turbulent quantities of the field. Therefore, the decay of $<U_k U_k>$--the turbulence energy of the family of eddies with a large initial value and alrge length scale--will be similar to the decay of the turbulence energy without the presence of the other family of energy-containing eddies of a small length scale. In this case, we can see $<\overline{U_k U_k}>$ decays in a manner analogous to the decay of $<\overline{W_k W_k}>$.

The decay of $<\overline{V_k V_k}>$ in Figure 4 shows that for large M, $<V_k V_k>$ decays faster than that for small M. If M is large, which indicates that initially the energy-containing eddies of family "b" are located in a farther large wave number region in the energy spectrum (compared to the energy-containing eddies of family "a"), then, this group of eddies of family "b" is smaller in size compared to that of small M, and th decay of family "b" energy-containing eddies takes a shorter time to reach equilibrium. Similar phenomena of the variations of $<\overline{V_k V_k}>$, when initial conditions are $<\overline{U_k U_k}>_o = 0.2$ and $<\overline{V_k V_k}>_o = 0.8$, are shown in Figure 5.

In Figure 5, $<\overline{U_k U_k}>_o$ has relatively small initial values compared to those of $<\overline{V_k V_k}>_o$. Although two families of energy-containing eddies are presented in the same field, the family of energy-containing eddies of a larger characteristic length scale will dominate the relaxation rate of the turbulence field. The rate of turbulence energy transfered from the energy-containing

eddies of family "b" (with small length scale Λ_b) to the equilibrium small eddies, has to be adjusted approximately to the rate of the energy pass-over from the energy-containing eddies of family "a" (with large length scale) to the family of eddies "b".

The imbalanced initial distribution of the turbulence energies between two families of nonequilibrium eddies as assigned to Figure 5 will cause a certain redistribution of turbulence energies between these two families of nonequilibrium eddies. This redistribution of turbulence energies makes $\langle U_k U_k \rangle$--the energy of the family of eddies with a larger length scale but a very small initial value--decay slower and sometimes causes it to gain energy instead of decay in the initial period of mixing of these two families of nonequilibrium eddies. These are shown in Figure 5.

Figures 6 and 7 describe the emergence and decay of the interacting turbulence energy $\langle \overline{U_k V_k} \rangle$. $\langle \overline{U_k V_k} \rangle$ begins with zero value, because there is no interaction between the two groups of nonequilibrium eddies before mixing begins. After mixing begins, through the interaction between these two families of nonequilibrium eddies, the interacting turbulence energy $\langle \overline{U_k V_k} \rangle$ begins to emerge as shown in the figures. After a certain redistribution of the turbulence energy between these two nonequilibrium eddies, there will be less interaction between them and the interacting turbulence energy will decline. This is also shown in the figures.

Figures 6 and 7 also show that the interacting turbulence energy $\langle \overline{U_k V_k} \rangle$ has a larger value when the length-scale ratio M is smaller than that which occurs when the length-scale ratio, M, is large. As mentioned before, the energy-containing eddies with larger length-scale control the dynamic behavior of the turbulence field. When M is small the two groups of energy-containing eddies are closer to each other in wave number space. Then, they will be

competing for control of the relaxation of the turbulence field. Therefore, when M is small the interaction between the two groups of nonequilibrium eddies will be stronger than that when M is large.

CHAPTER IV

GREEN'S FUNCTIONS OF THE KINETIC EQUATIONS

One of the immediate problems of the present kinetic theory is to solve the kinetic equations generated in the theory for the various engineering flow problems.

The remainder of this dissertation is devoted to the method of solution of the kinetic equations via construction of the appropriate Green's functions. We shall first consider the solution of the kinetic equations describing the turbulence field characterized by one family of nonequilibrium eddies. We shall then consider that for the field characterized by more than one family of the nonequilibrium eddies.

In the past, the bimodal method has been employed to solve the kinetic equations [see references (26 - 31)]. In this method, all distribution functions are a priori assumed to consist of two half-Maxwellian functions--one for $v > 0$ and the other for $v < 0$. Into these assumed forms of the distribution functions, an appropriate number of undetermined functions are imbedded. Appropriate moments of the kinetic equations are then employed to determine these imbedded functions.

As it was expected [see Chapter I and references (26 - 31)], the solution showed that the two half-Maxwellian functions are dissimilar and they together constitute a completely non-Maxwellian distribution function of chemical species for the chemically reactive problems analyzed.

We now confine ourselves to the free shear flow problems governed by the kinetic equations (II-8).

For the moment, if we discard the explicit reaction term ωf, then Eq. (II-8) for f, obtained by setting z to one, and the subsequent equations

for the z's (or F's) are all linear if we assume that the average quantities $\langle u_j \rangle$ and $\langle U_k U_k \rangle$ are known. Then we can construct the Green's functions (fundamental solutions) of these kinetic equations satisfying certain source conditions.

Utilizing this fact, we construct the solution of a given flow problem in the following manner. We first assume the values of $\langle u_j \rangle$ and $\langle U_k U_k \rangle$. Then, by appropriately summing the Green's functions, we construct a solution satisfying the initial and boundary conditions of the problem for f and F's. From these distribution functions, we evaluate $\langle u_j \rangle$ and $\langle U_k U_k \rangle$ and repeat the process until a suitable convergence is attained.

Now let us return to the chemical reaction term ωf. We confine our discussion to the chemical reactions which are either frozen or in equilibrium. Of course, $\omega f = 0$ for the frozen case. When the reaction is in equilibrium, one can define a set of new variables comprised of certain combinations of z's, such that the set of the Eqs. (II-8) can be replaced by a new set of equations, for the new variables, whose forms are identical to Eqs. (II-8), but which do not explicitly contain the reaction term. In this set, the reaction term degenerates to a separate algebraic equation [after Chung, reference (27)]. Therefore, the equilibrium reaction case can be solved in the manner described in the preceding paragraphs. These details will be presented in the next chapter.

IV.A. Green's Function of the Kinetic Equations Governed by One Nonequilibrium Degree of Freedom

The mathematical problem at hand is to obtain a set of fundamental solutions (Green's functions) of the equations of the form of Eq. (II-8) with its last term deleted. These solutions can be then employed to construct

the solutions for f and fz's of a variety of the flow problems with either frozen or equilibrium chemical reactions.

On the right side of Eq. (II-8), if we ignore $<z>$ in the term $\beta^{\nu} f(z - <z>)$ then this term $\beta^{\nu} f(z - <z>)$ can be approximated by the term $-\beta^{\nu}(\partial/\partial u_j)[fz(u_j - <u_j>)]$. This approximation does not change the moment equations for z through the second order [see reference (27), Eq. (10)]. If we further define a new parameter β as

$$\beta = \begin{cases} \beta_1 + \beta^{\nu} & \text{for equation of } f \\ \beta_1 + 2\beta^{\nu} & \text{for equation of } fz \end{cases} \qquad \text{(IV-1)}$$

then the equation for $F = fz$ will be identical in form to that for f. This will be shown in the following manner. Using the above mentioned approximation and employing the notation β as defined in Eq. (IV-1), Eq. (II-8) can be written (without chemical reaction term) as,

$$\frac{\partial F}{\partial t} + u_j \frac{\partial F}{\partial x_j} = \beta \frac{\partial}{\partial u_j}[(u_j - <u_j>)F] + \frac{\beta_1}{3} <U_k U_k> \frac{\partial^2 F}{\partial u_j \partial u_j} \qquad \text{(IV-2)}$$

We see that Eq. (IV-2) stands for the equation for fz (= F) and also, by setting z = 1, stands for the equation for f, and both are identical in form.

In order to obtain the fundamental solution of Eq. (IV-2), we will transform Eq. (IV-2) into a simpler form. We first rewrite it in the following manner:

$$\frac{\partial F}{\partial t} + (k_j - \beta u_j)\frac{\partial F}{\partial u_j} + u_j \frac{\partial F}{\partial x_j} = 3\beta F + q_1 \frac{\partial^2 F}{\partial u_j \partial u_j} \qquad \text{(IV-3)}$$

where

$$k_j = \beta \langle u_j \rangle$$

$$q_1 = \frac{1}{3}\beta_1 \langle U_k U_k \rangle \qquad \text{(IV-4)}$$

We will make two transformations on Eq. (IV-3). The first transformation is made to eliminate the first term on the right side of Eq. (IV-3). We let

$$F(\vec{x},\vec{u},t) = \overline{F}(\vec{x},\vec{u},t)e^{3\beta t} \qquad \text{(IV-5)}$$

Equation (IV-5) implies the following relations:

$$\frac{\partial F}{\partial x_j} = e^{3\beta t}\frac{\partial \overline{F}}{\partial x_j}$$

$$\frac{\partial F}{\partial u_j} = e^{3\beta t}\frac{\partial \overline{F}}{\partial u_j} \qquad \text{(IV-6)}$$

$$\frac{\partial F}{\partial t} = 3\beta e^{3\beta t}\overline{F} + e^{3\beta t}\frac{\partial \overline{F}}{\partial t}$$

$$\frac{\partial^2 F}{\partial u_j \partial u_j} = e^{3\beta t}\frac{\partial^2 \overline{F}}{\partial u_j \partial u_j}$$

With the aid of Eqs. (IV-6) and (IV-5), Eq. (IV-4) is transformed into the following form.

$$\frac{\partial \overline{F}}{\partial t} + (k_j - \beta u_j) \frac{\partial \overline{F}}{\partial u_j} + u_j \frac{\partial \overline{F}}{\partial x_j} = q_1 \frac{\partial^2 \overline{F}}{\partial u_j \partial u_j} \tag{IV-7}$$

The second transformation is undertaken to eliminate the first order derivatives (except with respect to t) in Eq. (IV-7). The six subsidary equations of Eq. (IV-7) are readily seen as,

$$\begin{cases} \dfrac{du_j}{dt} = -\beta u_j + k_j \\[2ex] \dfrac{dx_j}{dt} = u_j \end{cases} \tag{IV-8}$$

As mentioned before, we assume $\langle u_j \rangle$ and $\langle U_k U_k \rangle$ are known in Eq. (IV-2), hence, Eq. (IV-2) is linear and the solution will be obtained by iterating on $\langle u_j \rangle$ and $\langle U_k U_k \rangle$. In this scheme, β_1 and β^ν as defined on Eqs. (II-2) and (II-6) can also be considered as known. Therefore, β, as given in Eq. (IV-1), and k_j $(= \beta \langle w_j \rangle)$ in Eq. (IV-8) are considered as known values.

The transformation is then constructed as

$$\begin{cases} T_j = \left(u_j - \dfrac{k_j}{\beta}\right) e^{\beta t} \\[2ex] R_j = \left(x_j + \dfrac{u_j}{\beta} - \dfrac{k_j}{\beta} t\right) \end{cases} \tag{IV-9}$$

The Jacobian of the above transformation is found as

$$\frac{\partial(\vec{T},\vec{R})}{\partial(\vec{u},\vec{x})} = e^{3\beta t} \tag{IV-10}$$

which implies that our transformation has a one to one correspondence.

The function $\overline{F}(\vec{u},\vec{x},t)$ is transformed into $\overline{F}_1(\overline{T},\overline{R},t)$ in the following manner:

$$\frac{\partial\overline{F}}{\partial t} = \left(\frac{\partial\overline{F}_1}{\partial R_j}\right)\left(\frac{\partial R_j}{\partial t}\right) + \left(\frac{\partial\overline{F}_1}{\partial T_j}\right)\left(\frac{\partial T_j}{\partial t}\right) + \left(\frac{\partial\overline{F}_1}{\partial t}\right)\left(\frac{\partial t}{\partial t}\right)$$

$$\frac{\partial\overline{F}}{\partial u_j} = \left(\frac{\partial\overline{F}_1}{\partial T_k}\right)\left(\frac{\partial T_k}{\partial u_j}\right) + \left(\frac{\partial\overline{F}_1}{\partial R_k}\right)\left(\frac{\partial R_k}{\partial u_j}\right)$$

$$\frac{\partial\overline{F}}{\partial x_j} = \left(\frac{\partial\overline{F}_1}{\partial T_k}\right)\left(\frac{\partial T_k}{\partial x_j}\right) + \left(\frac{\partial\overline{F}_1}{\partial R_k}\right)\left(\frac{\partial R_k}{\partial x_j}\right)$$

$$\begin{aligned}\frac{\partial^2\overline{F}}{\partial u_j\partial u_j} = {} & \left(\frac{\partial^2\overline{F}_1}{\partial T_i\partial T_k}\right)\left(\frac{\partial T_i}{\partial u_j}\right)\left(\frac{\partial T_k}{\partial u_j}\right) + \left(\frac{\partial^2\overline{F}_1}{\partial R_i\partial T_k}\right)\left(\frac{\partial R_i}{\partial u_j}\right)\left(\frac{\partial T_k}{\partial u_j}\right) \\ & + \left(\frac{\partial^2 T_k}{\partial u_j\partial u_j}\right)\left(\frac{\partial\overline{F}_1}{\partial T_k}\right) \\ & + \left(\frac{\partial^2\overline{F}_1}{\partial T_i\partial R_k}\right)\left(\frac{\partial T_i}{\partial u_j}\right)\left(\frac{\partial R_k}{\partial u_j}\right) + \left(\frac{\partial^2\overline{F}_1}{\partial R_i\partial R_k}\right)\left(\frac{\partial R_i}{\partial u_j}\right)\left(\frac{\partial R_k}{\partial u_j}\right) \\ & + \left(\frac{\partial^2 R_k}{\partial u_j\partial u_j}\right)\left(\frac{\partial\overline{F}_1}{\partial R_k}\right)\end{aligned} \tag{IV-11}$$

From Eq. (IV-10) we see that

$$\frac{\partial T_i}{\partial u_j} = \delta_{ij} e^{\beta t} \quad , \quad \frac{\partial R_k}{\partial u_j} = \delta_{kj} \, (1/\beta) \tag{IV-12}$$

$$\frac{\partial^2 T_k}{\partial u_j \partial u_j} = 0 \quad , \quad \frac{\partial^2 R_k}{\partial u_j \partial u_j} = 0 \tag{IV-13}$$

Hence, Eq. (IV-8) is transformed into

$$\frac{\partial \overline{F}_1}{\partial t} = \left(a \frac{\partial^2 \overline{F}_1}{\partial T_k \partial T_k} + 2b \frac{\partial^2 \overline{F}_1}{\partial T_k \partial R_k} + c \frac{\partial^2 \overline{F}_1}{\partial R_k \partial R_k} \right) q_1 \tag{IV-14}$$

where, by the aid of Eqs. (IV-11), (IV-12) and (IV-13), we have

$$\begin{aligned} a &= e^{2\beta t} \\ b &= \frac{1}{\beta} e^{\beta t} \\ c &= \frac{1}{\beta^2} \end{aligned} \tag{IV-15}$$

The fundamental solution of Eq. (IV-14) can be obtained by employing Lemma II in reference (24). This Lemma II states: If a differential equation is given in the form

$$\frac{\partial P}{\partial t} = m_1(t)\frac{\partial^2 P}{\partial x^2} + 2m_2(t)\frac{\partial^2 P}{\partial x \partial y} + m_3(t)\frac{\partial^2 P}{\partial y^2} \qquad \text{(L-II-1)}$$

where $P = P(x,y,t)$, then the fundamental solution satisfying an initial condition

$$P(x,y,t/x_o,y_o,t_o) = \delta(x - x_o)\delta(y - y_o) \qquad \text{at } t = t_o$$

is given as

$$P(x,y,t/x_o,y_o,t_o) = \frac{\exp -\left[\dfrac{G(x - x_o)^2 + 2H(x - x_o)(y - y_o) + F(y - y_o)^2}{2(FH - H^2)}\right]}{2\pi(FG - H^2)^{1/2}}$$

(L-II-)

where δ represents the Dirac delta function and (x_o,y_o) is the initial position (x,y) at $t = t_o$.

Coefficients F, G and H are defined as

$$F = 2\int_{t_o}^{t} m_1(\xi)d\xi$$

$$G = 2\int_{t_o}^{t} m_3(\xi)d\xi \qquad \text{(L-II-3)}$$

$$H = -2\int_{t_o}^{t} m_2(\xi)d\xi$$

The above Lemma was verified by substituting Eq. (L-II-2) into Eq. (L-II-1) in reference (24).

We see that Eq. (IV-14) is a diffusion type equation and its variables can be separated into three parts which are (T_1,R_1,t), (T_2,R_2,t_2) and (T_3,R_3,t). The solution of $\overline{F}_1(\vec{T},\vec{R},t)$ can be expressed as,

$$\overline{F}_1(\vec{T},\vec{R},t) = \overline{F}_{11}(T_1,R_1,t)\overline{F}_{12}(T_2,R_2,t)\overline{F}_{13}(T_3,R_3,t) \qquad \text{(IV-16)}$$

The expression Eq. (IV-16) can be easily verified by taking Fourier transform of Eq. (IV-14) and by solving the resulting first order differential equation with respect to the independent variable t. Then, when we take an inverse transform of the resulting solution, the property of the separable variables becomes self-evident. This detailed process is shown in Appendix III where we have extended Lemma-II to the higher orders. In Appendix III it can be also seen that each explicit expression of $\overline{F}_{11}(T_1,R_1,t)$, $\overline{F}_{12}(T_2,R_2,t)$ and $\overline{F}_{13}(T_3,R_3,t)$ are derivable from Lemma-II. Thus, the fundamental solution of Eq. (IV-14) satisfying the initial condition

$$\overline{F}_1(\vec{T},\vec{R},t/\vec{T}_o,\vec{R}_o,t_o) = \delta(\vec{T} - \vec{T}_o)\delta(\vec{R} - \vec{R}_o) \quad \text{at } t = t_o$$

is obtained as,

$$\overline{F}_1(\vec{T},\vec{R},t/\vec{T}_o,\vec{R}_o,t_o)$$

$$= \frac{1}{8\pi^3(AC - B^2)^{3/2}} \exp\left\{\frac{-[C|\vec{T} - \vec{T}_o|^2 + 2B(\vec{T} - \vec{T}_o)\cdot(\vec{R} - \vec{R}_o) + A|\vec{R} - \vec{R}_o|^2]}{2(AC - B^2)}\right\}$$

(IV-17)

where

$$A = 2q_1 \int_{t_o}^{t} a(\xi)d\xi \qquad B = -2\int_{t_o}^{t} q_1 b(\xi)d\xi$$

$$C = 2\int_{t_o}^{t} q_1 c(\xi)d\xi \tag{IV-18}$$

and $(\vec{T}_o \vec{R}_o)$ is the initial position, $(\vec{T},\vec{R})$, at $t = t_o$.

From Eq. (IV-9), T_{oj} and R_{oj} can be expressed as

$$\begin{cases} T_{oj} = (u_{oj} - \dfrac{k_j}{\beta})\, e^{\beta t_o} \\ R_{oj} = x_{oj} + \dfrac{u_{oj}}{\beta} - \dfrac{k_j}{\beta} t_o \end{cases} \tag{IV-19}$$

Finally, with the aid of Eqs. (IV-5), (IV-9) and (IV-19), all independent variables of Eq. (IV-17), $(\vec{T},\vec{R},t|\vec{T}_o,\vec{R}_o,t_o)$, are transformed back to the original variables, $(\vec{x},\vec{u},t|\vec{x}_o,\vec{u}_o,t_o)$. We thus obtain the Green's function (fundamental solution) of Eq. (IV-2) as,

$$G_1(\vec{x},\vec{u},t|\vec{x}_o,\vec{u}_o,t_o) = \frac{1\ \exp(3\beta t)}{8\pi^3(AC - B^2)^{3/2}}$$

$$\exp - \left[\frac{\left\{ \begin{array}{l} C|(\vec{u} - \frac{\vec{k}}{\beta})e^{\beta t} - (\vec{u}_o - \frac{\vec{k}}{\beta})e^{\beta t_o}|^2 \\ + 2B[(\vec{u} - \frac{\vec{k}}{\beta})e^{\beta t} - (\vec{u}_o - \frac{\vec{k}}{\beta})\, e^{\beta t_o}] \cdot \\ [(\vec{x} - \vec{x}_o) + \frac{(\vec{u} - \vec{u}_o)}{\beta} - \frac{\vec{k}}{\beta}(t - t_o)] \\ + A|(\vec{x} - \vec{x}_o) + \frac{1}{\beta}(\vec{u} - \vec{u}_o) - \frac{\vec{k}}{\beta}(t - t_o)|^2 \end{array} \right\}}{2(AC - B^2)} \right] \tag{IV-20}$$

Here we use the notation G_1 to represent the Green's function or the fundamental solution of the kinetic equation, Eq. (IV-2), governing the turbulence field describable by one nonequilibrium degree of freedom.

IV.B. Green's Function of the Kinetic Equation Describing the Turbulent Field Governed by Two Nonequilibrium Degrees of Freedom and the Equilibrium Degrees of Freedom

In this chapter, we will obtain the Green's function of the kinetic equation, Eq. (III-1), which describes a turbulent field characterized by two significant dynamic length scales.

For our convenience in subsequent description (in this chapter) we will refer to the Green's function obtained in the previous section as the "single-mode G-function" and the Green's function of Eq. (III-1) (to be obtained in this section) as the "multi-mode G-function."

The multi-mode G-function will not be employed to solve any real physical problem in this dissertation. However, the single-mode G-function will be used to solve a specific physical problem in the next chapter.

As mentioned in previous chapters, many important turbulent flow fields are actually characterized by more than one significant dynamic length scale. Although we will not apply the multi-mode G-function to solve any physical problem in this dissertation, the determination of the multi-mode G-function is still within our interest for future application of the present (Chung's) theory for the solution of the multiscale turbulent flow problems.

In this section, we will employ a technique similar to that used in the previous section in obtaining the Green's function of Eq. (III-1). We will also make assumptions similar to those made in section IV.A., viz., $\langle v_j \rangle$, $\langle u_j \rangle$, $\langle U_k U_k \rangle$, $\langle U_k V_k \rangle$ and $\langle V_k V_k \rangle$ are known so that Eq. (III-1) can be

considered as a linear equation. In the future, if we apply the multi-mode G-function to solve multiscale turbulent problems, we will have to iterate on $\langle v_j \rangle$, $\langle u_j \rangle$, $\langle U_k U_k \rangle$, $\langle U_k V_k \rangle$ and $\langle V_k V_k \rangle$ when we try to obtain the associated momentum quantities. We will further assume that the problem is of the free shear layer turbulent flow type with negligible mean pressure gradients. $K_{a,k}$ and $K_{b,k}$ in Eq. (III-1) can thus be given as in Eq. (III-5). The characteristic dissipation rates, β_a, β_b and β_c, according to the previous analysis by Chung and Bywater[15,23,26] are given as in Eq. (III-2).

In order to obtain the Green's function of Eq. (III-1), we have to transform Eq. (III-1) into a simpler form. We first make a change of independent variables, $\vec{U}$, $\vec{V}$, $\vec{x}$, t of the function f_2, into the same function, f_2, of new independent variables, $\vec{u}$, $\vec{v}$, $\vec{x}$, t. Chain rules associated with this variable change are listed in Appendix I. With this change of independent variables, Eq. (III-1) becomes, after a little manipulation.

$$\frac{\partial f_2}{\partial t} + (k_{aj} - B_a u_j) \frac{\partial f_2}{\partial u_j} + (k_{bj} - B_b v_j) \frac{\partial f_2}{\partial v_j}$$

$$+ u_j \frac{\partial f_2}{\partial x_j} + v_j \frac{\partial f_2}{\partial x_j} = 3(B_a + B_b) f_2$$

$$+ q \left[\frac{\partial^2}{\partial u_j \partial u_j} + 2 \frac{\partial^2}{\partial u_j \partial v_j} + \frac{\partial^2}{\partial v_j \partial v_j} \right] f_2$$

$$f_2 = f_2(\vec{u}, \vec{v}, \vec{x}, t) \qquad \text{(IV-21)}$$

where

$$k_{a,j} = 2\beta_a\langle u_j\rangle + \beta_c\langle u_j\rangle - \beta_c\langle v_j\rangle$$

$$k_{b,j} = 2\beta_b\langle v_j\rangle + \beta_c\langle v_j\rangle - \beta_c\langle u_j\rangle$$

$$B_a = 2\beta_a + \beta_c \qquad \text{(IV-22)}$$

$$B_b = 2\beta_b + \beta_c$$

$$q = \frac{\beta_a\langle U_k U_k\rangle + \beta_b\langle V_k V_k\rangle + (\beta_a + \beta_b)\langle U_k V_k\rangle}{12}$$

Next, a transformation is undertaken in order to eliminate the first term on the right hand side of Eq. (IV-21). We let

$$f_2 = \bar{f}_2 e^{B_c t} \qquad \text{(IV-23)}$$

where $B_c = 3(B_a + B_b)$.

With the aid of Eq. (IV-23), Eq. (IV-21) is then transformed into

$$\frac{\partial \bar{f}_2}{\partial t} + (k_{a,j} - B_a u_j)\frac{\partial \bar{f}_2}{\partial u_j} + (k_{b,j} - B_b v_j)\frac{\partial \bar{f}_2}{\partial v_j}$$

$$+ u_j \frac{\partial \bar{f}_2}{\partial x_j} + v_j \frac{\partial \bar{f}_2}{\partial x_j} = q\left[\frac{\partial^2}{\partial u_j \partial u_j} + 2\frac{\partial^2}{\partial u_j \partial v_j} + \frac{\partial^2}{\partial v_j \partial v_j}\right]\bar{f}_2$$

(IV-24)

Detailed transformation from Eq. (IV-21) into Eq. (IV-24) is given in Appendix II.

The nine subsidiary equations of Eq. (IV-24) are readily seen as

$$\frac{du_j}{dt} = -B_a u_j + k_{a,j}$$

$$\frac{dv_j}{dt} = -B_b v_j + k_{b,j} \qquad \text{(IV-25)}$$

$$\frac{dx_j}{dt} = u_j + v_j$$

As mentioned before, $\langle v_j \rangle$, $\langle u_j \rangle$, $\langle U_k U_k \rangle$, $\langle U_k V_k \rangle$ and $\langle V_k V_k \rangle$ are assumed to be known values. Therefore, $k_{a,j}$, $k_{b,j}$, B_a and B_b as defined by Eq. (IV-23), can be considered as known values in Eq. (IV-25). A transformation of variables is then constructed as,

$$T_{a,j} = \left(u_j - \frac{k_{a,j}}{B_a}\right) e^{B_a t}$$

$$T_{b,j} = \left(v_j - \frac{k_{b,j}}{B_b}\right) e^{B_b t} \qquad \text{(IV-26)}$$

$$R_j = x_j + \frac{u_j}{B_a} + \frac{v_j}{B_b} - \left(\frac{k_{a,j}}{B_a} + \frac{k_{b,j}}{B_b}\right) t$$

The Jacobian of the above transformation is found as

$$\frac{\partial(\vec{T}_a, \vec{T}_b, \vec{R})}{\partial(\vec{u}, \vec{v}, \vec{x})} = e^{3(B_a + B_b)t} \qquad \text{(IV-27)}$$

which implies that our transformation has a one-to-one correspondence. With the above transformation, Eq. (IV-26), Eq. (IV-24) is transformed into the following form

$$\frac{\partial \bar{f}_2(\vec{T}_a,\vec{T}_b,\vec{R},t)}{\partial t} = q\left[a_2 \frac{\partial^2 \bar{f}_2(\vec{T}_a,\vec{T}_b,\vec{R},t)}{\partial T_{aj}\partial T_{aj}} + b_2 \frac{\partial^2 \bar{f}_2(\vec{T}_a,\vec{T}_b,\vec{R},t)}{\partial T_{bj}\partial T_{bj}}\right.$$

$$+ c_2 \frac{\partial^2 \bar{f}_2(\vec{T}_a,\vec{T}_b,\vec{R},t)}{\partial R_j \partial R_j} + 2d_2 \frac{\partial^2 \bar{f}_2(\vec{T}_a,\vec{T}_b,\vec{R},t)}{\partial T_{aj}\partial T_{bj}}$$

$$\left. + 2e_2 \frac{\partial^2 \bar{f}_2(\vec{T}_a,\vec{T}_b,\vec{R},t)}{\partial T_{aj}\partial R_j} + 2g_2 \frac{\partial^2 \bar{f}_2(\vec{T}_a,\vec{T}_b,\vec{R},t)}{\partial T_{bj}\partial R_j}\right] \qquad \text{(IV-28)}$$

where

$$a_2 = \exp(2B_a t)$$

$$b_2 = \exp(2B_b t)$$

$$c_2 = \left(\frac{1}{B_a} + \frac{1}{B_b}\right)^2$$

$$d_2 = \exp[(B_a + B_b)t] \qquad \text{(IV-29)}$$

$$e_2 = \left(\frac{B_a + B_b}{B_a B_b}\right) \exp(B_a t)$$

$$g_2 = \left(\frac{B_a + B_b}{B_a B_b}\right) \exp(B_b t)$$

Detailed processes of the transformation from Eq. (IV-24) into Eq. (IV-28) are given in Appendix II.

In order to obtain the fundamental solution of Eq. (IV-28), two mathematical lemmas will be proposed next. These two lemmas are the extension of Lemma I and Lemma II in reference (24), which will provide the fundamental solutions of certain types of diffusion equations. The differential equation cited in Lemma I of reference (24) has the form

$$\frac{\partial P}{\partial t} = \psi(t) \frac{\partial^2 P}{\partial x \partial x} \qquad \text{(L-I-1)}$$

We will refer to Eq. (L-I-1) as the "single-direction with non-coupled" diffusion equation. Equation (L-II-1) in the previous section (Lemma II) will be referred to as the "single-direction with two coupled" diffusion equation, and Eq. (IV-14) can be called the "three-direction with two coupled" diffusion equation. Lemma I and Lemma II of reference (24) give the fundamental solutions of Eq. (L-I-1) and Eq. (L-II-1). Lemma III will give the fundamental solution of a "single-direction with three-coupled" (so to speak) diffusion equation and Lemma III-A will provide the fundamental solution of a "three-direction with three-coupled" diffusion equation. These two Lemmas will be presented in the following.

Lemma III

If the differential equation is given in the form

$$\frac{\partial Y}{\partial t} = \phi_1(t)\frac{\partial^2 Y}{\partial x_1 \partial x_1} + \phi_2(t)\frac{\partial^2 Y}{\partial x_2 \partial x_2} + \phi_3(t)\frac{\partial^2 Y}{\partial x_3 \partial x_3}$$

$$+ 2\phi_{12}(t)\frac{\partial^2 Y}{\partial x_1 \partial x_2} + 2\phi_{13}(t)\frac{\partial^2 Y}{\partial x_1 \partial x_3} + 2\phi_{23}\frac{\partial^2 Y}{\partial x_2 \partial x_3} \qquad \text{(L-III-1)}$$

in which $Y = Y(x_1,x_2,x_3,t)$, the fundamental solution of Eq. (L-III-1) which satisfies the initial condition

$$Y(x_1,x_2,x_3,t)\Big|_{t=t_o} = \delta(x_1 - x_{1o})\delta(x_2 - x_{2o})\delta(x_3 - x_{3o}) \qquad \text{(L-III-1a)}$$

is given as

$$Y(x_1,x_2,x_3,t|x_{1o},x_{2o},x_{3o},t) = \frac{1}{(2\pi)^{3/2}\underline{\Delta}_3^{1/2}}$$

$$\exp\left\{-\frac{1}{2\underline{\Delta}_3}\left[\begin{array}{l}\underline{\Delta}_{11}(x_1 - x_{1o})^2 + \underline{\Delta}_{22}(x_2 - x_{2o})^2 + \underline{\Delta}_{33}(x_3 - x_{3o})^2 \\ + 2\underline{\Delta}_{12}(x_1 - x_{1o})(x_2 - x_{2o}) + 2\underline{\Delta}_{13}(x_1 - x_{1o})(x_3 - x_{3o}) \\ + 2\underline{\Delta}_{23}(x_2 - x_{2o})(x_3 - x_{3o})\end{array}\right]\right\}$$

(L-III-2)

where

$$(x_{1o},x_{2o},x_{3o}) = (x_1,x_2,x_3)_{t=t_o} \qquad \text{(L-III-3)}$$

and

$$\underline{\Delta}_3 = 2^3 \begin{vmatrix} M_{11} & M_{12} & M_{13} \\ M_{21} & M_{22} & M_{23} \\ M_{31} & M_{32} & M_{33} \end{vmatrix} \qquad \underline{\Delta}_{11} = 2^2 \begin{vmatrix} M_{22} & M_{23} \\ M_{32} & M_{33} \end{vmatrix}$$

$$\underline{\Delta}_{12} = -2^2 \begin{vmatrix} M_{21} & M_{23} \\ M_{31} & M_{33} \end{vmatrix} \qquad \underline{\Delta}_{13} = 2^2 \begin{vmatrix} M_{21} & M_{22} \\ M_{31} & M_{32} \end{vmatrix}$$

$$\underline{\Delta}_{23} = -2^2 \begin{vmatrix} M_{11} & M_{12} \\ M_{31} & M_{32} \end{vmatrix} \qquad \text{(L-III-4)}$$

in which

$$M_{11} = \int_{t_o}^{t} \phi_1(\xi)d\xi \,, \qquad M_{22} = \int_{t_o}^{t} \phi_2(\xi)d\xi \,, \qquad M_{33} = \int_{t_o}^{t} \phi_3(\xi)d\xi$$

$$M_{12} = M_{21} = \int_{t_o}^{t} \phi_{12}(\xi)d\xi \,, \qquad M_{13} = M_{31} = \int_{t_o}^{t} \phi_{13}(\xi)d\xi$$

$$M_{23} = M_{32} = \int_{t_o}^{t} \phi_{23}(\xi)d\xi \qquad \text{(L-III-5)}$$

Lemma III-A

If the differential equation is given in the form

$$\frac{\partial Y_a}{\partial t} = \phi_1(t)\frac{\partial^2 Y_a}{\partial x_{1j}\partial x_{1j}} + \phi_2(t)\frac{\partial^2 Y_a}{\partial x_{2j}\partial x_{2j}} + \phi_3(t)\frac{\partial^2 Y_a}{\partial x_{3j}\partial x_{3j}}$$

$$+ 2\phi_{12}(t)\frac{\partial^2 Y_a}{\partial x_{1j}\partial x_{2j}} + 2\phi_{13}(t)\frac{\partial^2 Y_a}{\partial x_{1j}\partial x_{3j}} + 2\phi_{23}(t)\frac{\partial^2 Y_a}{\partial x_{2j}\partial x_{3j}}$$

(L-III-6)

where j is the cartesian tensor index, j =1, 2, 3.

The fundamental solution of Eq. (L-III-6) satisfying the initial condition

$$Y_a(\vec{x}_1,\vec{x}_2,\vec{x}_3,t)_{t=t_o} = \delta(x_{11} - x_{11o})\delta(x_{12} - x_{12o})\delta(x_{13} - x_{13o})$$

$$\delta(x_{21} - x_{21o})\delta(x_{22} - x_{22o})\delta(x_{23} - x_{23o})$$

$$\delta(x_{31} - x_{31o})\delta(x_{32} - x_{32o})\delta(x_{33} - x_{33o})$$

(L-III-7)

where

$$(x_{ij})_{t=t_o} = x_{ijo}$$

is given as

$$Y_a(\vec{x}_1,\vec{x}_2,\vec{x}_3,t|\vec{x}_{1o},\vec{x}_{2o},\vec{x}_{3o},t_o) = \frac{1}{(2\pi)^{9/2}\cdot \underline{\Delta}_3^{3/2}}$$

$$\exp\left\{-\frac{\left[\begin{array}{l}\underline{\Delta}_{11}|\vec{x}_1-\vec{x}_{1o}|^2+\underline{\Delta}_{22}|\vec{x}_2-\vec{x}_{2o}|^2+\underline{\Delta}_{33}|\vec{x}_3-\vec{x}_{3o}|^2\\ +2\underline{\Delta}_{12}(\vec{x}_1-\vec{x}_{1o})\cdot(\vec{x}_2-\vec{x}_{2o})+2\underline{\Delta}_{13}(\vec{x}_1-\vec{x}_{1o})\cdot(\vec{x}_3-\vec{x}_{3o})\\ +2\underline{\Delta}_{23}(\vec{x}_2-\vec{x}_{2o})\cdot(\vec{x}_3-\vec{x}_{3o})\end{array}\right]}{2\underline{\Delta}_3}\right\} \tag{L-III-9}$$

where $\underline{\Delta}_3$ and Δ_{ij} are the same as in Eq. (L-III-4). Lemma III and Lemma III-A are verified in Appendix III.

From Lemma III-A, the Green's function of Eq. (IV-29) is readily obtained as

$$\overline{G}_2(\vec{T}_a,\vec{T}_b,\vec{R},t|\vec{T}_{ao},\vec{T}_{bo},\vec{R}_o\ t_o) = \frac{1}{(2\pi)^{9/2}\Delta_3^{3/2}}$$

$$\exp\left\{-\frac{\left[\begin{array}{l}\Delta_{11}|\vec{T}_a-\vec{T}_{ao}|^2+\Delta_{22}|\vec{T}_b-\vec{T}_{bo}|^2+\Delta_{33}|\vec{R}-\vec{R}_o|^2\\ +2\Delta_{12}(\vec{T}_a-\vec{T}_{ao})\cdot(\vec{T}_b-\vec{T}_{bo})+2\Delta_{13}(\vec{T}_a-\vec{T}_{ao})\cdot(\vec{R}-\vec{R}_o)\\ +2\Delta_{23}(\vec{T}_b-\vec{T}_{bo})\cdot(\vec{R}-\vec{R}_o)\end{array}\right]}{2\Delta_3}\right\} \tag{IV-30}$$

where $(\vec{T}_{ao},\vec{T}_{bo},\vec{R}_o,t_o)$ is the initial condition of $(\vec{T}_a,\vec{T}_b,\vec{R},t)$ at $t = t_o$, and

$$\Delta_3 = 2^3 \begin{vmatrix} A_{11} & A_{12} & A_{13} \\ A_{21} & A_{22} & A_{23} \\ A_{31} & A_{32} & A_{33} \end{vmatrix} \qquad \Delta_{11} = 2^2 \begin{vmatrix} A_{22} & A_{23} \\ A_{32} & A_{33} \end{vmatrix}$$

$$\Delta_{12} = -2^2 \begin{vmatrix} A_{21} & A_{23} \\ A_{31} & A_{33} \end{vmatrix} \qquad \Delta_{13} = 2^2 \begin{vmatrix} A_{21} & A_{22} \\ A_{31} & A_{32} \end{vmatrix}$$

$$\Delta_{23} = -2^2 \begin{vmatrix} A_{11} & A_{12} \\ A_{31} & A_{32} \end{vmatrix} \tag{IV-31}$$

Also,

$$A_{11} = q \int_{t_o}^{t} a_2(\xi)d\xi \ , \quad A_{22} = q \int_{t_o}^{t} b_2(\xi)d\xi \ , \quad A_{33} = q \int_{t_o}^{t} c_2(\xi)d\xi$$

$$A_{12} = A_{21} = q \int_{t_o}^{t} d_2(\xi)d\xi \ , \quad A_{13} = A_{31} = q \int_{t_o}^{t} e_2(\xi)d\xi$$

$$A_{23} = A_{32} = q \int_{t_o}^{t} g_2(\xi)d\xi \tag{IV-32}$$

Here we use the notation $\overline{G}_2$ to represent the Green's function (G) in the transformed space $(\vec{T}_a,\vec{T}_b,\vec{R},t)$,(-), of the two nonequilibrium degrees of freedom (2) kinetic equation.

Finally, the independent variables in Eq. (IV-31) are transformed back to the original variables. By employing relations (IV-23) and (IV-27), the Green's function of Eq. (IV-21) is obtained as,

$$G_2(\vec{u},\vec{v},t|\vec{u}_o,\vec{v}_o,t_o) = \frac{e^{B_c t}}{(2\pi)^{9/2}\Delta^{3/2}} \times$$

$$\exp\left[-\frac{\begin{aligned}&\Delta_{11}\left|(\vec{u}-\frac{\vec{k}_a}{B_a})e^{B_a t}-(\vec{u}_o-\frac{\vec{k}_a}{B_a})e^{B_a t_o}\right|^2\\ &+\Delta_{22}\left|(\vec{v}-\frac{\vec{k}_b}{B_b})e^{B_b t}-(\vec{v}_o-\frac{\vec{k}_b}{B_b})e^{B_b t_o}\right|^2\\ &+\Delta_{33}\left|(\vec{x}-\vec{x}_o)+\frac{\vec{u}}{B_a}-\frac{\vec{u}_o}{B_a}+\frac{\vec{v}}{B_b}-\frac{\vec{v}_o}{B_b}-(\frac{\vec{k}_a}{B_a}+\frac{\vec{k}_b}{B_b})(t-t_o)\right|^2\\ &+2\Delta_{12}\left((\vec{u}-\frac{\vec{k}_a}{B_a})e^{B_a t}-(\vec{u}_o-\frac{\vec{k}_a}{B_a})e^{B_a t_o}\right)\cdot\left((\vec{v}-\frac{\vec{k}_b}{B_b})e^{B_b t}\right.\\ &\left.-(\vec{v}_o-\frac{\vec{k}_b}{B_b})e^{B_b t_o}\right)+2\Delta_{13}\left((\vec{u}-\frac{\vec{k}_b}{B_a})e^{B_a t}-(\vec{u}_o-\frac{\vec{k}_a}{B_a})e^{B_a t_o}\right)\\ &\cdot\left((\vec{x}-\vec{x}_o)+\frac{\vec{u}-\vec{u}_o}{B_a}+\frac{\vec{v}-\vec{v}_o}{B_b}-(t-t_o)(\frac{\vec{k}_a}{B_a}+\frac{\vec{k}_b}{B_b})\right)\\ &+2\Delta_{23}\left((\vec{v}-\frac{\vec{k}_a}{B_b})e^{B_a t}-(\vec{v}_o-\frac{\vec{k}_b}{B_b})e^{B_b t_o}\right)\cdot\\ &\left((\vec{x}-\vec{x}_o)+\frac{\vec{u}-\vec{u}_o}{B_a}+\frac{\vec{v}-\vec{v}_o}{B_b}-(t-t_o)(\frac{\vec{k}_a}{B_a}+\frac{\vec{k}_b}{B_b})\right)\end{aligned}}{2\Delta_3}\right] \tag{IV-33}$$

where $\vec{u}$, $\vec{v}$, $\vec{k}_a$, $\vec{k}_b$ are vectors, and $(\vec{x}_o,\vec{u}_o,\vec{v}_o,t_o) = (\vec{x},\vec{u},\vec{v},t)_{t=t_o}$ in the phase space.

CHAPTER V

SPECIFIC SOLUTION

The single-mode Green's function obtained will be employed to solve a two parallel stream turbulent shear flow problem with and without chemical reactions.

As mentioned in the previous chapter, the kinetic equations for f and for F [Eq. (IV-2)] are linear if we assume $\langle u_j \rangle$ and $\langle U_k U_k \rangle$ are known. The Green's function of Eq. (IV-2), without considering chemical reaction term, ωf, is then obtained as described in Chapter IV.

The following simple chemical reaction will be considered in this chapter for chemically reactive flow:

$$\underset{\text{fuel}}{a} + \underset{\text{oxidant}}{b} \xrightarrow{K_f} \underset{\text{product}}{d} \tag{V-1}$$

$$\omega_\alpha = K_\alpha \exp\left(-\frac{E}{z_t}\right) z_r^a z_s^b \tag{V-1a}$$

In the above, the subscript α represents either of the subscripts t, r, s, or p, which denote the temperature, fuel, oxidant and combustion product, respectively. By introducing new variables, the kinetic equations (IV-2) for the F's can be manipulated into two equations which are identical to that of Eq. (IV-2) without the chemical reaction term. Also, in the limit of an infinitely fast chemical reaction rate, the chemical reaction term of Eq. (IV-2) can be degenerated into a set of algebraic equations. Therefore, the obtained single-mode G-function, in which the chemical reaction

term was not considered, can be employed to solve the infinitely fast chemically reactive flow problems. This method was derived by Chung[26,27] and details of this process will be given later in this chapter.

Since we assumed that $\langle u_j \rangle$ and $\langle U_k U_k \rangle$ are known when we were solving for the Green's function of the kinetic equation, we will first assume the value of $\langle u_j \rangle$ and $\langle U_k U_k \rangle$. Then, by appropriate summing of the Green's functions according to the flow conditions of the given physical problem, we will construct a solution for f and F's. From these distribution functions, we evaluate $\langle u_j \rangle$ and $\langle U_k U_k \rangle$ and repeat the process until a suitable convergence is attained. This detailed process will be shown later in this chapter.

The physical problem given here is similar to a pair of parallel streams flowing out continuously at the x = 0 plane with given mean velocities and turbulence energies. (See Figure 8.) The upper stream contains fuel and the lower stream contains oxidant and inert species. The temperature is given as uniform at the x = 0 plane.

The above mentioned flow problem has been of interest since the late 1880's.[34-48] Most former researchers[34-48] only investigated the momentum flow field without considering chemical reactions. The analytical work of Tollmein,[37] Goertler,[39] Lessen,[40] Chiarulli[41] and Lin, et al.[38] in one way or the other employed a Bousinesq relationship. Among these investigations of the turbulent mixing problem which are based on the idealized initial velocity profiles (Figure 8), the main difference in the analyses has been in the expression chosen to represent the eddy viscosity in the mixing region. Tollmein,[37] in 1926, first obtained the analytical solution by using Prandtl's mixing-length theory. His solution shows that the second order derivatives of mean velocity are discontinuous at the edges of the mixing layer and the velocity in the mixing region does not asymptotically

approach the free stream values. Liepmann and Laufer[43] demonstrated that their experimental results could be brought into reasonable agreement with the mean velocity distributions obtained from either the solution of Tollmein or that of Goertler. However, turbulent stress measurements and back calculations of the mixing length and the exchange coefficient showed that both varied across the mixing region. Thus, they concluded that neither Prandtl's mixing-length hypothesis nor the exchange coefficient hypothesis adequately describes the turbulence characteristics of the mixing region. Schlichting[44] pointed out that Tollmein's discontinuity solution is a general property of all solutions based on Prandtl's mixing-length hypothesis and called this an esthetical deficiency of the hypothesis. The inadequacy of the gradient-type approach of turbulent momentum transport has been fairly described in Chapter II.

Possibly because of a lack of proper expression for Reynold's stress in the mixing region, Baker and Weinstein's[46,47] experimental and analytical studies of this problem in 1968 did not give any curve of Reynolds stress in the mixing region.

The analytical solutions of the momentum field obtained by former investigators are usually adjusted by changing the already embedded parameter when they employed Prandtl's approach or by adding new parameters in order to compare the experimental data. The analytical results of Tollmein, Goertler and others[44-46] show that there exist similarity solutions of the momentum field. These are evidenced by experimental results. Experimental data of this type of problem of a uniform density fluid has been taken by Albertson,[48] Reichardt,[49] Liepmann and Laufer,[43] Baker and Weinstein[47] and others, and most recently by Spencer.[50] Spencer has conducted the most complete and thorough experimental studies of this turbulent mixing problem.

Our main interest is in employing Chung's theory to solve chemically

reactive flow problems. In order to assure our calculations, the momentum field to be obtained later in this chapter will be compared with Spencer's experimental data. However, the experimental combustion data of the present problem analyzed is not available now.

Chung's model is the only existing kinetic theory for turbulent chemically reactive flow. The solutions to be obtained in this chapter will reconfirm some salient features of Chung's theory which have mostly been revealed in previous analyses[26-31] by the bimodal method. The present Green's function method only provides a more refined method for applying Chung's theory. Although the previous bimodal method embedded certain discontinuities in the distribution function and so resulted in discontinuities at the flame edges of the mean quantity profiles, the assumed two half-Maxwellian functions are dissimilar and together they constitute a completely non-Maxwellian distribution function of chemical species for the chemically reactive problems analyzed. This is what we would expect, since the Maxwellian distribution implies a completely homogeneous, isotropic field which is of little interest to engineers.

The conventional approach has been the use of one-point averaged equations derived from the Navier-Stokes equation, and the species and energy conservation equations, which are not closed. The closure techniques of the above mentioned equations are mainly based on Boussinesq's relationship or Prandtl's approach, which are basically inadequate to describe turbulent transport as pointed out first by Chung[15] and later by Spalding,[11] and these have been explained in Chapters I and II. Not only is the mean-gradient type closure technique, which ascribes the turbulent transport as analogous to laminar transport and results in a flame sheet solution in the turbulent combustion flame, inadequate, but also the basic physics of the problem, concerning the mixing and reactions, cannot be described successfully by the moment equations alone.

These basic physical descriptions of mixing and reactions will be briefly mentioned herein.

We will repeat a portion of the physical description given earlier by Chung.[26,15,22,27] As an illustration, let us consider the turbulent mixing of two groups of fluid elements containing two different chemical species, say the fuel and oxidant, across the plane A-A' in Figure 9. As far as the transport of the momentum, energy, and the chemical species in the absence of chemical reaction are concerned, this fluid-element transport (eddy transport) completely describes the mixing. This mixing of the fluid elements, however, will not allow chemical reaction between the two chemical species. Chemical reaction is a molecular process, and the chemical species must molecularly mix between the two groups of the fluid elements before a reaction can commence. Crossing of the fluid elements across the plane A-A' in itself does not necessarily imply mixing as far as the chemical processes are concerned.

The molecular mixing between the fluid elements (dissipation) takes a finite amount of time. Therefore, the chemical reaction zone of the two initially unmixed reactants of Figure 9 should be of finite thickness even in the limit of an infinitely fast reaction rate [$K_f \to \infty$ in Eq. (V-1)]. In spite of this fact, if one employs Prandtl's approach, discussed previously for the mixing and reaction problem at hand, one obtains an infinitesimally thin combustion sheet (diffusion flame sheet) in the limit of $K_f \to \infty$, as it is in the laminar flame [see, for instance, Libby (1962), reference 53].

There have been several experimental results published in the past which tried to allude to this fact, such as Hawthorne[54] et al., Wooldridge and Muzzy,[55] and Vranos[56] et al. Figure 10 shows the early experimental results of Hawthorne et al., who established a diffusion flame between a turbulent hydrogen jet and the surrounding air. These results show that the

flame (combustion zone) wherein both the reactants co-exist in the average is of finite thickness, and the flame structure is basically different from that predicted by Prandtl's theory. These points have been pointed out and discussed by Chung.[15,26,27,32]

Let us consider, again as an illustration, the idealized cases shown in Figure 11. Consider that point B is being alternately occupied by the fluid elements containing either the species r or s, whereas point B' is being occupied in tandem by the fluid elements containing various molecular mixtures of the two species. We further consider that the concentrations of the species r and s in the fluid elements occupying B and those comprising the molecular mixtures of the fluid element occupying B' are such that the mean concentrations of r and s observed at B are equal respectively to those observed at B'. We now see that the chemical reaction of Eq. (V-1) is prohibited at B whereas it can proceed at B' even though

$$\begin{aligned} \langle z_r \rangle_B &= \langle z_r \rangle_{B'} \\ \langle z_s \rangle_B &= \langle z_s \rangle_{B'} \\ \langle z_r \rangle_B \langle z_s \rangle_B &= \langle z_r \rangle_{B'} \langle z_s \rangle_{B'} \end{aligned} \qquad \text{(V-2)}$$

What is different between B and B' is the simultaneous probability of finding the species r and s. This probability is zero at B, whereas it is finite at B', and, therefore, $\langle z_r z_s \rangle_B = 0$ whereas $\langle z_r z_s \rangle_{B'} \neq 0$.

Now, let us consider for B' that the temperatures of the fluid elements are substantially different from each other, which is usually the case in combustion. Then the chemical reaction rate in each fluid element will be given by Eq. (V-1a) where z_t is the temperature of that fluid element and is

not directly related to the average temperature $\langle z_t \rangle$ which one would observe at B'. The average chemical reaction rate observed at B' will simply be the average of the chemical reaction rates in the fluid elements, $\langle K_\alpha \exp(-E/z_t) \cdot z_r^a z_s^b \rangle$. Replacement of this quantity by $K_\alpha \exp(-E/z_t) \langle z_r \rangle^a \langle z_s \rangle^b$ as is done in the conventional approach of turbulent chemically reactive flow is not physically meaningful.

The above illustrations show the fact that each averaged quantity in a chemically reacting flow implicitly embodies specific information of a certain process taking place in the flow field. Therefore, replacement of a particular higher order average by a collection of certain lower order averages--that is, direct modeling between the averages--could lead to an erroneous consequence.

Chung's theory is statistically more general in the sense of generating moments. The solutions to be obtained in this chapter will reflect more evidence of the physical phenomena described before.

In the subsequent analysis, we will assume that the momentum flow field will not be affected by chemical reactions.

V.A. Governing Equations

Our governing equation is the kinetic equation, Eq. (IV-2). The chemical reaction to be considered is given as Eq. (V-1).

K_f in Eq. (V-1) is the specific rate coefficient which is given as

$$K_f = K_o \, e^{-\Delta E/Rz_t} \tag{V-3}$$

where K_o is a constant. ΔE, R and z_t denote the activation energy, the gas constant, and the absolute temperature, respectively. K in Eq. (V-1a) is

given as

$$K = k_o\left(\frac{dM_p}{M_r^a M_s^b}\right)\rho^{a+b-1} \exp\left[-\frac{\Delta E}{Rz_t^*}\right] \tag{V-4}$$

where z_t^* represents the mean chemical equilibrium value at one of the flame edges.

The instantaneous rates of generation of the fuel ω_r, the oxidant ω_s, and the temperature ω_t by chemical reaction are related to those of the combustion product ω_p, by the relationship

$$\begin{aligned} \omega_r &= -\frac{a}{d}\left(\frac{M_r}{M_p}\right)\omega_p \\ \omega_s &= -\frac{b}{d}\left(\frac{M_s}{M_p}\right)\omega_p \\ \omega_t &= \left(\frac{\Delta h^o}{c_p}\right)\omega_p \end{aligned} \tag{V-5}$$

where Δh^o and c_p are the heat of combustion and the specific heat, respectively.

For convenience of later reference, we repeat the kinetic equation, Eq. (IV-2)

$$\frac{\partial F_\ell}{\partial t} + u_j\frac{\partial F_\ell}{\partial x_j} = \beta\frac{\partial}{\partial u_j}(F_\ell U_j) + \frac{\beta_1}{3}\langle U_k U_k\rangle\frac{\partial^2 F_\ell}{\partial u_j \partial u_j} + \omega_\ell f \tag{IV-2}$$

where $F_\ell = fz_\ell$.

The symbol ℓ represents either of the following functions

$$\ell = \begin{cases} r & \text{fuel} \qquad\qquad p \quad \text{product} \\ s & \text{oxidant} \qquad\qquad c \quad \text{inert species} \\ t & \text{temperature} \end{cases} \tag{V-6}$$

when ℓ represents c, $\omega_c = 0$.

Equation (IV-2) will be manipulated to eliminate the chemical reaction term in the following manner. We first define the nondimensional variables

$$h = \left(\frac{c_p}{\Delta h^o}\right) z_t$$

$$m = \left(\frac{dM_p}{aM_r}\right) z_r \qquad \text{(V-7)}$$

$$n = \left(\frac{dM_p}{bM_s}\right) z_s$$

and

$$\alpha = m + h$$

$$\beta = n + h \qquad \text{(V-8)}$$

Now we rewrite Eq. (IV-2) in terms of the new variables h, α and β, and we obtain the following equations,

$$\frac{\partial F_\alpha}{\partial t} + u_j \frac{\partial F_\alpha}{\partial x_j} = \beta \frac{\partial}{\partial u_j}(F_\alpha U_j) + \frac{\beta_1 \langle U_k U_k \rangle}{3} \frac{\partial^2 F_\alpha}{\partial u_j \partial u_j} \qquad \text{(V-9)}$$

$$\frac{\partial F_\beta}{\partial t} + u_j \frac{\partial F_\beta}{\partial x_j} = \beta \frac{\partial}{\partial u_j}(F_\beta U_j) + \frac{\beta_1 \langle U_k U_k \rangle}{3} \frac{\partial^2 F_\beta}{\partial u_j \partial u_j} \qquad \text{(V-10)}$$

$$\frac{\partial F_h}{\partial t} + u_j \frac{\partial F_h}{\partial x_j} = \beta \frac{\partial}{\partial u_j}(F_h U_j) + \frac{\beta_1 \langle U_k U_k \rangle}{3} \frac{\partial^2 F_h}{\partial u_j \partial u_j} + \omega_p f \qquad \text{(V-11)}$$

$$\frac{\partial F_m}{\partial t} + u_j \frac{\partial F_m}{\partial x_j} = \beta \frac{\partial}{\partial u_j} (F_m U_j) + \frac{\beta_1 \langle U_k U_k \rangle}{3} \frac{\partial^2 F_m}{\partial u_j \partial u_j} - \omega_p f \qquad \text{(V-12)}$$

$$\frac{\partial F_n}{\partial t} + u_j \frac{\partial F_n}{\partial x_j} = \beta \frac{\partial}{\partial u_j} (F_n U_j) + \frac{\beta_1 \langle U_k U_k \rangle}{3} \frac{\partial^2 F_n}{\partial u_j \partial u_j} - \omega_p f \qquad \text{(V-13)}$$

where

$$F_\alpha = \alpha f , \qquad F_\beta = \beta f$$

$$F_m = mf , \qquad F_n = nf \qquad \text{(V-14)}$$

$$F_h = hf$$

We notice that Eqs. (V-9) and (V-10) have the same form as that of Eq. (IV-2) without the chemical reaction term. The single-mode G-function obtained in the previous chapter can be used for solutions for F_α and F_β. If we further define $(F_m)_i$ and $(F_n)_i$ as F_m and F_n without chemical reactions, from Eq. (IV-2) with the aid of Eqs. (V-12) and (V-13) we can readily see the following relations,

$$(F_m)_i - (F_n)_i = F_m - F_n \qquad \text{(V-15)}$$

Since $(F_m)_i$ and $(F_n)_i$ are governed by Eq. (IV-2) without the chemical reaction term, the single-mode G-function can be used for the solutions of $(F_m)_i$ and $(F_n)_i$.

The governing equations have now become the set of equations (V-9) through (V-13). Equation (V-11) will be degenerated into a set of algebraic equations in the limit of $K \to \infty$ (or $K_f \to \infty$). With the aid of Eq. (V-7), the equation for ω_p, Eq. (V-1a), can be written as,

$$\omega_p = K \exp\left[-\frac{\Delta E}{Rz_t}\right]\left(\frac{a}{d}\right)^a\left(\frac{M_r}{M_p}\right)^a\left(\frac{b}{d}\right)^b\left(\frac{M_s}{M_p}\right)^b m^a n^b \tag{V-16}$$

Hence, we have

$$\omega_p f = K \exp\left[-\frac{\Delta E}{Rz_t}\right]\left(\frac{a}{d}\right)^a\left(\frac{M_r}{M_p}\right)^a\left(\frac{b}{d}\right)^b\left(\frac{M_s}{M_d}\right)^b f^{1-a-b} F_m^a F_n^b \tag{V-17}$$

Substituting Eq. (V-17) into Eq. (V-11) and dividing each term by K, we obtain

$$\frac{1}{K}\left\{\frac{\partial F_n}{\partial t} + u_j \frac{\partial F_n}{\partial x_j} - \beta \frac{\partial}{\partial u_j}(F_h U_j) - \frac{\beta_1}{3}\langle U_k U_k\rangle \frac{\partial^2 F_n}{\partial u_j \partial u_j}\right\}$$

$$= F_m^a F_n^b \exp\left[-\frac{\Delta E}{Rz_t}\right]\left(\frac{a}{d}\right)^a\left(\frac{M_r}{M_p}\right)^a\left(\frac{b}{d}\right)^b\left(\frac{M_s}{M_d}\right)^d f^{1-a-b} \tag{V-18}$$

In the above, when the chemical reaction rate is infinitely large, i.e. $K \to \infty$, we get the following equation

$$F_m^a F_n^b = 0 \tag{V-19}$$

Since a and b are positive numbers, Eq. (V-19) may be written as

$$F_m F_n = 0 \tag{V-20}$$

The above equation gives us some explanation of the physical phenomena of mixing and reaction, in the limit of $K \to \infty$, as described earlier in this chapter. We would like to recall that the definition of F_m (or F_n) is the probability density function of finding the fluid element containing species r (or s) with concentrations m (or n) [dimensionless form of z_r (or z_s)] having the velocities between $\vec{u}$ and $\vec{u} + d\vec{u}$ in velocity space. As mentioned before, chemical reaction is a molecular process which takes a certain time for two different chemical species (in our case they are originally contained in different fluid elements) to diffuse into each other (between fluid elements) in the course of turbulent mixing (eddy transport) so that the chemical reaction can happen. In the limit of $K \to \infty$, as soon as two different species r and s appear in the same fluid element--so that they are in the same probability cell in the velocity space--the combustion will take place and complete simultaneously. Thus, Eq. (V-20) describes the prohibition of the coexistence of the two species r and s in the same fluid element (which occupies the same probability cell in the velocity space).

The existence of one of the species r or s at a given phase point $(\vec{x},\vec{u})$ can be determined if the amount of the species appearing in the fluid element, less the amount of that species required for a complete chemical reaction, is positive.

For the convenience of later calculations we will let

$$\frac{aM_r}{dM_p} = \frac{bM_s}{dM_p} = 0.5 \tag{V-21}$$

Thus, an equal amount of two species r and s is required for a complete chemical reaction of Eq. (V-1).

Equation (V-20) will be further degenerated into the following algebraic equations. We first divide the velocity space into two domains as,

$$\begin{cases} \vec{u} \in (\vec{u})_m & \text{if} \quad \left[(F_m)_i - (F_n)_i\right] \geq 0 \\ \vec{u} \in (\vec{u})_n & \text{if} \quad \left[(F_n)_i - (F_m)_i\right] \leq 0 \end{cases} \tag{V-22}$$

According to our explanations in previous paragraphs on Eq. (V-20), F_m and F_n can be determined as follows,

$$\begin{cases} F_m = (F_m)_i - (F_n)_i & \text{for } \vec{u} \in (\vec{u})_m \\ F_n = 0 \end{cases} \tag{V-23}$$

$$\begin{cases} F_m = 0 \\ F_n = (F_n)_i = (F_m)_i & \text{for } \vec{u} \in (\vec{u})_n \end{cases} \tag{V-24}$$

Thus, our governing equations finally become Eqs. (V-9), (V-10), (V-23) and (V-24).

V.B. Properties of the Green's Functions

The kinetic equations we employed previously are homogeneous. The Fokker-Planck type equation such as Eq. (IV-2) is a diffusion type equation. The fundamental solutions obtained in the previous chapter are the instantaneous point source solutions. These solutions are similar to that of an ordinary diffusion equation.

In a mass diffusion field, if C represents the mass concentrations, its diffusion equation is given as

$$\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial x^2} \tag{V-25}$$

The Green's function of Eq. (V-25) is well known as a Gaussian kernel, which is

$$P = \frac{1}{\sqrt{2\pi D(t - t_o)}} \exp\left[- \frac{(x - x_o)^2}{2D(t - t_o)}\right] \tag{V-26}$$

P is exactly the solution of Eq. (V-25) representing the solution of an instantaneous point source with unit intensity given at $x = x_o$ when $t = t_o$. P as well as G are delta functions at $t = t_o$, at a given physical point x_o, or at the phase point $(\vec{x}_o, \vec{u}_o)$. Obviously, from the conservation of mass, P satisfies the following relation

$$\int_{-\infty}^{\infty} P(x,t|x_o,t_o)dx = 1 \tag{V-27}$$

Similarly, the Green's function which represents the unit intensity point source solution of Eq. (IV-2) has the following property

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} G_1(\vec{x},\vec{u},t|\vec{x}_o,\vec{u}_o,t_o)d\vec{x}d\vec{u} = 1 \tag{V-28}$$

Equation (V-28) is easily verified by first considering the integral

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \overline{F}_1(\vec{T},\vec{R},t|\vec{T}_o,\vec{R}_o,t_o)d\vec{T}d\vec{R} = 1 \tag{V-29}$$

which is self-evident. Then, by employing Eq. (IV-5) the left hand side of Eq. (V-29) can be written as

$$\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} G_1(\vec{x},\vec{u},t|\vec{x}_o,\vec{u}_o,t_o)\ e^{-3\beta t}\ \frac{\partial(\vec{T},\vec{R})}{\partial(\vec{u},\vec{x})}\ d\vec{u}d\vec{x} \tag{V-30}$$

Since the Jacobian $\frac{\partial(\vec{T},\vec{R})}{\partial(\vec{u},\vec{x})} = e^{3\beta t}$, Eq. (V-30) readily gives the result of Eq. (V-28).

V.C. Source Conditions

The flow conditions at $x = 0$ of the present physical problem are idealized as shown in Figure 8. The velocity profiles at $x = 0$ are so-called plug velocity profiles. In the real physical picture, one should have a certain mechanism for supplying fluids flowing continuously in the $x < 0$ region, and the two streams separated at the $y = 0$ plane should be kept unmixed. In many experimental studies such as Baker's and Spencer's experiments, in their wind tunnel the section before the test section, i.e., the $x < 0$ region, the two

streams are separated by a smooth plate which usually causes certain boundary layers on both sides of the plate. They both tried to minimize these boundary layers by smoothing the separating plate and by reducing the free stream turbulence energies to as low as possible. However, after a certain distance downstream, the effects of the original boundary layers near $x = 0$ on the other momentum quantity is no longer important.

The flow region of interest is in the region of $x > 0$ where turbulent mixing and reaction take place.

In the present analysis, we will idealize that the fluids flowing out from the $x = 0$ plane have plug velocity profiles with given turbulent energies for both streams which are originally unmixed.

The kinetic equation considered in the present analysis is linear and homogeneous, Eq. (IV-2). The Green's function obtained in the previous chapter is an instantaneous point source solution of the kinetic equation. If we properly define the distributions of the sources according to the flow conditions of the present physical problem, the Duhamel principle can be applied to superimpose all solutions caused by these sources.

In order to utilize the Green's function--the single-mode G-function--which is an instantaneous point source solution of the kinetic equation, Eq. (IV-2), we have to specify the distributions of the sources which will suitably describe the given flow conditions of the present physical problem. As far as the probability density function of the fluid elements, which carry the chemical species, z, are concerned, the distributions of the sources--according to the flow conditions mentioned in the previous paragraph--can be considered as continuous probability density fluxes (at the $x = 0$ plane) per unit area per unit time with Gaussian intensities. These are Gaussian sources with respect to their own mean velocities and turbulence energies. The condi-

tion of the source distributions is thus defined as follows,

$$S_o = [z_o f_o(\vec{u}_o)] u_o H(u_o) \delta(x_o) \tag{V-31}$$

where

$$f_o(\vec{u}_o) = \begin{cases} \dfrac{1}{(\frac{2}{3}\pi \langle U_k U_k \rangle_{o+})^{3/2}} \exp\left[-\dfrac{[(u_o - \langle u \rangle_\infty)^2 + v_o^2 + w_o^2]}{\frac{2}{3}\langle U_k U_k \rangle_{o+}}\right], & y > 0 \\[2ex] \dfrac{1}{(\frac{2}{3}\pi \langle U_k U_k \rangle_{o-})^{3/2}} \exp\left[-\dfrac{[(u_o - \langle u \rangle_{-\infty})^2 + v_o^2 + w_o^2]}{\frac{2}{3}\langle U_k U_k \rangle_{o-}}\right], & y < 0 \end{cases} \tag{V-32}$$

and

$$H(u_o) = \begin{cases} 1 & u_o > 0 \\ 0 & u_o \leq 0 \end{cases} \tag{V-33}$$

z_o denotes the species concentration given at the sources. All subscripts o denote the quantities given at the source. $H(u_o)$ denotes that only those fluid elements with positive u_o values can go into the region of $x > 0$ where mixing and reaction take place.

In the present analysis we will let $\langle U_k U_k \rangle_{o+}$ and $\langle U_k U_k \rangle_{o-}$ be significantly small compared to $\langle u \rangle_\infty^2$. In the subsequent analyses we will let

$$\frac{\langle U_k U_k \rangle_{o^+}}{\langle u \rangle_\infty^2} = 2 \times 10^{-5}$$

$$\frac{\langle U_k U_k \rangle_{o^-}}{\langle u \rangle_\infty^2} = 2 \times 10^{-5} \tag{V-34}$$

The value of u_o is given as

$$u_o = \langle u \rangle_{\pm\infty} + U_o \tag{V-35}$$

which can be approximately written as

$$f(u_o) \sim 0 \quad \text{unless} \quad |u_o - \langle u \rangle_\infty| \leq \langle U_k U_k \rangle_o^{1/2} \tag{V-36}$$

From Eq. (V-32) we see that most fluid elements given at x = 0 have the x-component velocities of the value of $\langle u \rangle_\infty$ (or $\langle u \rangle_{-\infty}$). Under the condition of Eq. (V-32) we also can see from Eq. (V-30) that the probability of finding the fluid elements with negative values of u_o is exponentially very small. Therefore, Eq. (V-31) is approximated as,

$$S_o \doteq [z_o f_o(\vec{u}_o)] \langle u \rangle_\infty \, \delta(x_o) \tag{V-37}$$

The above approximation will simplify some manipulations in later analyses.

In the case of chemically frozen flow, we will let $z_o = 1$ in Eq. (V-31). When the chemical reactions are undertaken we assume that the upper stream (y > 0) contains fuel (r) and the lower stream (y < 0) contains oxidant (s) and inert species (c). In the present analysis, these chemical species con-

centrations at the source are given as follows.

In the upper stream ($y > 0$, $x \leq 0$):

$$z_{r_o} = 1.0$$
$$h_o^+ = 0.5 \tag{V-38}$$

In the lower stream ($y < 0$, $x \geq 0$)

$$z_{s_o} = 0.7$$
$$z_{c_o} = 0.3 \tag{V-39}$$
$$h_o^- = 0.5$$

We should notice that from Eqs. (V-5) and (V-21), we have

$$z_r = \frac{1}{2} m$$
$$z_s = \frac{1}{2} n \tag{V-40}$$

Therefore, the m_o and n_o at the source are readily given as

$$\left.\begin{aligned} m_o &= 2.0, \\ n_o &= 0 \end{aligned}\right\} y > 0,\ x \leq 0$$
$$\left.\begin{aligned} m_o &= 0 \\ n_o &= 1.4\ , \end{aligned}\right\} y < 0,\ x \leq 0 \tag{V-41}$$

V.D. Solutions

We will use the Green's function--the single-mode G-function--to construct the solutions for f and F's. As mentioned in the previous section, the kinetic equation employed is linear and homogeneous, and its solution can be obtained by properly summing up the sources distributed in the physical space. With the distributions of the sources specified in the previous section and by employing the Duhamel principle, the solution for F and f can be constructed as follows (without chemical reaction).

$$F(\vec{u},\vec{x},t) = \int_{t_o=0}^{t} dt_o \int_{-\infty}^{\infty} dw_o \int_{-\infty}^{\infty} dv_o \int_{-\infty}^{\infty} du_o \int_{-\infty}^{\infty} dz_o \int_{-\infty}^{\infty} dx_o \int_{-\infty}^{\infty} dy_o \; G_1(\vec{x},\vec{u},t|\vec{x}_o,\vec{u}_o,t_o)\, S_o \tag{V-42}$$

and f is obtained by setting all z's equal to 1.

$$f = (F)_{z=1} \tag{V-43}$$

Since the fluids are continuously flowing out at the x = 0 plane, after a certain considerable time, i.e., t >> 1, all the solutions to be obtained in the region $\infty > x > 0$ will reach their steady state. In our subsequent calculation we will tend to obtain steady state solutions.

The integrations on the right hand side of Eq. (V-42) and Eq. (V-43) can be evaluated by suitable application of integration tables and little manipulation except with respect to t_o. The last step of integration with respect to time is left to the computer for numerical integration.

Once the distribution functions are determined, the various one-point

correlation functions can readily be obtained. Let $Q(\vec{u})$ represent the general momentum quantities. The averaged $Q(\vec{u})$ can be obtained as follows,

$$\langle Q \rangle = \frac{1}{N} \int_{-\infty}^{\infty} Qf(\vec{u},\vec{x})d\vec{u} \tag{V-44}$$

In later calculation we will let $Q = u$ and $U_k U_k$, which are essentially needed for further calculation of combustion diffusion flame.

N in Eq. (V-44) is the normalization factor, which is

$$N = \int_{-\infty}^{\infty} f(\vec{u},\vec{x})d\vec{u} \tag{V-45}$$

N is sometimes called the particle density. When we defined the conditions of our sources we made certain approximations which took a very little amount of the fluids with negative u_o velocities at $x = 0$ into our solutions. Ideally, N should be exactly 1. In our calculation for the given original turbulence energy and approximation made before, the result of N in the free stream has the value of 1.000104, and with little variation in the mixing region. We count N as the particle density and all the calculations are normalized by N. The necessary parameters and iteration scheme on $\langle u_j \rangle$ and $\langle U_k U_k \rangle$ will be given and discussed later in this chapter.

As we have assumed before, the momentum field will not be affected by chemical reactions.

Once the distribution functions, F's, are determined as given by Eq. (V-42), the various quantities of mean species concentration and their mean turbulent transport can be easily determined. This will be given subsequently.

The determination of $F_m(\vec{u})$ and $F_n(\vec{u})$ is given by Eqs.(V-23), (V-24) and (V-42). Equation (V-20) prohibits the coexistence of the fuel and oxidant

in the same fluid element which has been explained in Section V.A. Our physical problem gives the two separated streams with one stream containing fuel and the other one containing oxidant and inert species. These two streams are originally unmixed. The intermixing between these two streams and the associated interdiffusion of oxidant and fuel between fluid elements, which originally contained different species, will be mainly undergone through vertical mixing and transport. We then approximate that the requirement, in the limit of $K \to \infty$, that the two chemical species, fuel and oxidant, be "in phase" in velocity space ~~in the limit of k~~, is necessary only in the vertical direction. Thus, Eq. (V-20) is approximated as follows,

$$F_{m,v} F_{n,v} = 0 \tag{V-46}$$

where

$$F_{m,v} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F_m(\vec{u})\,dw\,du \tag{V-47}$$

$$F_{n,v} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} F_n(\vec{u})\,dw\,du \tag{V-48}$$

Equation (V-46) prohibits the coexistence of fuel and oxidant appearing in the probability density cell on the vertical velocity v-axis. Equation (V-46) can be further written as,

$$\text{For } [(F_{m,v})_i \geq (F_{n,v})_i] , \quad v \in v_m \tag{V-49}$$

and

$$F_{m,v} = (F_{m,v})_i - (F_{n,v})_i$$

$$\& \qquad F_{n,v} = 0 \tag{V-50}$$

For $[(F_{n,v})_i \geq (F_{m,v})_i]$, $v \in v_n$ (V-51)

and

$$F_{n,v} = (F_{n,v})_i - (F_{m,v})_i$$

$$F_{m,v} = 0 \tag{V-52}$$

where

$$(F_{m,v})_i = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} (F_m)_i dwdu$$

$$(F_{n,v})_i = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty} (F_n)_i dwdu \tag{V-53}$$

The expressions of Eqs. (V-49) through (V-52) are equivalent to Eqs. (V-22) through (V-24) in section V.A. We only reduce the velocity domain of interest, $\vec{u}_m$ (or $\vec{u}_n$), to that of the v-component, v_m (or v_n).

We would like to mention here again that the single-mode G-function, G_1, is the Green's function of Eq. (IV-2) without the chemical reaction term. The solutions for the F's given by Eq. (V-42) can be used for F_α, F_β, $(F_m)_i$ and $(F_n)_i$.

With the aid of Eq. (V-42) and Eqs. (V-49) through (V-52), the various quantities of the mean species concentration can be readily defined as follows,

$$\langle m \rangle = \int_{v_m} F_{m,v} dv$$

$$\langle z_r \rangle = \frac{\langle m \rangle}{2} \tag{V-54}$$

$$\langle n \rangle = \int_{v_n} F_{n,v} dv$$

$$\langle z_s \rangle = \frac{\langle n \rangle}{2} \tag{V-55}$$

$$\langle z_c \rangle = \int_{-\infty}^{\infty} F_c(\vec{u},\vec{x}) d\vec{u} \tag{V-56}$$

From the conservation of species, $\langle z_p \rangle$ can be obtained as follows:

$$\langle z_p \rangle = 1 - \langle z_r \rangle - \langle z_s \rangle - \langle z_c \rangle \tag{V-57}$$

Since the kinetic equations for F_α and F_β do not contain chemical reaction terms, the solution for the F's given by Eq. (V-42) can be used for F_α and F_β. Thus, $\langle \alpha \rangle$ and $\langle \beta \rangle$ can be readily obtained as

$$\langle \alpha \rangle = \int_{-\infty}^{\infty} F_\alpha(\vec{u},\vec{x}) d\vec{u} \tag{V-58}$$

$$\langle\beta\rangle = \int_{-\infty}^{\infty} F_{\beta}(\vec{u},\vec{x})d\vec{u} \tag{V-59}$$

and

$$\langle h\rangle = \langle\alpha\rangle - \langle m\rangle$$

or (V-60)

$$\langle h\rangle = \langle\alpha\rangle - \langle n\rangle$$

In Eq. (V-21) we let $\frac{aM_r}{dM_p} = \frac{bM_s}{dM_p} = 0.5$, i.e., equal amounts of the mass of fuel (m) and oxidant (n) are required for a complete chemical reaction.

In the domain of $v \in v_m$, all the oxidant appearing (before chemical reaction occurs) in the fluid element will be totally committed to combustion and will become product. Therefore, $F_{p,v}$, the distribution function for the species of the product can be readily obtained as [from Eqs. (V-49) through (V-52)],

$$F_{p,v} = \begin{cases} (F_{n,v})_i , & v \in v_m \\ (F_{m,v})_i , & v \in v_n \end{cases} \tag{V-61}$$

Therefore, $\langle z_p\rangle$ can also be determined as follows,

$$\langle z_p\rangle = \int_{-\infty}^{\infty} F_{p,v}dv \tag{V-62}$$

In our later calculation, the results of $\langle z_p\rangle$ calculated from Eq. (V-62) and Eq. (V-57) are almost identical.

From Eqs. (V-49) through (V-52) and Eq. (V-61), the mean turbulent transport of various species can be obtained as follows,

$$\langle Vm\rangle = \int_{v_m} VF_{m,v}dv$$

$$\langle Vz_r\rangle = \frac{1}{2}\langle V_m\rangle \tag{V-63}$$

$$\langle Vn\rangle = \int_{v_n} VF_{n,v}dv$$

$$\langle Vz_s\rangle = \frac{1}{2}\langle Vn\rangle \tag{V-64}$$

and

$$\langle Vz_p\rangle = \int_{-\infty}^{\infty} VF_{p,v}dv \tag{V-65}$$

If we define ω_h as the dimensionless temperature due to chemical reaction, we may write, from Eq. (V- 7),

$$\omega_h = \left(\frac{c_p}{\Delta h^o}\right)\omega_t \tag{V-66}$$

By comparing Eqs. (V-66) and (V- 5), we have

$$\omega_h = \omega_p \tag{V-67}$$

which gives

$$h_p = z_p \quad \text{and} \quad \langle Vh_p\rangle = \langle Vz_p\rangle \tag{V-68}$$

where h_p is the dimensionless temperature (product) due to chemical reaction. If h_i represents the dimensionless temperature of the flow field for a chemically frozen case, then h can be written as

$$h = h_i + h_p \tag{V-69}$$

and the vertical turbulent transport is

$$\langle Vh \rangle = \langle Vh_i \rangle + \langle Vh_p \rangle \tag{V-70}$$

Since we have originally uniform temperature, $h_o = 0.5$ for all y at $x = 0$, there will be no net heat transfer under chemical frozen conditions. Therefore, we have

$$\langle Vh_i \rangle = 0 \tag{V-71}$$

With the aid of Eqs. (V-68) and (V-71), Eq. (V-70) becomes

$$\langle Vh \rangle = \langle Vz_p \rangle \tag{V-72}$$

In calculating the solutions cited above there are certain parameters which must be determined and which will be discussed in the next section. For the convenience of calculation, all quantities to be calculated will be non-dimensionalized by some reference quantities.

V.E. Determination of Parameters and the Similarity Solutions

As mentioned in the previous chapter, our solutions will be iterated on $\langle u_j \rangle$ and $\langle U_k U_k \rangle$ until a certain convergence is attained. In our present physical problem, as described earlier, the mean velocities given at $x = 0$ (source) are only in the x-direction, i.e., $\langle v \rangle_\infty = 0$, $\langle w \rangle_\infty = 0$. Even in the mixing region $\langle w \rangle = 0$, which results from the nature of the problem being two-dimensional. $\langle w \rangle = 0$ is also shown in our calculations. In the mixing layer there is $\langle v \rangle$, which is relatively very small compared to $\langle u \rangle$ ($\langle v \rangle / \langle u \rangle \sim 0.005$). Also, our preliminary calculations show that the calculated $\langle u \rangle$ is relatively insensitive to that of the assumed $\langle u \rangle$ and the chosen $\langle U_k U_k \rangle$. Even when we merely assumed $\langle u \rangle = \frac{1}{2} (\langle u \rangle_{-\infty} + \langle u \rangle_\infty)$, the resulting $\langle u \rangle$ is very close to the error function and comparable to the experimental data. In the subsequent analysis the iteration of $\langle u_j \rangle$ will be simplified on $\langle u \rangle$ only.

There are some parameters, associated with the guessing of $\langle u \rangle$ and $\langle U_k U_k \rangle$, which will be discussed subsequently. Later in this section we will also see that by properly defining the integral length scale in the mixing layer we will obtain similarity solutions. Similarity solutions of the present problem have been given before[38,39,45] and were also shown by experimental results.[47,48,50] However, the present approach is quite different from the conventional ones[38,39,45] and the former investigators were restricted to obtaining the momentum field only.

First, β has to be determined. β is given as the sum of β_1 and β^ν which are given by Eqs. (II-2) and (II-6). β_1 and β^ν can be related by introducing the turbulent Reynold's number which is

$$Re_\Lambda = \frac{\langle U_k U_k \rangle^{1/2} \Lambda}{\nu} \tag{V-73}$$

From Eqs. (II-2), (II-6) and (V-68), β^ν can be written in terms of β_1 as

$$\beta^\nu = b'\beta_1 \tag{V-74}$$

where

$$b' = \frac{1}{2}\left(\frac{\Lambda}{\lambda}\right)^2 / Re_\Lambda \tag{V-74a}$$

Therefore, β becomes

$$\beta = \begin{cases} (1 + 2b')\beta_1, & \text{for } F \\ (1 + b')\beta_1, & \text{for } f \end{cases} \tag{V-75}$$

Analogous to β_1, we define β as

$$\beta = \frac{\langle U_k U_k \rangle^{1/2}}{2\Lambda'} \tag{V-76}$$

where Λ' is similar to a length scale which represents the length scale corresponding to the dissipation rate β and the turbulence energy $\langle U_k U_k \rangle$.

The growth of the mixing layer thickness is approximately a linear function of x, which is shown in both Baker's and Spencer's experimental results. This enables us to assume that Λ and Λ' are also linear functions of x. The integral length scale is approximately of the order of one half of the mixing layer thickness. Therefore, we let

$$\Lambda = \ell_s x$$

$$\Lambda' = \ell_s' x \tag{V-77}$$

where ℓ_s and ℓ_s' are constants to be determined later.

The two dimensionless spatial variables appearing in our solution are in the x-direction $x' = x/\Lambda'$, and in the y-direction $y' = y/\Lambda'$. By using Λ' as a linear function of x, x' and y' become

$$x' = \frac{x}{\Lambda'} = \frac{1}{\ell_s'}$$

$$y' = \frac{y}{\Lambda'} = \frac{y}{x}\,\frac{1}{\ell_s'} \tag{V-78}$$

The above functions of the dimensionless spatial variables automatically give us the similarity solutions with the similarity variable

$$\eta = \frac{y}{x} \tag{V-79}$$

Thus, all the quantities to be obtained will be functions of η only.

Many investigators (Tollmein, Goertler, Baker, Spencer, et al.) defined the similarity parameter as

$$\xi = \frac{\sigma y}{x} \tag{V-80}$$

where σ is a constant to be determined by experiments which also will indicate how fast the mixing layer grows.

Goertler's error function of mean velocity profiles gives the dividing line--where the mean velocity is the average mean of the free stream's velocities--as being on the x-axis. This dividing line given by Goertler does not agree with the experimental results. If we properly add one parameter η_o which will adjust the dividing line in Goertler's error function, the mean velocity distributions of both Baker's and Spencer's data are very close to the following form.

$$\frac{\langle u\rangle}{\langle u\rangle_\infty} = \frac{1}{2}\left\{\left(1 + \mathrm{erf}[\sigma(\eta - \eta_o)]\right) + \frac{\langle u\rangle_{-\infty}}{\langle u\rangle_\infty}\left(1 - \mathrm{erf}[\sigma(\eta - \eta_o)]\right)\right\} \tag{V-81}$$

The velocity ratio $\frac{\langle u\rangle_{-\infty}}{\langle u\rangle_\infty}$ will be chosen as 0.3. From Spencer's experimental data, those parameters, σ, Λ, λ, Re_Λ, and b, needed for our calculation are as follows

For $\frac{\langle u\rangle_{-\infty}}{\langle u\rangle_\infty} = 0.3$

η_o	σ	Λ/λ	Re_Λ	b'	Λ
-0.02	20.43	3.26	$\sim$ 1600	0.012	$0.044(x - x_o)$

where x_o is the virtual origin point of Spencer's experiments and has a very small negative value. As we can see from the above list of parameters, b is relatively small as compared to 1, and we approximate Λ' as

$$\Lambda' = 0.044x \qquad [\text{i.e., } \ell_s' = 0.044 \text{ in Eq. (V-77)}] \tag{V-82}$$

By using the above parameters, the calculated $\langle u \rangle$ is almost identical to that given by Eq. (V-81). These results of $\langle u \rangle$ and their comparison with Spencer's data will be given in the next section.

In calculating $\langle U_k U_k \rangle$ we need more iteration work. From both Spencer's and Baker's (Baker only measured the turbulent intensity, $\langle U^2 \rangle^{1/2}$, instead of the turbulent energy profile) data, we propose the following formula for the turbulent energy profiles

$$\frac{\langle U_k U_k \rangle}{\langle u \rangle_\infty^2} = E_m \, e^{-\Gamma(\eta-\eta_o)^2} \tag{V-83}$$

where Γ is a constant parameter to be determined later. E_m is the maximum value of $\langle U_k U_k \rangle$ which is given by the experimental data. Equation (V-83) is evolved based on Baker's turbulent intensity profile and Spencer's turbulence energy profiles. Finally, a proper choice of $\Gamma = 1.4$ (for $\frac{\langle u \rangle_{-\infty}}{\langle u \rangle_\infty} = 0.3$) is found to have very good agreement between both the given and the calculated values. The results of $\langle U_k U_k \rangle$ which will be compared with Spencer's experimental data will be given in the next section.

V.F. Results of the Iteration on $\langle u \rangle$ and $\langle U_k U_k \rangle$

We will let Ep and E represent the given and the calculated $\frac{\langle U_k U_k \rangle}{\langle u \rangle_\infty^2}$, respectively, and $\frac{\langle u \rangle}{\langle u \rangle_\infty}$ and UK represent the calculated and the given $\frac{\langle u \rangle}{\langle u \rangle_\infty}$, respectively. All the necessary parameters for the calculation are defined in Chapter V. The resulting Ep, E, $\langle u \rangle$ and UK are listed in the following table.

$$\frac{\langle u\rangle_{-\infty}}{\langle u\rangle_{\infty}} = 0.3$$

$\eta = y/x$	Ep	E	UK	$\langle u\rangle/\langle u\rangle_{\infty}$
0.06	0.00062	0.0004168	0.9927	0.9978
0.05	0.00200	0.00232	0.9849	0.9900
0.04	0.00420	0.0054721	0.9729	0.9709
0.03	0.00801	0.008797	0.9480	0.9501
0.02	0.01347	0.013652	0.9178	0.91325
0.01	0.02027	0.0201724	0.8648	0.8724
0.0	0.02715	0.027106	0.8028	0.8125
-0.01	0.03235	0.0325176	0.72957	0.7403
-0.02	0.03430	0.034707	0.650	0.6613
-0.03	0.03235	0.033013	0.5703	0.5827
-0.04	0.02715	0.028117	0.4972	0.5121
-0.05	0.02027	0.0217065	0.43513	0.4557
-0.06	0.01347	0.01582	0.3867	0.410
-0.07	0.0080	0.0100	0.352	0.371
-0.09	0.00196	0.00181	0.3151	0.3115
-0.10	0.00082	0.00072	0.3072	0.3043

V.G. Results

With the solution cited in section V.D. and the calculation scheme of $\langle u \rangle$ and $\langle U_k U_k \rangle$ given in section V.G., the results of $\frac{\langle u \rangle}{\langle u \rangle_\infty}$ and $\frac{\langle U_k U_k \rangle}{\langle u \rangle_\infty^2}$ are given in Figures 12 and 13. These figures show that the comparison with Spencer's experimental data has a very good agreement.

Once the momentum field is determined, no further iteration is needed for further calculation of the combustion data. The distribution functions $F_{m,v}$ and $F_{n,v}$ of fuel and oxidant species in the combustion zone at different positions η are given in Figures 14 and 15. These two figures show the non-Gaussian nature of the distribution functions of the different species in the mixing layer.

The combustion diffusion flame structure is given in Figure 16. Figure 16 presents the various mean species concentration profiles and also shows the finite thickness of the diffusion flame which is approximately of the order of half of the mixing layer thickness.

Finally, the mean turbulent transport of various different species is given in Figure 17. Figure 17 shows that in some region of the mixing layer, the heat transfer direction does not depend on mean temperature gradients. All the results will be discussed in the next section.

V.H. Discussion of the Results

The results for the momentum field, both for mean velocity profile and mean turbulence energy profile have very good agreement in comparison with Spencer's experimental results. Those parameters needed for calculation which are determined in a previous section are based on Spencer's data.

From the results shown in Figures 12 and 13, it seems that the present Green's function method is satisfactorily accessible in applying Chung's theory.

For the present two dimensional shear flow problem, the mean velocity distribution can well be described by certain error functions. These have been shown by many former investigators[37-48] both analytically and experimentally. Although the present kinetic approach is totally different from the former conventional approach, the error function distribution of the mean velocity profiles can be seen from our solution, one step before we integrate with respect to time. This error function distribution of the mean velocity can be considered as the nature of the problem.

The present similarity solutions are automatically obtained after suitably choosing the expression of the integral length scale Λ'. We do not intend to obtain similarity solutions in the beginning of the present analysis. Since σ is a constant (to be determined by experiments) our present similarity variable, $\eta = y/x$, and the similarity variable defined by others,[39,47] $\xi = \sigma y/x$, function in the same manner.

In the real physical picture, as mentioned before, there is a separating plate between the two streams in the region of $x \leq 0$, and the resulting boundary layers do affect the velocity profile and turbulence energy profiles in the initial part of the mixing region. In between these two regions, both Baker's and Spencer's experimental results show that the measured turbulent intensity, $\langle U^2 \rangle^{\frac{1}{2}}$ and the turbulence energy distribution are constants on the centerline, $\eta \sim \eta_o$, and the mean velocity profiles are nearly similar. However, our present analysis has assumed ideal plug velocity profiles at $x = 0$ and no wall effects of the wind tunnel; therefore, our solutions are similar everywhere (along the x axis).

From Figure 12, we see that the deflection point of the mean velocity profile is near $\eta = \eta_o$, which gives the maximum shear stress near that point. Since our original turbulence energy given at $x = 0$ (source) is negligibly small, the turbulence energies are produced by shear stress in the mixing layer. The maximum turbulence energy as shown in Figure 13 is near the region of $\eta = \eta_o$ which corresponds to the deflection point (maximum shear stress) near the region of $\eta = \eta_o$ in Figure 12.

The distribution functions of $F_{m,v}$ and $F_{n,v}$ at two different positions of η in the mixing layer are given in Figures 14 and 15. As it was explained in sections V.A. and V.C. of this chapter, the governing set of fundamental solutions for this problem consists of single-mode G-functions and an algebraic equation which is the degenerate of the reaction term, ωf. This algebraic equation, Eq. (V-46), prohibits the coexistence of the fuel and oxidant in the same fluid element since $K \to \infty$ demands the immediate combustion of all molecularly mixed reactants until one of the reactants disappears. This fact manifests itself in the present solution, as the prohibition of coexistence of the fuel and oxidant within the same velocity cell for a given t and $\vec{x}$. The above phenomena are evident in the distribution functions of the chemical species shown in Figures 14 and 15. In these figures, the completely non-Maxwellian nature of the distribution functions is evident in these results.

Figure 16 shows the structure of the combustion diffusion flame. As we expected, the flame is of finite thickness, and its thickness is close to one half of the mixing layer thickness (local integral scale). These features of the combustion diffusion flame have been revealed in the previous analyses[26-31] by using the bimodal method. As we have explained before, chemical reaction is a molecular process, and the chemical species must molecularly

diffuse into each other (they are originally contained in different fluid elements) so that the chemical reaction can commence. The molecular diffusion of chemical species between the fluid elements has to take a finite amount of time, and, therefore, the combustion zone must be of finite thickness even in the limit of $K \to \infty$. As a matter of fact, the existing experimental results[53-55] of the turbulent diffusion flames bear out the above mentioned aspect of combustion.

Since the chemical species are carried by the fluid elements, the rate of momentum mixing (eddy transport) will control the rate of mixing and, meanwhile, the interdiffusion of two different chemical species. The rate of momentum mixing is β_1, and in a complete momentum mixing the fluid element will travel a distance of the order of the integral length scale. Therefore, the complete combustion of the reactants will take place in a flame whose thickness is of the order of Λ. This is shown in Figure 16.

We also see that the maximum $\langle z_p \rangle$ appears near $\eta - \eta_o = -0.02$. Since the species from both streams have to cross the centerline region, $\eta = \eta_o$, in the course of mixing and reaction, the area near the centerline region would have a better chance of more complete mixing and chemical reaction between these two chemical species. Therefore, the maximum $\langle z_p \rangle$ appears in this region, $\eta - \eta_o = 0$. However, the mass rate of supply of fuel from the upper stream is faster with larger momentum than that of the oxidant from the lower stream. We see that the maximum value of $\langle z_p \rangle$ is located near $\eta - \eta_o = -0.02$ which is slightly lower than the centerline $\eta - \eta_o = 0$.

Figure 17 presents the mean turbulent transport of various chemical species and the mean temperature distributions, $\langle h \rangle$. Our source conditions specify that we have originally uniform temperature in both streams. The heat production (or temperature increase) in the mixing layer is mainly

contributed by the heat of combustion. Therefore, the profile of $\langle h \rangle$ is distributed in a manner analogous to that of $\langle z_p \rangle$.

In Figure 17 we also can see that $\langle nV \rangle$ has positive values and $\langle mV \rangle$ has negative values. Since the oxidant is supplied from the lower stream and the fuel is coming from the upper stream, the former species have to move upward while the latter have to be transported downward in order to particpate in the mixing and reaction in the mixing region.

From the curves of $\langle z_p \rangle$ and $\langle h \rangle$ we can see that much of the production appeared in the core region of the mixing layer. The vertical transport of z_p and h, i.e., $\langle Vz_p \rangle$ and $\langle Vh \rangle$, will emanate from this region to both the upper and lower directions. These are shown on the curve of $\langle Vz_p \rangle$ and $\langle Vh \rangle$ in Figure 17.

As mentioned earlier, the original two streams have uniform temperature. The temperature increase or the heat production in the mixing layer are mainly obtained from chemical reaction. Therefore, the immediate turbulent transport of z_p and h would behave in the same manner. This is shown in Figure 17.

One interesting phenomenon which has also been revealed by the previous bimodal method, as shown in Figure 17, is that in some region of the combustion zone, heat transfer, $\langle Vh \rangle$, takes place against the conventional negative mean temperature gradient. In the region of $-0.02 < \eta - \eta_o < -.005$, $\langle Vh \rangle$ has negative values which implies that heat transfer is taking place in the $-(\eta - \eta_o)$ direction, while the mean temperature profile, $\langle h \rangle$, has negative gradient values along the $+(\eta - \eta_o)$ direction. This manifests the inadequacy of the conventional gradient-type approach in which turbulent transport has been analogous to laminar transport and is in terms of local mean properties. The inadequacy of the mean gradient-type approach and the insufficiency of the

one-point moment equation in describing the turbulent mixing and combustion have been well explained before and will not be repeated here.

Most of the salient features of Chung's theory of turbulent chemically reactive flow as discussed in the previous paragraphs have been revealed in the previous analyses by the bimodal method.[26-31] The present solutions do not show the discontinuities in gradients of the mean concentrations at the two flame edges seen in the bimodal solutions. It seems logical that such discontinuities should be a natural consequence of the bimodal approximation. As it was explained in Chapter IV, in a bimodal approximation, all distribution functions are a priori approximated by two dissimilar half-Maxwellian functions. Therefore, for the completely non-Maxwellian combustion problems, the distribution functions have imbedded discontinuity at $v = 0$. Furthermore, in the bimodal method, one divides the fluid elements into two families in velocity space with one for $v > 0$ and the other one for $v < 0$, respectively. All reactants $\underline{s}$ in $v > 0$, for instance, are considered to be molecularly mixed and may react simultaneously. No distinction is possible among the fluid elements and the chemical species with varying positive values of v.

Obviously, all chemical species $\underline{s}$ moving with the positive v (see Figure 9) will not molecularly mix with $\underline{r}$ at the same rate. Ones with greater v will mix before those with smaller v. Therefore, the beginning or end of a flame zone is reached in a continuous manner and not discontinuously. A description of these detailed phenomena, however, has been precluded in a bimodal approximation, and the discontinuities in the mean profile gradients resulted.

CHAPTER VI

CONCLUDING REMARKS

A study of turbulent mixing and combustion according to the kinetic theory due to Chung has been presented in this dissertation. A further study of the multiscale turbulent kinetic theory generated from Chung's theory has also been studied.

We first thoroughly reviewed Chung's theory, its basic physical standing and its engineering-wise applicability which distinguishes Chung's theory from the conventional phenomenological and classical statistical theories.

In Chapter III, the extended kinetic equation from Chung's theory characterized by two-length-scales was employed to analyze the behavior of the mixing and decay of a multiscale turbulence field. The decay and interaction of the two nonequilibrium degrees and the behavior of the apparent length scale representing the hypothetical turbulence field characterized by one length-scale was studied through the kinetic theory approach for the first time. The relaxation of a multiscale turbulence field is found to be in basic agreement with that analyzed in the classical statistical theories that the group of energy-containing eddies with a larger length scale controls the relaxation rate of the turbulence field. The variations of the apparent length scale are quantitatively revealed during the decay of a multiscale turbulence field. The apparent length scale is found to tend to reach a steady value, for large T, of approximately the average value of the two given length scales. We also found that the interaction between the two nonequilibrium degrees is stronger when they are closer in wave space in the energy spectrum.

The analysis presented in Chapter IV provides the mathematical scheme

of finding the fundamental solutions of the kinetic equations given by Chung's theory. In principle, if one should find it necessary to seek for the higher order (more than two) kinetic equations according to Chung's theory (only at the expense of mathematical complications) the mathematical techniques are implicitly given in Chapter IV, and the generalized fundamental solutions can be obtained by extending the mathematical lemmas given in Appendix III.

The results in Chapter V show that the present Green's function method of applying Chung's theory improves qualitatively the results obtained by the former bimodal method. The present solutions removed the discontinuities of the mean gradient quantities in the diffusion flame structure which are caused by the approximation of the bimodal method in the previous analyses.[26-31] Our solutions reconfirm the finite thickness of the diffusion flame, and they reconfirm that the flame thickness is of the order of the integral length scale, both of which have been revealed by the bimodal method in previous analyses.[26-31] We also noticed that the heat transfer could take place against the negative mean temperature gradient in certain regions of combustion zone. All these salient features of turbulent chemically reacting flow mentioned above enlightened the present kinetic theory approach of turbulent chemically reacting flow.

It is our main purpose to study Chung's theory of turbulent chemically reacting flow. None of the other existing kinetic theories of turbulence are modeled for chemically reacting flow. We have provided a better method and improved the results in applying Chung's theory. We also studied the decay of a multiscale turbulence field and we do realize the need for a multiscale turbulence theory, which enables us to have an equation to describe the length scale, but there is no chemical species equation for a multiscale

turbulent flow. The establishment of a chemical species kinetic equation for a multiscale turbulent chemically reacting flow will be of great interest in the near future.

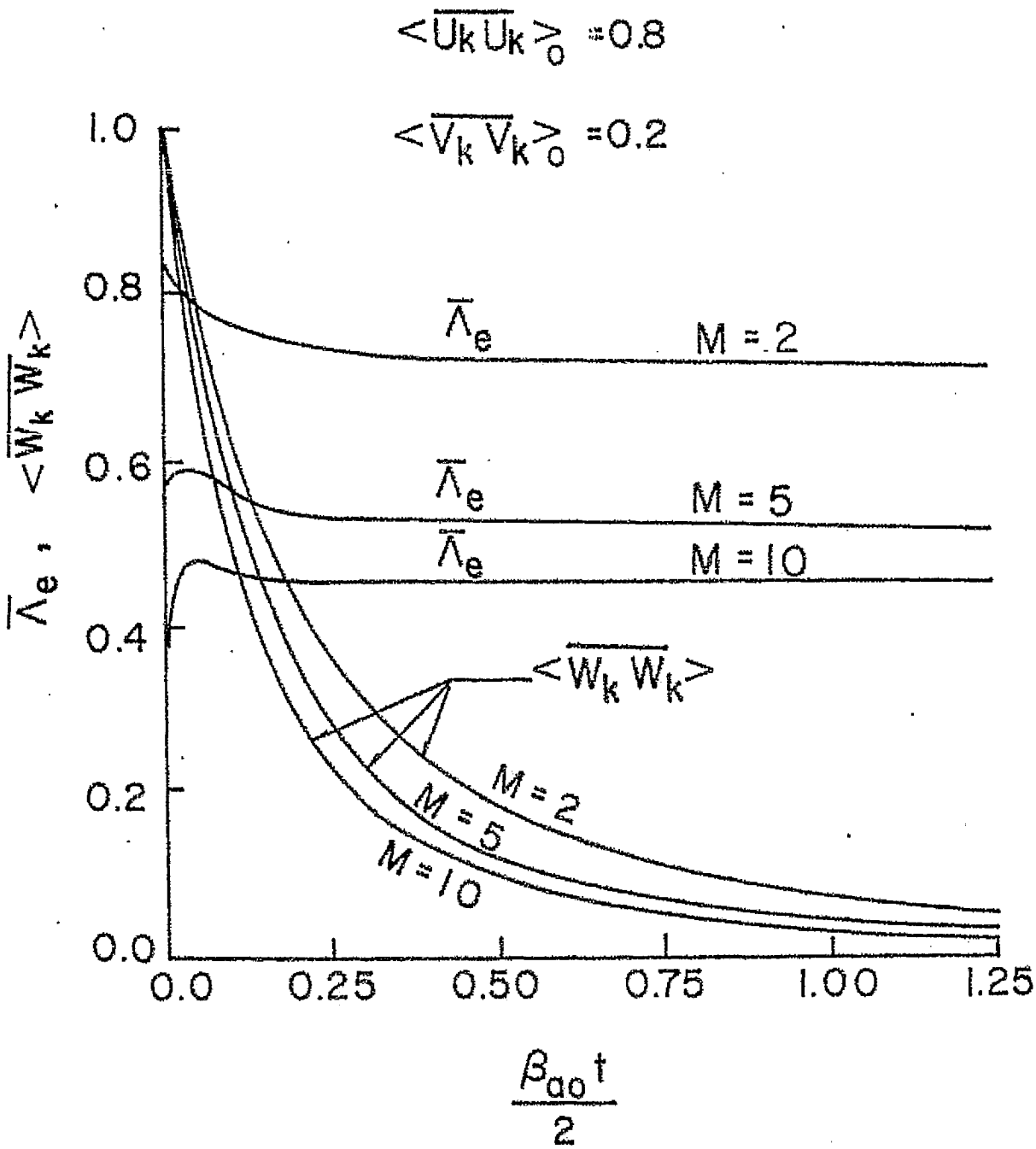


Figure 2 Decay of the turbulence energy, $\langle \overline{W_k W_k} \rangle$, and the variation of the apparent length scale, $\overline{\Lambda}_e$, with initial conditions $\langle \overline{U_k U_k} \rangle_o = 0.8$, $\langle \overline{V_k V_k} \rangle_o = 0.2$.

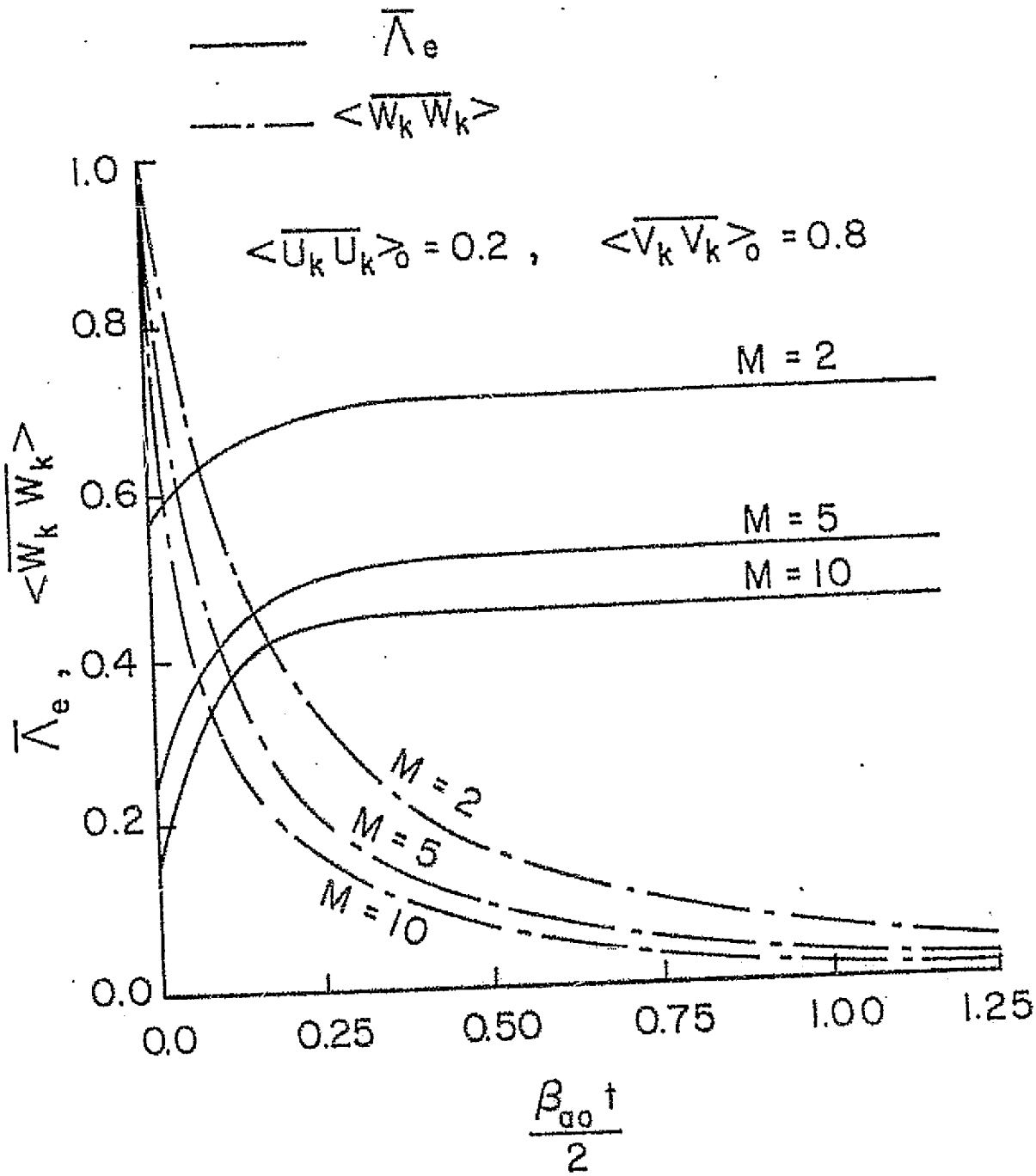


Figure 3 Decay of the turbulence energy, $\langle\overline{W_k W_k}\rangle$, and the variation of the apparent length scale, $\overline{\Lambda}_e$, with initial conditions $\langle\overline{U_k U_k}\rangle_o = 0.2$, $\langle\overline{V_k V_k}\rangle_o = 0.8$.

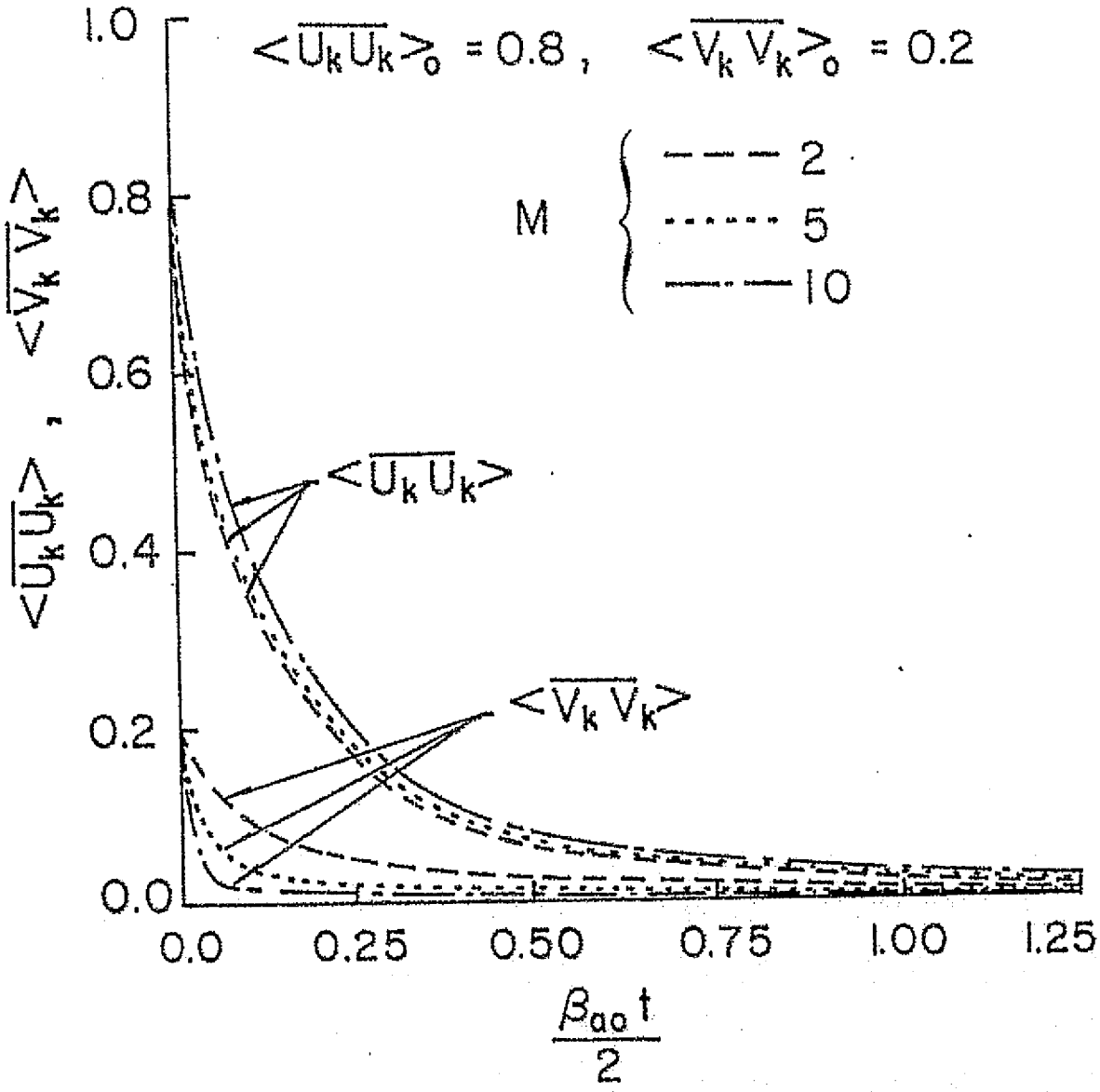


Figure 4 Decay of $\langle\overline{U_k U_k}\rangle$ and $\langle\overline{V_k V_k}\rangle$ with initial conditions $\langle\overline{U_k U_k}\rangle_o = 0.8$ $\langle\overline{V_k V_k}\rangle_o = 0.2$.

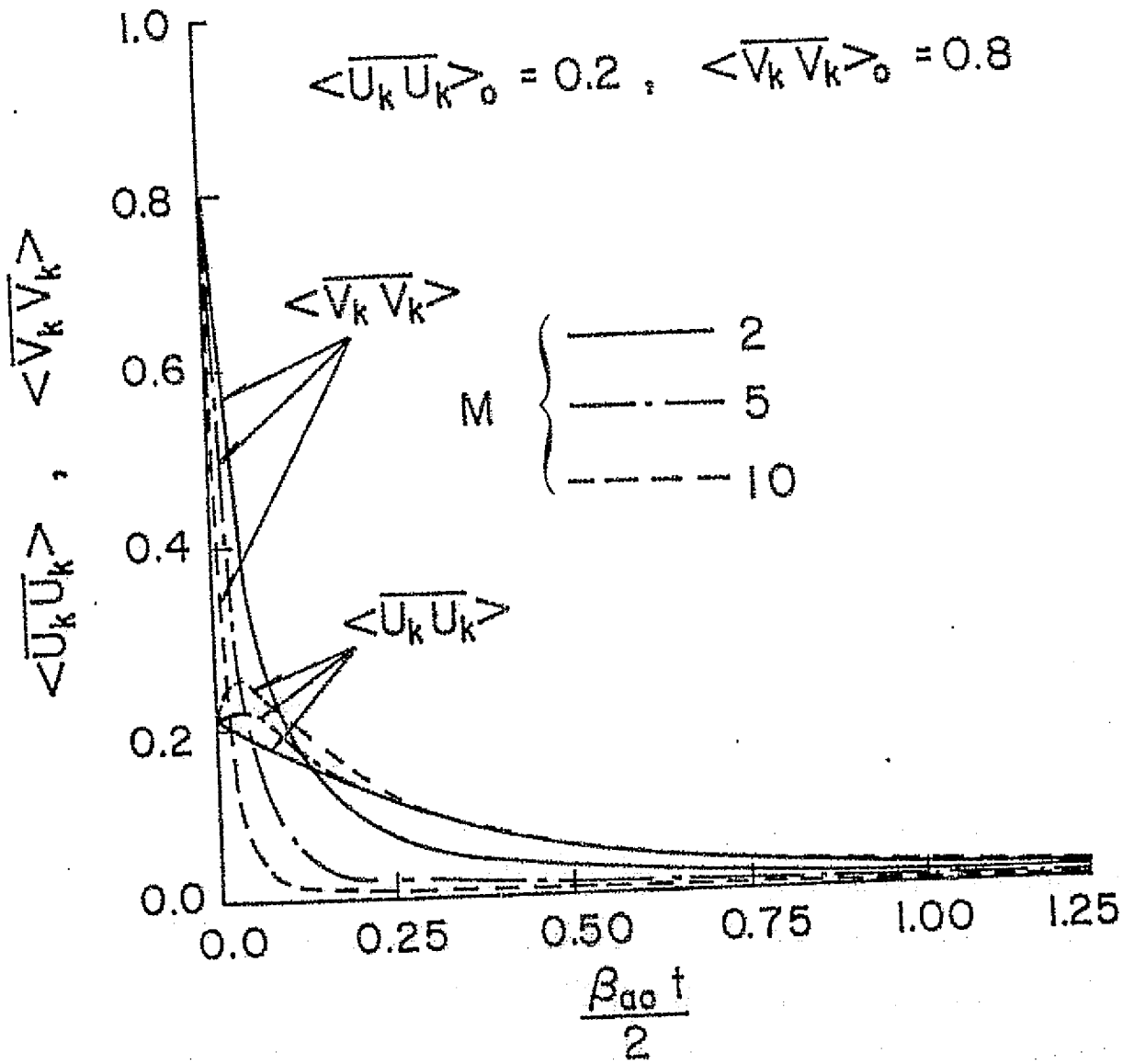


Figure 5 Decay of $\langle\overline{U_k U_k}\rangle$ and $\langle\overline{V_k V_k}\rangle$ with initial conditions $\langle\overline{U_k U_k}\rangle_o = 0.2$, $\langle\overline{V_k V_k}\rangle_o = 0.8$.

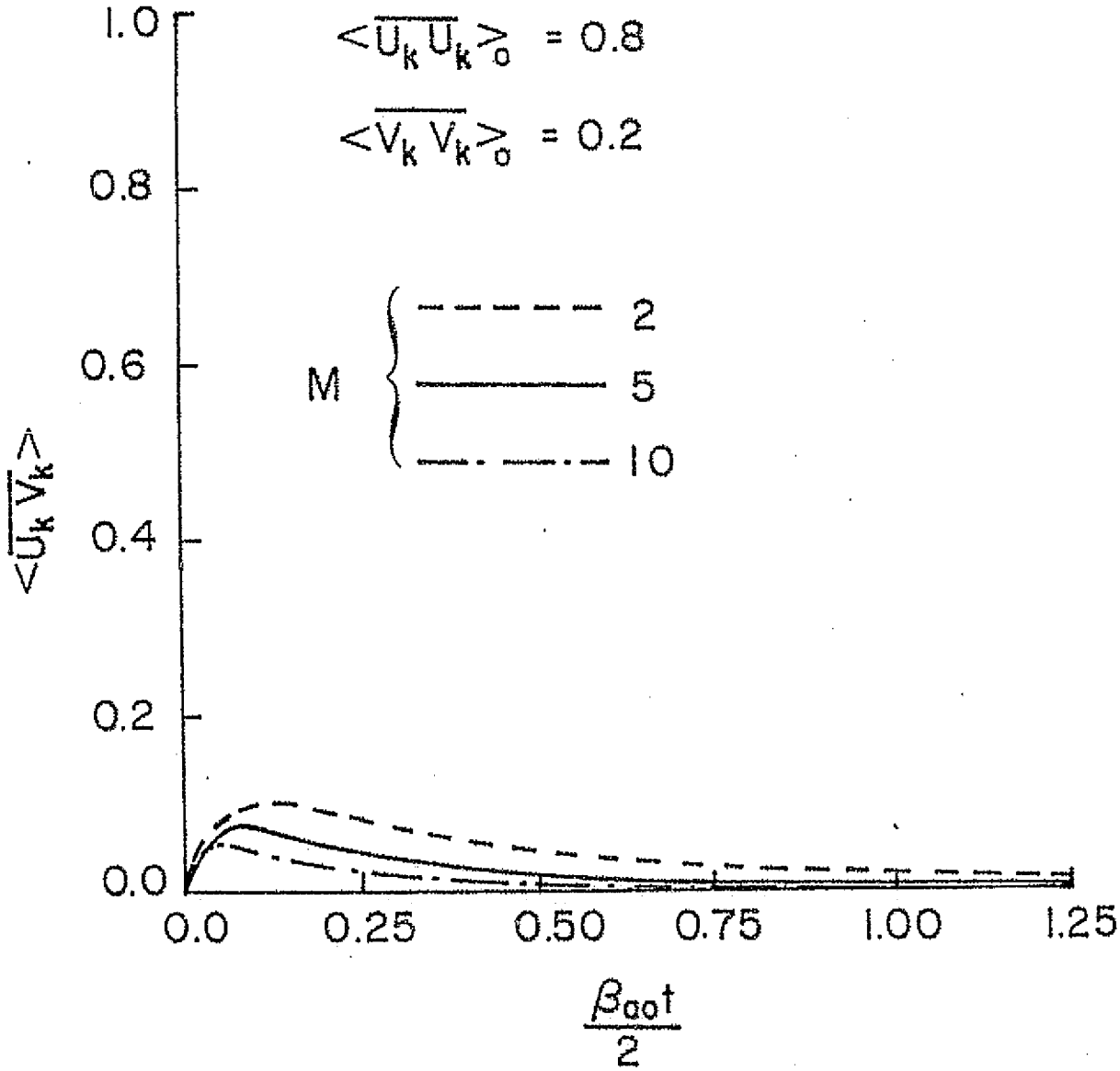


Figure 6 The behavior of the normalized interacting turbulence energy $\langle \overline{U_k V_k} \rangle$ with the initial conditions of $\langle \overline{U_k U_k} \rangle_o = 0.8$, $\langle \overline{V_k V_k} \rangle_o = 0.2$.

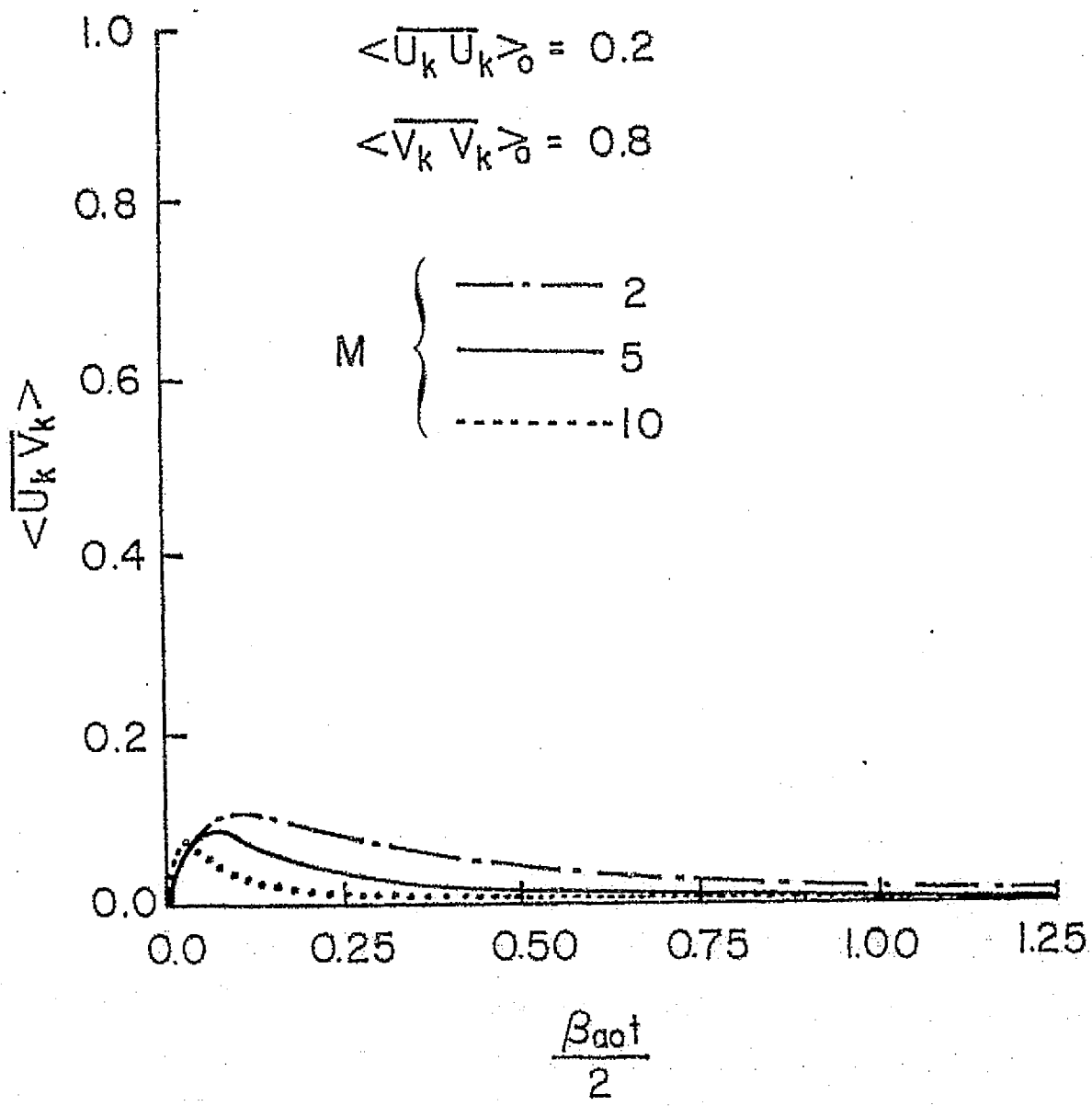


Figure 7 The behavior of the normalized interaction turbulence energy $\langle\overline{U_k V_k}\rangle$ with the initial conditions of $\langle\overline{V_k V_k}\rangle_o = 0.2$, $\langle\overline{U_k U_k}\rangle_o = 0.8$.

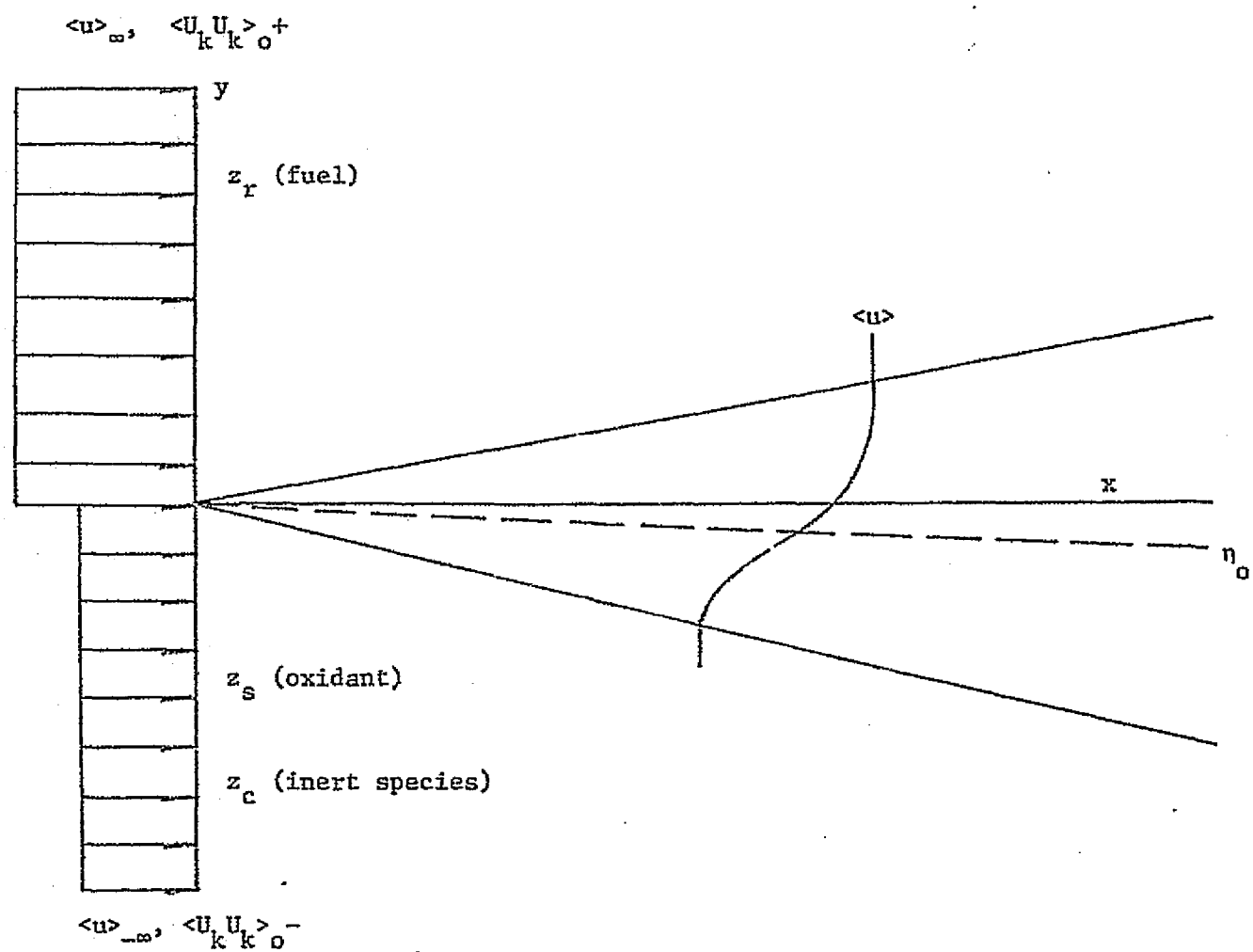


Figure 8 Two-Dimensional turbulent shear flow

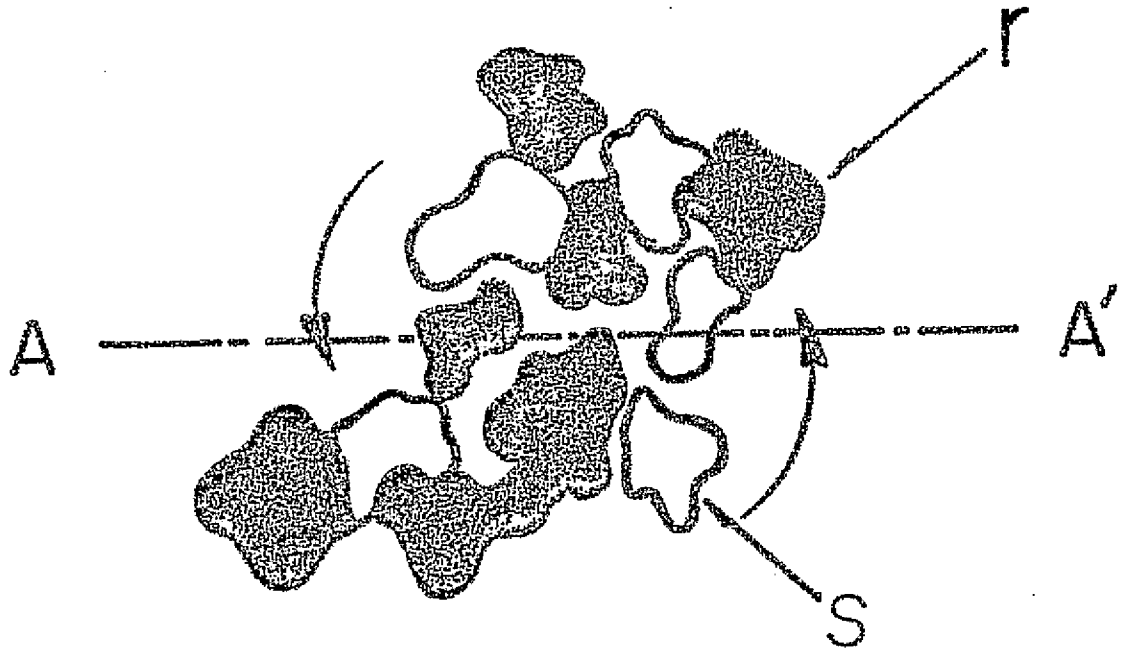
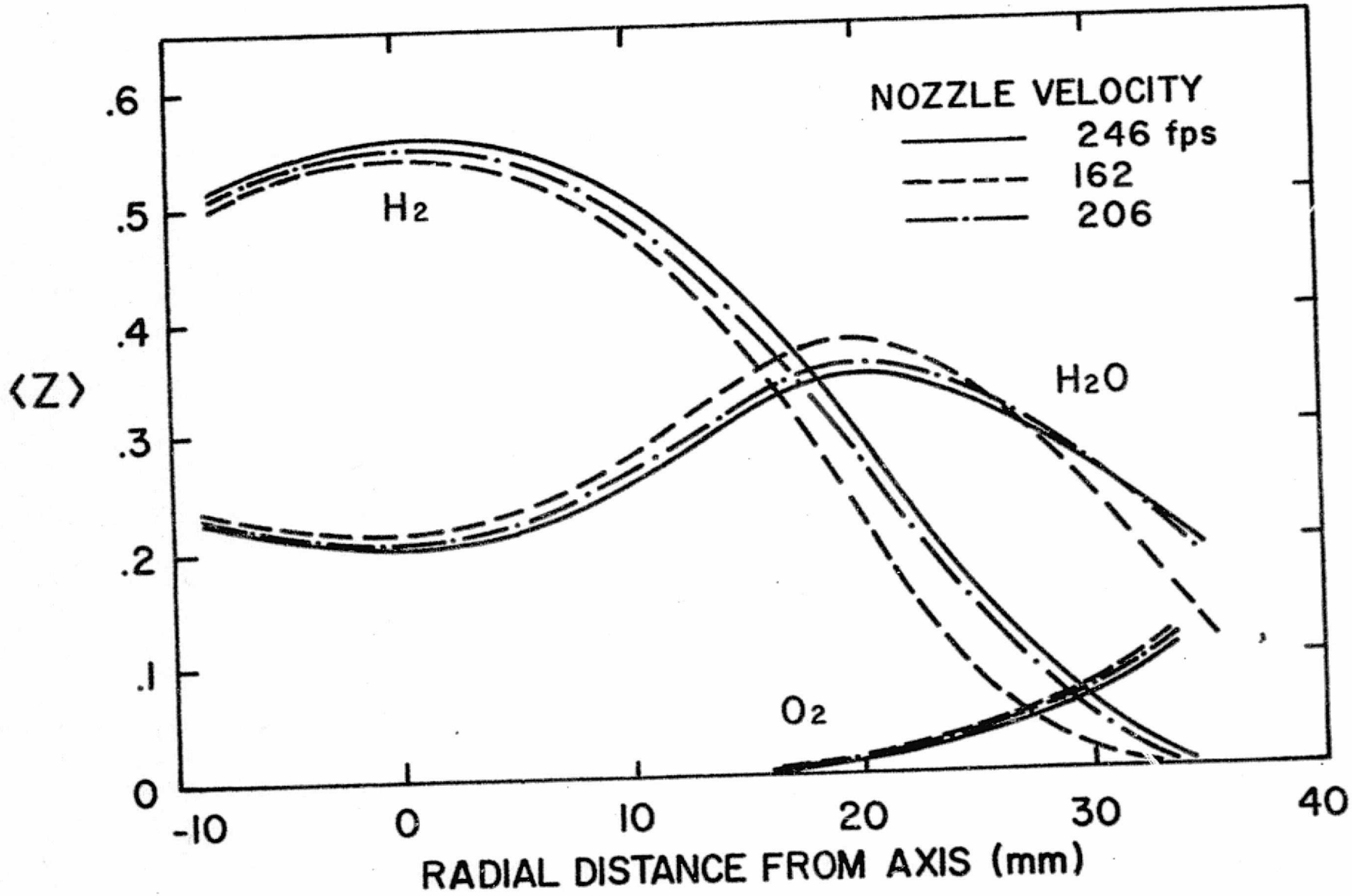


Figure 9 Turbulent mixing of fluid elements with different chemical species


NOZZLE VELOCITY
246 fps
162
206
H2
H2O
O2
⟨Z⟩
.6
.5
.4
.3
.2
.1
0
-10
0
10
20
30
40
RADIAL DISTANCE FROM AXIS (mm)

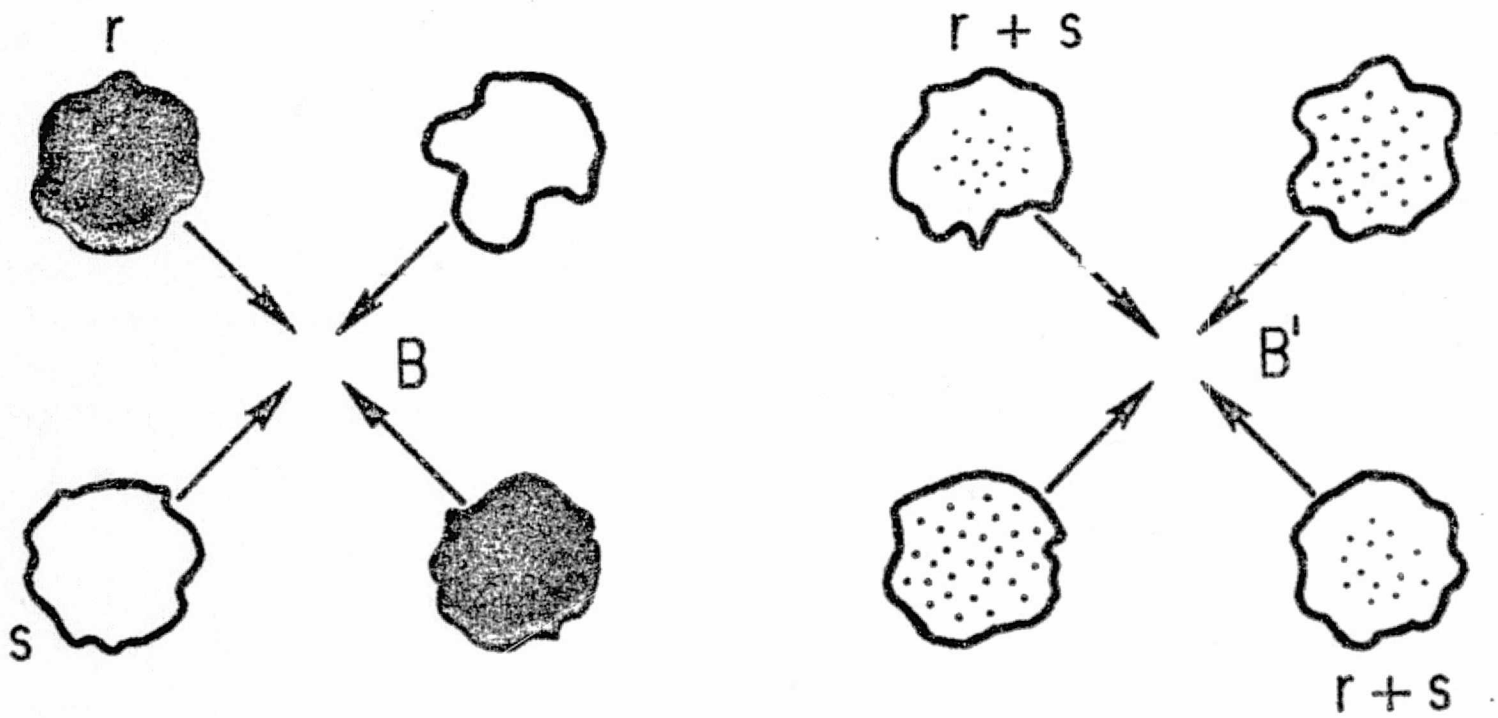


Figure 11 Chemical species, r and s, observed at two different points, B and B'

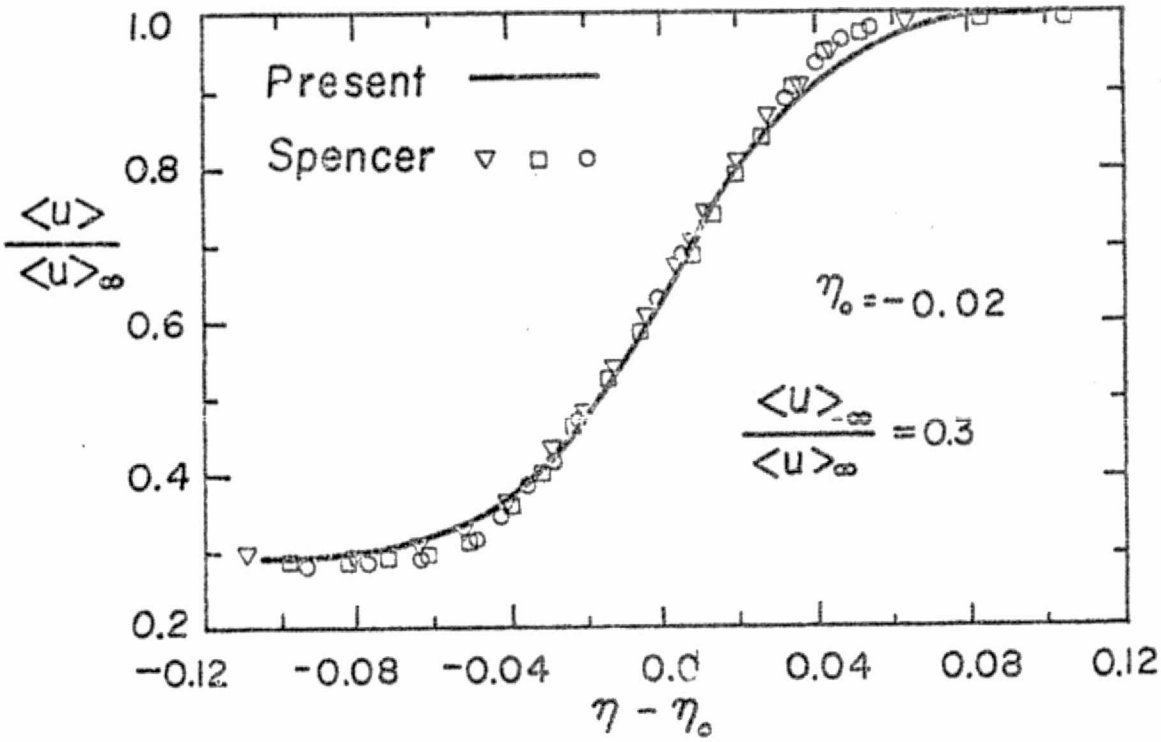


Figure 12 Averaged-velocity profile for plane free shear layer, $\eta = y/x$. η_o = dividing streamline. Present solution compared with the experimental data of Spencer (1970).

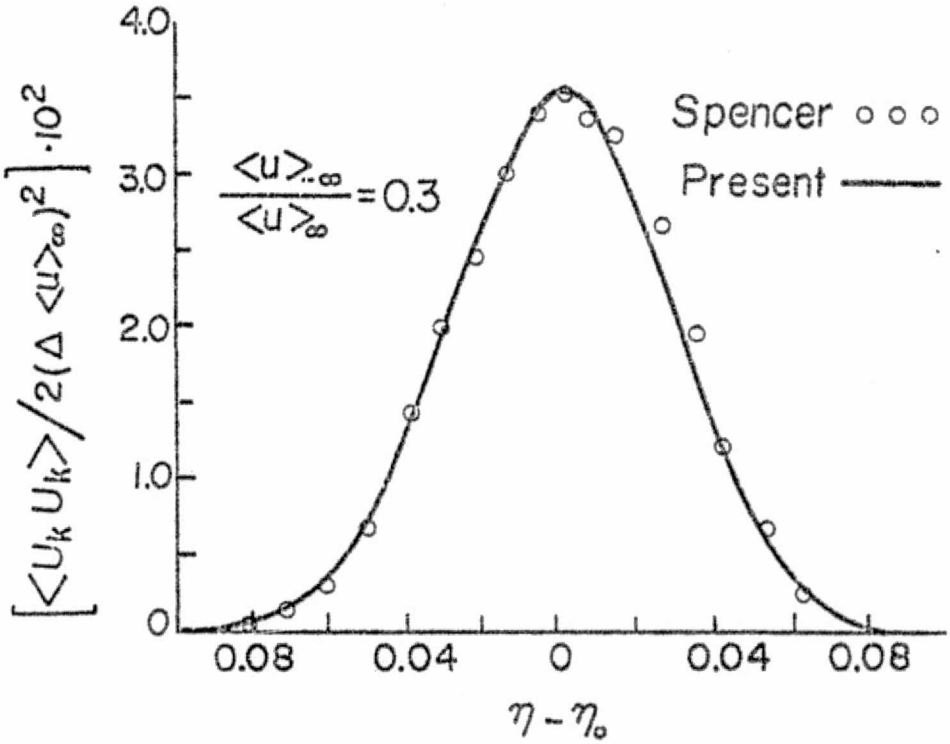


Figure 13 Turbulent-energy profile for plane free shear layer. $\Delta\langle u \rangle_\infty = \langle u \rangle_\infty - \langle u \rangle_{-\infty}$, $\eta_o = -.02$. Present solution compared with the experimental data of Spencer (1970).

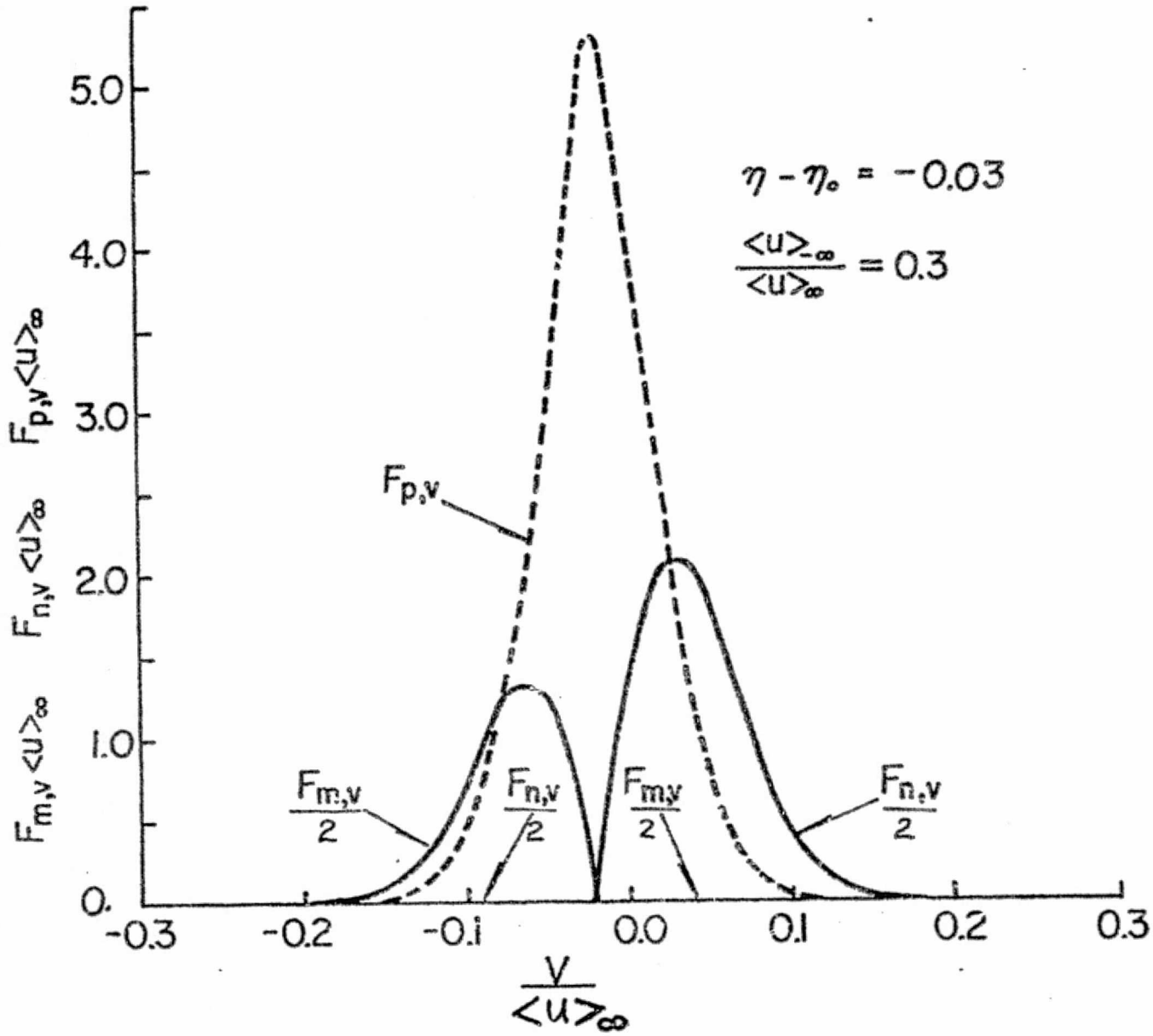


Figure 14 Distribution function at $\eta - \eta_o = -0.03$, of fuel (m), oxidant (n), and combustion product (p), normalized by $\langle u \rangle_\infty$.

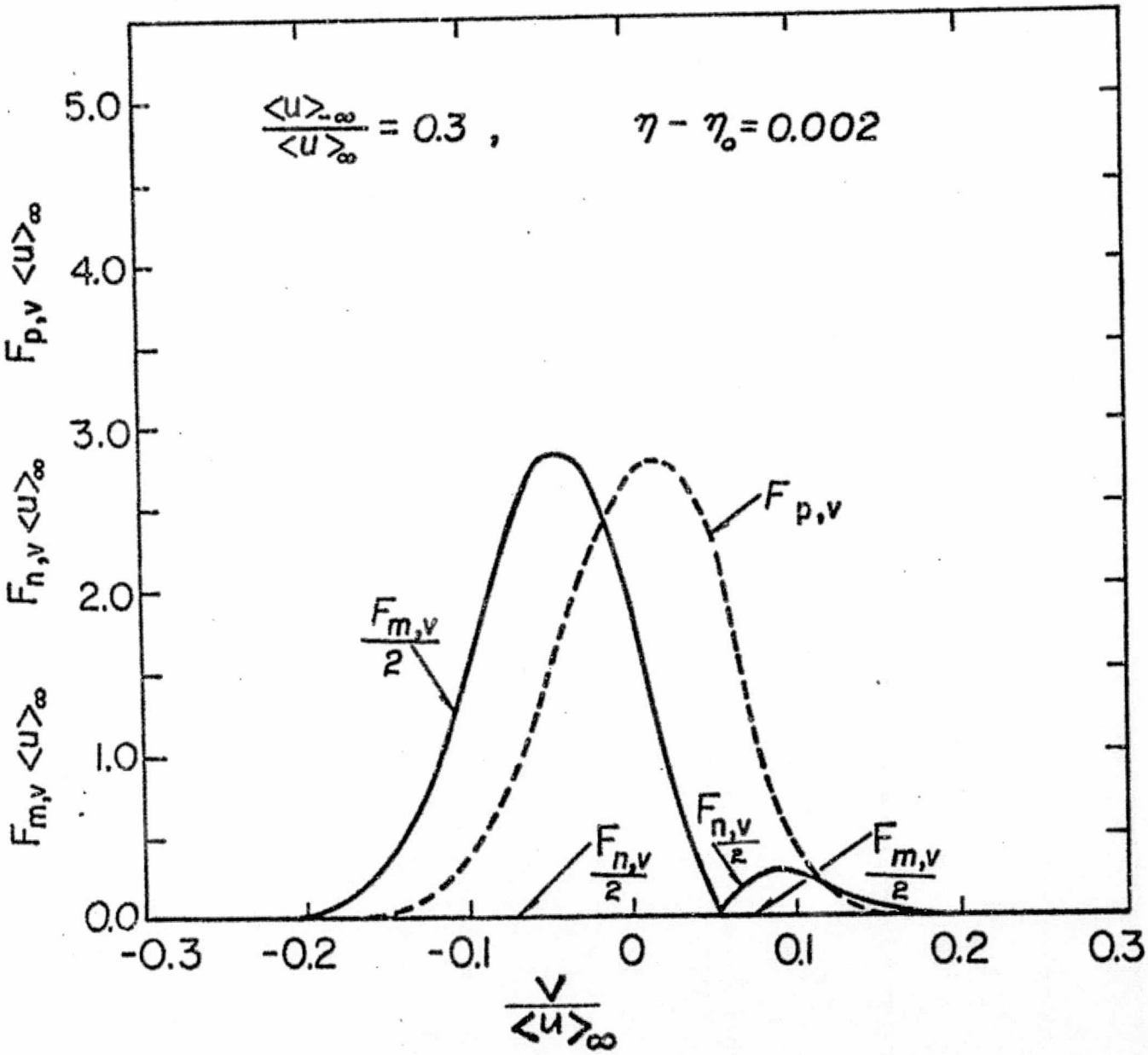


Figure 15 Distribution function at $\eta - \eta_o = 0.002$, of fuel (m), oxidant (n), and combustion product (p), normalized by $\langle u\rangle_\infty$.

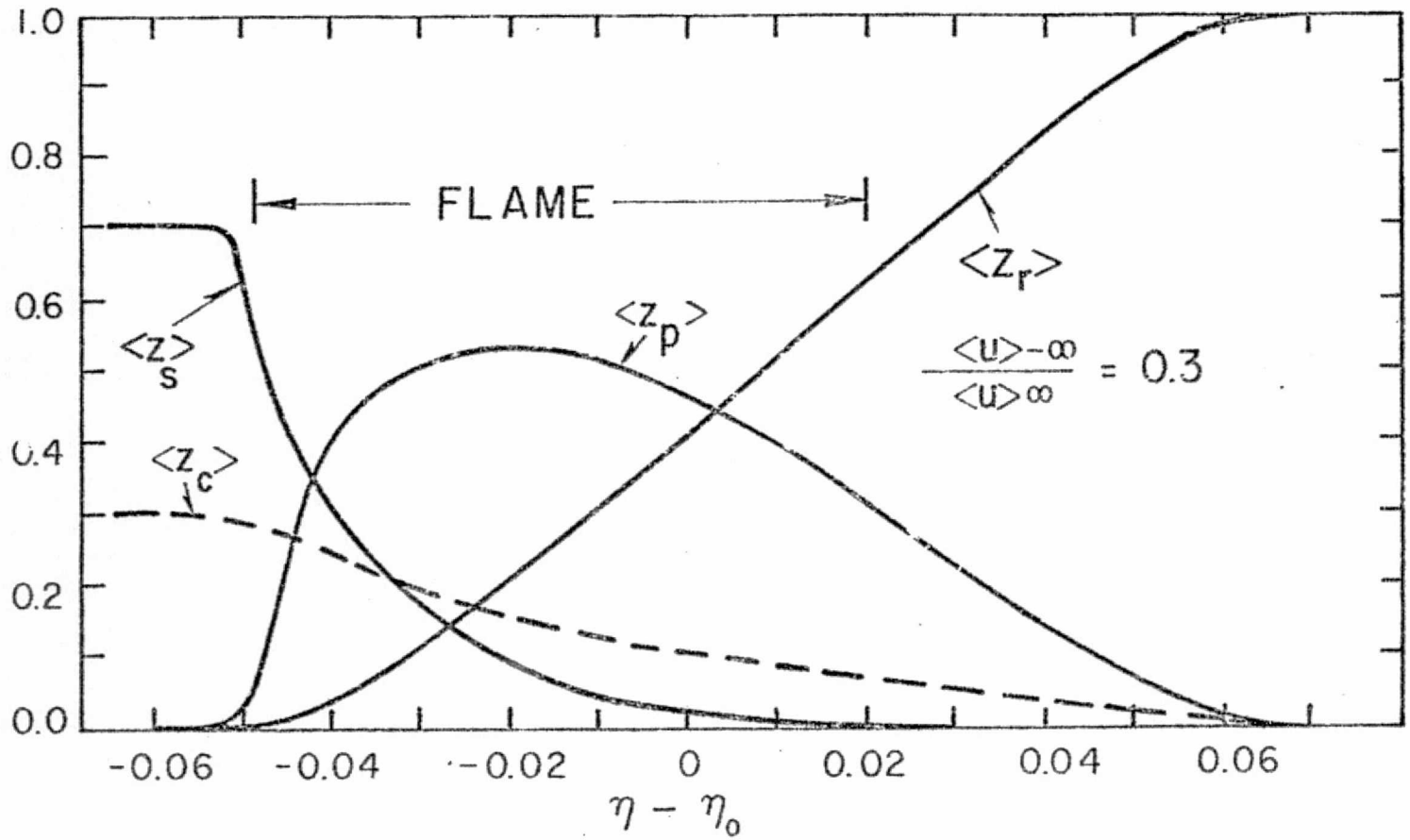


Figure 16 Equilibrium diffusion flame structure across the plane shear layer.

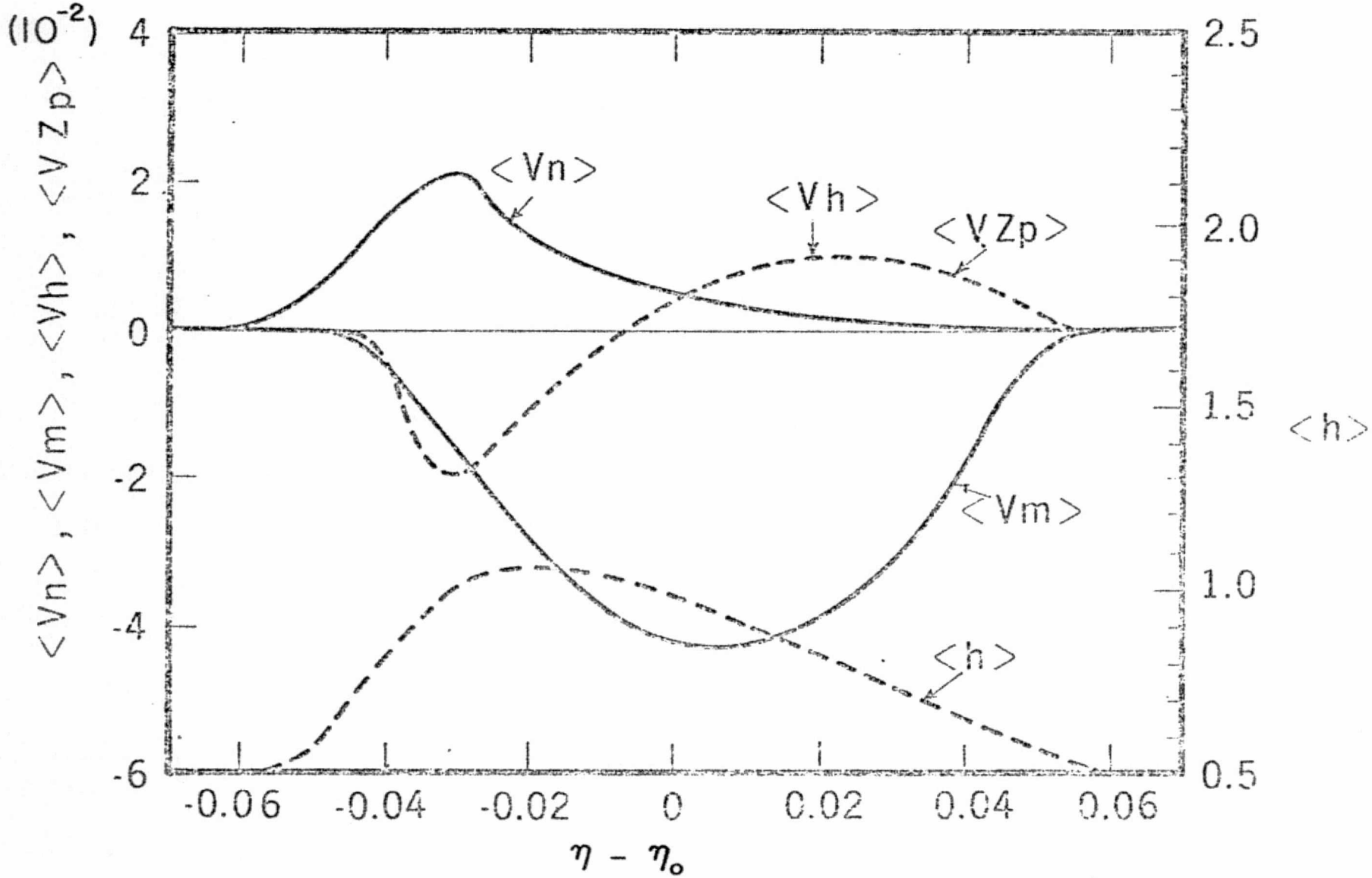


Figure 17 Averaged vertical turbulent transport of fuel, oxidant and combustion product, and the mean temperature <h> profile across the plane shear layer. V is normalized by $\langle u \rangle_\infty$.

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APPENDIX I

Changes of Independent Variables of f_2

The following chain rules are employed in order to change the independent variables from $f_2(\vec{U},\vec{V},\vec{x},t)$ to $f_2(\vec{u},\vec{v},\vec{x},t)$.

$$(\vec{U},\vec{V},\vec{x},t) \longrightarrow (\vec{u},\vec{x},\vec{v},t) \tag{AI-1}$$

$$\left(\frac{\partial}{\partial t}\right)_{\vec{U},\vec{V},\vec{x}} = \left(\frac{\partial}{\partial u_k}\right)_{\vec{v},\vec{x},t}\left(\frac{\partial u_k}{\partial t}\right)_{\vec{U},\vec{V},\vec{x}} + \left(\frac{\partial}{\partial v_k}\right)_{\vec{u},\vec{x},t}\left(\frac{\partial v_k}{\partial t}\right)_{\vec{U},\vec{V},\vec{x}} + \left(\frac{\partial}{\partial t}\right)_{\vec{u},\vec{v},t} \tag{AI-2}$$

$$\left(\frac{\partial}{\partial x_j}\right)_{\vec{U},\vec{V},t} = \left(\frac{\partial}{\partial u_k}\right)_{\vec{v},\vec{x},t}\left(\frac{\partial u_k}{\partial x_j}\right)_{\vec{U},\vec{V},t} + \left(\frac{\partial}{\partial v_k}\right)_{\vec{u},\vec{x},t}\left(\frac{\partial v_k}{\partial x_j}\right)_{\vec{U},\vec{V},t} + \left(\frac{\partial}{\partial x_j}\right)_{\vec{u},\vec{v},t} \tag{AI-3}$$

$$\left(\frac{\partial}{\partial U_j}\right)_{\vec{V},\vec{x},t} = \left(\frac{\partial}{\partial u_k}\right)_{\vec{v},\vec{x},t}\left(\frac{\partial u_k}{\partial U_j}\right)_{\vec{V},\vec{x},t} + \left(\frac{\partial}{\partial v_k}\right)_{\vec{u},\vec{x},t}\cancelto{0}{\left(\frac{\partial v_k}{\partial U_j}\right)_{\vec{V},\vec{x},t}} \tag{AI-4}$$

$$\left(\frac{\partial}{\partial V_j}\right)_{\vec{U},\vec{x},t} = \left(\frac{\partial}{\partial v_k}\right)_{\vec{v},\vec{x},t}\left(\frac{\partial v_k}{\partial V_j}\right)_{\vec{U},\vec{x},t} + \left(\frac{\partial}{\partial u_k}\right)_{\vec{u},\vec{x},t}\cancelto{0}{\left(\frac{\partial u_k}{\partial V_j}\right)_{\vec{U},\vec{x},t}} \tag{AI-5}$$

It should be noted that

$$\begin{aligned} \langle u\rangle_i &= \iint u_i f_2 d\vec{u}d\vec{v} \\ \langle v\rangle_i &= \iint v_i f_2 d\vec{u}d\vec{v} \end{aligned} \tag{AI-6}$$

$$U_i = u_i - \langle u_i \rangle \quad , \qquad V_i = v_i - \langle v_i \rangle \tag{AI-7}$$

Since f_2 is a function of $\vec{x}$ and t as well as $\vec{u}$ and $\vec{v}$, the integrals in Eqs. (AI-6) and, hence, $\langle u \rangle_i$ and $\langle v \rangle_i$, are also functions of $\vec{x}$ and t. Obviously from Eq. (AI-7), it also shows that u_i and v_i are functions of $\vec{x}$ and t, because of $\langle u \rangle_j$ and $\langle v \rangle_j$.

By employing (AI-7) we also see that

$$\left(\frac{\partial u_k}{\partial t}\right)_{\vec{U},\vec{V},\vec{x}} = \frac{\partial}{\partial t}\left[U_k + \langle u \rangle_k\right]_{\vec{U},\vec{V},\vec{x}} = \frac{\partial \langle u \rangle_k}{\partial t}$$

Similarly,

$$\left(\frac{\partial v_k}{\partial t}\right)_{\vec{U},\vec{V},\vec{x}} = \frac{\partial \langle v \rangle_k}{\partial t}$$

and

$$\left(\frac{\partial u_k}{\partial x_i}\right)_{\vec{U},\vec{V},t} = \frac{\partial}{\partial x_i}\left[U_k + \langle u \rangle_k\right]_{\vec{U},\vec{V},t} = \frac{\partial \langle u \rangle_k}{\partial x_i}$$

$$\left(\frac{\partial v_k}{\partial x_i}\right)_{\vec{U},\vec{V},t} = \frac{\partial \langle v \rangle_k}{\partial x_i}$$

$$\frac{\partial u_k}{\partial U_j} = \delta_{kj}$$

$$\frac{\partial v_k}{\partial V_j} = \delta_{kj}$$

$$\frac{\partial x_k}{\partial x_i} = \delta_{ki}$$

With the above expressions, those for the derivatives finally become:

$$\left(\frac{\partial}{\partial t}\right)_{\vec{x},\vec{U},\vec{V}} = \left(\frac{\partial}{\partial t}\right)_{\vec{x},\vec{u},\vec{v}} + \frac{\partial \langle u\rangle_k}{\partial t}\left(\frac{\partial}{\partial u_k}\right)_{t,\vec{x},\vec{v}} + \frac{\partial \langle v\rangle_k}{\partial t}\left(\frac{\partial}{\partial v_k}\right)_{t,\vec{x},\vec{u}}$$

$$\left(\frac{\partial}{\partial x_i}\right)_{t,\vec{U},\vec{V}} = \left(\frac{\partial}{\partial x_i}\right)_{t,\vec{u},\vec{v}} + \frac{\partial \langle u\rangle_k}{\partial x_i}\left(\frac{\partial}{\partial u_k}\right)_{t,\vec{x},\vec{v}} + \frac{\partial \langle v\rangle_k}{\partial x_i}\left(\frac{\partial}{\partial v_k}\right)_{t,\vec{x},\vec{u}}$$

$$\left(\frac{\partial}{\partial U_i}\right)_{t,\vec{x},\vec{V}} = \left(\frac{\partial}{\partial u_i}\right)_{t,\vec{x},\vec{v}}$$

$$\left(\frac{\partial}{\partial V_i}\right)_{t,\vec{x},\vec{U}} = \left(\frac{\partial}{\partial v_i}\right)_{t,\vec{x},\vec{u}} \qquad \text{(AI-10)}$$

Second order terms follow in a straightforward manner from the last two terms. Using (AI-10), Eq. (III-1) was changed to Eq. (IV-21).

APPENDIX II

Verification of the Transformation from Eqs. (IV-21) to (IV-28)

From Eq. (III-23) we have

$$\frac{\partial f_2(\vec{u},\vec{v},\vec{x},t)}{\partial t} = e^{B_c t} \frac{\partial \bar{f}_2(\vec{u},\vec{v},\vec{x},t)}{\partial t}$$

$$+ \quad B_c \, e^{B_c t} \, \bar{f}_2(\vec{u},\vec{v},\vec{x},t)$$

$$\frac{\partial f_2}{\partial u_j} = e^{B_c t} \frac{\partial \bar{f}_2}{\partial u_j} , \qquad \frac{\partial^2 f_2}{\partial u_j \partial u_j} = e^{B_c t} \frac{\partial \bar{f}_2}{\partial u_j \partial u_j} \tag{AII-1}$$

$$\frac{\partial f_2}{\partial v_j} = e^{B_c t} \frac{\partial \bar{f}_2}{\partial v_j} , \qquad \frac{\partial^2 f_2}{\partial v_j \partial v_j} = e^{B_c t} \frac{\partial \bar{f}_2}{\partial v_j \partial v_j}$$

$$\frac{\partial^2 f_2}{\partial u_j \partial v_j} = e^{B_c t} \frac{\partial^2 \bar{f}_2}{\partial u_j \partial v_j}$$

By using relation (IV-23) and (AII-1), Eq. (III-21) becomes

$$e^{B_c t}\frac{\partial \bar{f}_2}{\partial t} + B_c e^{B_c t}\,\bar{f}_2(\vec{u},\vec{v},\vec{x},t) + e^{B_c t}(k_{a,j} - B_a u_j)\frac{\partial \bar{f}_2}{\partial u_j}$$

$$+ e^{B_c t}(k_{b,j} - B_b v_j)\frac{\partial \bar{f}_2}{\partial v_j} + u_j\frac{\partial \bar{f}_2}{\partial x_j} + v_j\frac{\partial \bar{f}_2}{\partial x_j}\,e^{B_c t}$$

$$= B_c e^{B_c t}\,\bar{f}_2 + q\left(\frac{\partial^2}{\partial u_j \partial u_j} + 2\frac{\partial^2}{\partial u_j \partial v_j} + \frac{\partial^2}{\partial v_j \partial v_j}\right)\bar{f}_2\;e^{B_c t} \tag{AII-2}$$

By canceling $e^{B_c t}(e^{B_c t} \neq 0)$ and the common term $B_c e^{B_c t}\bar{f}_2$ on both sides of the equal sign, Eq. (AII-2) reads:

$$\frac{\partial \bar{f}_2}{\partial t} + (k_{a,j} + B_a u_j)\frac{\partial \bar{f}_2}{\partial u_j} + (k_{b,j} - B_b v_j)\frac{\partial \bar{f}_2}{\partial v_j} + (u_j + v_j)\frac{\partial \bar{f}_2}{\partial x_j}$$

$$= q\left(\frac{\partial^2}{\partial u_j \partial u_j} + 2\frac{\partial^2}{\partial u_j \partial v_j} + \frac{\partial^2}{\partial v_j \partial v_j}\right)\bar{f}_2 \tag{AII-3}$$

Now, we will use relation (IV-26) to change Eq. (AII-3) into Eq. (IV-28). Obviously, we are making the transformation $\bar{f}_2(\vec{u},\vec{v},\vec{x},t) \rightarrow \bar{f}_2(\vec{T}_a,\vec{T}_b,\vec{R},t)$, which we shall designate as Eq. (AII-4)

Chain rules of changes of variables are as follows:

$$\frac{\partial}{\partial u_i} = \frac{\partial}{\partial T_{a,j}} \frac{\partial T_{a,j}}{\partial u_i} + \frac{\partial}{\partial T_{b,j}} \frac{\partial T_{b,j}}{\partial u_j} + \frac{\partial}{\partial R_j} \frac{\partial R_j}{\partial u_i}$$

$$\frac{\partial}{\partial v_i} = \frac{\partial}{\partial T_{a,j}} \frac{\partial T_{a,j}}{\partial v_i} + \frac{\partial}{\partial T_{b,j}} \frac{\partial T_{b,j}}{\partial v_i} + \frac{\partial}{\partial R_j} \frac{\partial R_j}{\partial v_i}$$

$$\frac{\partial}{\partial x_i} = \frac{\partial}{\partial T_{a,j}} \frac{\partial T_{a,j}}{\partial x_i} + \frac{\partial}{\partial T_{b,j}} \frac{\partial T_{b,j}}{\partial x_i} + \frac{\partial}{\partial R_j} \frac{\partial R_j}{\partial x_i} \qquad \text{(AII-5)}$$

$$\frac{\partial}{\partial t} = \frac{\partial}{\partial T_{a,j}} \frac{\partial T_{a,j}}{\partial t} + \frac{\partial}{\partial T_{b,j}} \frac{\partial T_{b,j}}{\partial t} + \frac{\partial}{\partial R_j} \frac{\partial R_j}{\partial t} + \frac{\partial}{\partial t}$$

We see from Eq. (IV-26) that we have

$$\frac{\partial T_{a,j}}{\partial u_j} = e^{B_a t} \quad , \quad \frac{\partial T_{a,j}}{\partial v_j} = 0 \quad , \quad \frac{\partial T_{a,j}}{\partial t} = B_a u_j - \frac{k_{a,j}}{B_a} \cdot e^{B_a t}$$

$$\frac{\partial T_{b,j}}{\partial u_j} = 0 \quad , \quad \frac{\partial T_{b,j}}{\partial v_j} = e^{B_b t} \quad , \quad \frac{\partial T_{b,j}}{\partial t} = B_b v_j - \frac{k_{b,j}}{B_b} e^{B_b t}$$

$$\frac{\partial T_{a,j}}{\partial x_j} = 0 \quad , \quad \frac{\partial T_{b,j}}{\partial x_j} = 0 \quad , \quad \frac{\partial R_j}{\partial u_j} = \frac{1}{B_a} \quad , \quad \frac{\partial R_j}{\partial v_j} = \frac{1}{B_b} \quad ,$$

$$\frac{\partial R_j}{\partial t} = -\left(\frac{k_{a,j}}{B_a} + \frac{k_{b,j}}{B_b}\right) \qquad \text{(AII-5a)}$$

With the aid of Eq. (AII-5), the left hand side of Eq. (AII-3) can be written as,

$$\frac{\partial \bar{f}_2(\vec{T}_a,\vec{T}_b,\vec{R},t)}{\partial t} + \frac{\partial \bar{f}_2}{\partial T_{a,j}}\left[\frac{\partial T_{a,j}}{\partial t} + (u_i + v_i)\frac{\partial T_{a,j}}{\partial x_i}\right]$$

$$+ \frac{\partial \bar{f}_2}{\partial T_{b,j}}\left[\frac{\partial T_{b,j}}{\partial t} + (u_i + v_i)\frac{\partial T_{b,j}}{\partial x_i}\right.$$

$$\left. + (k_{a,i} - B_a u_i)\frac{\partial T_{b,j}}{\partial u_i} + (k_{b,i} - B_b v_i)\frac{\partial T_{b,j}}{\partial v_i}\right]$$

$$+ \frac{\partial \bar{f}_2}{\partial R_j}\left[\frac{\partial R_j}{\partial t} + (u_i + v_i)\frac{\partial R_j}{\partial x_i} + (k_{a,i} - B_a u_i)\frac{\partial R_j}{\partial u_i}\right.$$

$$\left. + (k_{b,i} - B_b v_i)\frac{\partial R_j}{\partial v_i}\right]$$

Substituting Eq. (AII-5a) into the above, we have,

$$\frac{\partial \bar{f}_2(\vec{T}_a,\vec{T}_b,\vec{R},t)}{\partial t} + \frac{\partial \bar{f}_2}{\partial T_{a,j}}(0) + \frac{\partial \bar{f}_2}{\partial T_{b,j}}(0) + \frac{\partial \bar{f}_2}{\partial R_j}(0)$$

$$= \frac{\partial \bar{f}_2(\vec{T}_a,\vec{T}_b,\vec{R},t)}{\partial t} \qquad \text{(AII-6)}$$

Now we look at the right hand side of Eq. (AII-3).

$$\frac{\partial^2}{\partial u_j \partial u_j} = \left[\left(\frac{\partial}{\partial T_{a,i}}\right)\left(\frac{\partial T_{a,i}}{\partial u_j}\right) + \left(\frac{\partial}{\partial T_{b,i}}\right)\left(\frac{\partial T_{b,i}}{\partial u_j}\right) + \left(\frac{\partial}{\partial R_i}\right)\left(\frac{\partial R_i}{\partial u_j}\right)\right]$$

$$\times \left[\left(\frac{\partial}{\partial T_{a,k}}\right)\left(\frac{\partial T_{a,k}}{\partial u_j}\right) + \left(\frac{\partial}{\partial T_{b,k}}\right)\left(\frac{\partial T_{b,k}}{\partial u_j}\right) + \left(\frac{\partial}{\partial R_k}\right)\left(\frac{\partial R_k}{\partial u_j}\right)\right]$$

$$\frac{\partial^2}{\partial u_j \partial v_j} = \left[\left(\frac{\partial}{\partial T_{a,i}}\right)\left(\frac{\partial T_{a,i}}{\partial u_j}\right) + \left(\frac{\partial}{\partial T_{b,i}}\right)\left(\frac{\partial T_{b,i}}{\partial u_j}\right) + \left(\frac{\partial}{\partial R_i}\right)\left(\frac{\partial R_i}{\partial u_j}\right)\right]$$

$$\times \left[\left(\frac{\partial}{\partial T_{a,k}}\right)\left(\frac{\partial T_{a,k}}{\partial v_j}\right) + \left(\frac{\partial}{\partial T_{b,k}}\right)\left(\frac{\partial T_{b,k}}{\partial v_j}\right) + \left(\frac{\partial}{\partial R_k}\right)\left(\frac{\partial R_k}{\partial v_j}\right)\right] \qquad \text{(AII-7)}$$

$$\frac{\partial^2}{\partial v_j \partial v_j} = \left[\left(\frac{\partial}{\partial T_{a,i}}\right)\left(\frac{\partial T_{a,i}}{\partial v_j}\right) + \left(\frac{\partial}{\partial T_{b,i}}\right)\frac{\partial T_{b,i}}{\partial v_j}\right) + \left(\frac{\partial}{\partial R_i}\right)\left(\frac{\partial R_i}{\partial v_j}\right)\right]$$

$$\times \left[\left(\frac{\partial}{\partial T_{a,k}}\right)\left(\frac{\partial T_{a,k}}{\partial v_j}\right) + \left(\frac{\partial}{\partial T_{b,k}}\right)\left(\frac{\partial T_{b,k}}{\partial v_j}\right) + \left(\frac{\partial}{\partial R_k}\right)\left(\frac{\partial R_k}{\partial v_j}\right)\right]$$

If we substitute Eq. (AII-5a) into Eq. (AII-7), and after minor manipulation, Eq. (AII-7) becomes

$$\frac{\partial^2}{\partial u_j \partial u_j} = e^{2B_a t}\left(\frac{\partial^2}{\partial T_{a,j}\partial T_{a,j}}\right) + \frac{e^{B_a t}}{B_a}\left(\frac{\partial^2}{\partial T_{a,j}\partial R_j}\right) + \frac{1}{B_a^2}\left(\frac{\partial^2}{\partial R_j \partial R_j}\right)$$

$$\frac{\partial^2}{\partial u_j \partial v_j} = e^{(B_a+B_b)t}\left(\frac{\partial^2}{\partial T_{a,j}\partial T_{b,j}}\right) + \left(\frac{\partial^2}{\partial R_j \partial T_{b,j}}\right)\frac{e^{B_b t}}{B_a} + \left(\frac{1}{B_a} + \frac{1}{B_b}\right)\left(\frac{\partial^2}{\partial R_j \partial R_j}\right)$$

$$\frac{\partial^2}{\partial v_j \partial v_j} = e^{2B_b t}\left(\frac{\partial^2}{\partial T_{b,j}\partial T_{b,j}}\right) + \frac{e^{B_b t}}{B_b}\left(\frac{\partial^2}{\partial T_{b,j}\partial R_j}\right) + \frac{1}{B_b^2}\left(\frac{\partial^2}{\partial R_j \partial R_j}\right) \qquad \text{(AII-8)}$$

By the aid of Eq. (AII-7) and Eq. (AII-8), the right hand side of Eq. (AII-3) is changed to the following:

$$q \left[a_2 \left(\frac{\partial^2}{\partial T_{a,j} \partial T_{a,j}} \right) + b_2 \left(\frac{\partial^2}{\partial T_{b,j} \partial T_{b,j}} \right) + c_2 \left(\frac{\partial^2}{\partial R_j \partial R_j} \right) + 2d_2 \left(\frac{\partial^2}{\partial T_{a,j} \partial T_{b,j}} \right) \right.$$

$$\left. + 2e_2 \left(\frac{\partial^2}{\partial T_{a,j} \partial R_j} \right) + 2g_2 \left(\frac{\partial^2}{\partial T_{b,j} \partial R_j} \right) \right] \bar{f}_2(\vec{T}_a, \vec{T}_b, \vec{R}, t) \tag{AII-9}$$

where

$$a_2 = e^{2(B_a t)} \quad , \qquad g_2 = \left(\frac{1}{B_a} + \frac{1}{B_b} \right) e^{B_b t}$$

$$b_2 = e^{2B_b t} \quad , \qquad e_2 = \left(\frac{1}{B_b} + \frac{1}{B_a} \right) e^{B_a t} \tag{AII-10}$$

$$c_2 = \left(\frac{1}{B_a} + \frac{1}{B_b} \right)^2 \quad , \qquad d_2 = e^{(B_a + B_b)t}$$

Finally, by putting Eq. (AII-6) and (AII-9) together we get:

$$\frac{\partial \bar{f}_2(\vec{T}_a, \vec{T}_b, \vec{R}, t)}{\partial t} = q \left[a_2 \frac{\partial^2}{\partial T_{a,j} \partial T_{a,j}} + b_2 \frac{\partial^2}{\partial T_{b,j} \partial T_{b,j}} + c_2 \frac{\partial^2}{\partial R_j \partial R_j} \right.$$

$$+ 2d_2 \frac{\partial^2}{\partial T_{a,j} \partial T_{b,j}} + 2e_2 \frac{\partial^2}{\partial T_{a,j} \partial R_j}$$

$$\left. + 2g_2 \frac{\partial^2}{\partial T_{b,j} \partial R_j} \right] \bar{f}_2(\vec{T}_a, \vec{T}_b, \vec{R}, t) \tag{AII-11}$$

which is exactly as Eq. (IV-28).

APPENDIX III

Verification of Lemma III and Lemma III-A

In reference (24) similar lower order mathematical lemmas were developed by Chandrasekhar. Both Lemma I and Lemma II were verified by substituting the solution into the original equations. In order to solve the present kinetic equations, the higher order extensions of these mathematical lemmas are needed. We shall derive Lemma III and Lemma III-A in a more direct manner with the purpose of generalizing the lemmas.

III.A. Verification of Lemma III

We begin with Eq. (L3-1),

$$\frac{\partial Y}{\partial t} = \phi_{11}(t)\frac{\partial^2 Y}{\partial x_1^2} + \phi_{22}(t)\frac{\partial^2 Y}{\partial x_2 \partial x_2} + \phi_{33}(t)\frac{\partial^2 Y}{\partial x_3 \partial x_3}$$

$$+ 2\phi_{12}(t)\frac{\partial^2 Y}{\partial x_1 \partial x_2} + 2\phi_{13}(t)\frac{\partial^2 Y}{\partial x_1 \partial x_3} + 2\phi_{23}(t)\frac{\partial^2 Y}{\partial x_2 \partial x_3} \qquad \text{(L-III-1)}$$

where $Y = Y(x_1, x_2, x_3, t)$.

We assume $Y(x_1, x_2, x_3, t)$ is piecewise differentiable and also

$$\iiint_{-\infty}^{\infty} |Y| \, dx_1 dx_2 dx_3 \qquad \text{(AIII-1)}$$

is finite.

For our interest, Y represents a probability density function, such as $\overline{F}_1$.

Due to the properties peculiar to the probability density function (distribution functions) such functions obviously satisfy condition (AIII-1) The convergence of the distribution function is well described in reference (36), Chapter 4. It is also obvious that the velocity probability density function which is the subject matter of our kinetic equation is continuous in phase space. Therefore, we may take a Fourier transform of this type of function. We make an integral transform of $Y(x_1,x_2,x_3,t)$ as

$$Y_3(\xi_1,\xi_2,\xi_3,t) = \iiint_{-\infty}^{\infty} Y(x\ t)e^{i(\xi_1x_1+\xi_2x_2+\xi_3x_3)}\, dx_1dx_2dx_3 \qquad \text{(AIII-2)}$$

where ξ_1, ξ_2, and ξ_3 are auxiliary variables in transformed space. By making this transformation, Eq. (L-III-1) becomes:

$$\frac{\partial Y_3}{\partial t} = -\left[\phi_{11}(t)\xi_1^2 + \phi_{22}(t)\xi_2^2 + \phi_{33}(t)\xi_3^2 + 2\xi_1\xi_2\phi_{12}(t) + 2\xi_1\xi_3\phi_{13}(t) + 2\xi_2\xi_3\phi_{23}(t)\right]\cdot Y_3 \qquad \text{(AIII-3)}$$

Solution of Eq. (AIII-3) is easily obtained as:

$$Y_3 = Y_{3o}\ \exp\left\{-\left(\begin{array}{l}\xi_1^2\int_{t_o}\phi_1(R)d\tau + \xi_2^2\int_{t_o}\phi_2(\tau)d\tau + \xi_3^2\int_{t_o}\phi_3(\tau)d\tau \\ + 2\xi_1\xi_2\int_{t_o}\phi_{12}(\tau)d\tau + 2\xi_1\xi_3\int_{t_o}\phi_{13}(\tau)d\tau \\ + 2\xi_2\xi_3\int_{t_o}\phi_{23}(\tau)d\tau\end{array}\right)\right\} \qquad \text{(AIII-4)}$$

where $Y_{3o} = Y_3(\xi_1,\xi_2,\xi_3,t)_{t=t_o}$.

We know from Eq. (L-III-1a) that $(Y)_{t=t_o}$ is a Dirac delta function, which is

$$(Y)_{t=t_o} = \delta(x_1 - x_{1o})\delta(x_2 - x_{2o})\delta(x_3 - x_{3o}) \qquad \text{(L-III-1a)}$$

With the aid of Eq. (AIII-2), Eq. (L-III-1a) becomes

$$Y_{3o} = \iiint_{-\infty}^{\infty} (Y)_{t=t_o} \, e^{i(\xi_1 x_1+\xi_2 x_2+\xi_3 x_3)} \, dx_1 dx_2 dx_3 \qquad \text{(AIII-5)}$$

Therefore,

$$Y_{3o} = e^{-i(\xi_1 x_{1o}+\xi_2 x_{2o}+\xi_3 x_{3o})} \qquad \text{(AIII-6)}$$

Substituting Eq. (AIII-6) into Eq. (AIII-4), and by taking an inverse integral transform of the resulting equation, we have (where $M_{ij} = \int_{t_o} \phi_{ij}(\tau)d\tau$ has been employed)

$$Y(x_1,x_2,x_3,t/x_{1o},x_{2o},x_{3o},t_o)$$

$$= \frac{1}{(2\pi)^3} \iiint_{-\infty}^{\infty} e^{-(M_{11}\xi_1^2+M_{22}\xi_2^2+M_{33}\xi_3^2+2M_{12}\xi_1\xi_2+2M_{13}\xi_1\xi_3+2M_{23}\xi_2\xi_3)}$$

$$\times \; e^{-i[\xi_1(x_1-x_{1o})+\xi_2(x_2-x_{2o})+\xi_3(x_3-x_{3o})]} \, d\xi_1 d\xi_2 d\xi_3 \qquad \text{(AIII-7)}$$

where Eq. (AIII-6) has also been employed. The right hand side of Eq. (AIII-7) can be readily evaluated. After some manipulation, there results,

$$Y(x_1,x_2,x_3,t/x_{1o},x_{2o},x_{3o},t_o) =$$

$$\frac{1}{(2\pi)^3}(\sqrt{\pi})^3 \exp\left[-\frac{\begin{array}{l}(x_1-x_{1o})^2(M_{22}M_{33}-M_{23}^2)+(x_2-x_{2o})^2(M_{11}M_{33}-M_{13}^2)\\ +(x_3-x_{3o})^2(M_{11}M_{22}-M_{12}^2)-2(x_1-x_{1o})(M_{23}M_{12}-M_{13}M_{23})\\ -2(x_1-x_{1o})(x_2-x_{2o})(M_{22}M_{13}-M_{12}M_{23})\\ -2(x_2-x_{2o})(x_3-x_{3o})(M_{11}M_{23}-\delta_{12}\delta_{13})\end{array}}{4(M_{11}M_{22}M_{33}+2M_{12}M_{13}M_{23}-M_{22}M_{13}^2-M_{11}M_{23}^2-M_{33}M_{12}^2)}\right]$$

$$\overline{(M_{11}M_{22}M_{33}+2M_{12}M_{13}M_{23}-M_{11}M_{23}^2-M_{22}M_{13}^2-M_{33}M_{12}^2)^{1/2}}$$

(AIII-8)

Equation (AIII-8) is already the solution of Eq. (L-III-1). It is our intention to find a formal solution of the general diffusion-type equation described earlier. We see from Eq. (AIII-8), that one may write

$$Y = \frac{1}{(2\pi)^{3/2}\Delta_3^{1/2}} \exp\left\{-\frac{\left[\begin{array}{l}\Delta_{11}(x_1-x_{1o})^2+\Delta_{22}(x_2-x_{2o})^2+\Delta_{33}(x_3-x_{3o})^2\\ +2\Delta_{12}(x_1-x_{1o})(x_2-x_{2o})+2\Delta_{13}(x_1-x_{1o})(x_3-x_{3o})\\ +2\Delta_{23}(x_2-x_{2o})(x_3-x_{3o})\end{array}\right]}{2\Delta_3}\right\}$$

(AIII-9)

where

$$\Delta_3 = 2^3 \, || M_{ij} ||$$

$|| M_{ij} ||$ is the determinant composed of M_{ij}

Δ_{ij} = the cofactor of $|| M_{ij} ||$ 2^3 for the ith row and the jth column element

III.B. Verification of Lemma-III-A

Lemma III is easily extended to Lemma-III-A. This is shown in the following. We first rewrite Eq. (L-III-6) as follows.

$$\begin{aligned}\frac{\partial Y_a(x_{1,j},x_{2,j},x_{3,j},t)}{\partial t} = {} & \phi_1(t)\frac{\partial^2 Y_a}{\partial x_{1,j}\partial x_{1,j}} + \phi_2(t)\frac{\partial^2 Y_a}{\partial x_{2,j}\partial x_{2,j}} \\ & + \phi_3(t)\frac{\partial^2 Y_a}{\partial x_{3,j}\partial x_{3,j}} + 2\phi_{12}(t)\frac{\partial^2 Y_a}{\partial x_{1,j}\partial_{2,j}} \\ & + 2\phi_{13}(t)\frac{\partial^2 Y_a}{\partial x_{1,j}\partial x_{3,j}} + 2\phi_{23}(t)\frac{\partial^2 Y_a}{\partial x_{2,j}\partial x_{3,j}}\end{aligned} \tag{L-III-6}$$

where j is the cartesian tensor index.

Again, we require that Y_a be at least piecewise differentiable and its integral be finite in all domains. Then we make an integral transform as,

$$Y_{3a} = \iiint_{-\infty}^{\infty} Y_a \, e^{-i(\xi_{1,k}x_{1,k}+\xi_{2,k}x_{2,k}+\xi_{3,k}x_{3,k})} \, d\vec{x}_1 d\vec{x}_2 d\vec{x}_3 \qquad \text{(AIII-10)}$$

By this transformation, Eq. (L-III-5) becomes

$$\frac{\partial Y_3(\vec{\xi}_1,\vec{\xi}_2,\vec{\xi}_3,t)}{\partial t} = -[\phi_1\xi_{1,j}\xi_{1,j} + \phi_2(t)\xi_{2,j}\xi_{2,j} + \phi_3(t)\xi_{3,j}\xi_{3,j}$$

$$+ 2\phi_{12}(t)\xi_{1,j}\xi_{2,j} + 2\phi_{13}(t)\xi_{1,j}\xi_{3,j} + 2\phi_{23}(t)\xi_{2,j}\xi_{3,j}]$$

(AIII-11)

where $j = 1, 2, 3$, and $\xi_{1,k}$, $\xi_{2,k}$, and $\xi_{3,k}$ are auxiliary variables.

The solution of Eq. (AIII-11) is readily obtained as,

$$Y_3(\vec{\xi}_1,\vec{\xi}_2,\vec{\xi}_3,t/\vec{\xi}_{1o},\vec{\xi}_{2o},\vec{\xi}_{3o},t_o)$$

$$= Y_{3o} \exp\left\{-\left[\xi_{1,j}\xi_{1,j}\int_{t_o}\phi_1(\tau)d\tau + \xi_{2,j}\xi_{2,j}\int_{t_o}\phi_2(\tau)d\tau\right.\right.$$

$$+ \xi_{3,j}\xi_{3,j}\int_{t_o}\phi_3(\tau)d\tau + 2\xi_{1,j}\xi_{2,j}\int_{t_o}\phi_{12}(\tau)d\tau$$

$$\left.\left. + 2\xi_{1,j}\xi_{3,j}\int_{t_o}\phi_{13}(\tau)d\tau + 2\xi_{2,j}\xi_{3,j}\int_{t_o}\phi_{23}(\tau)d\tau\right]\right\} \qquad \text{(AIII-12)}$$

where

$$Y_{3ao} = Y_{3a}(\vec{\xi}_1,\vec{\xi}_2,\vec{\xi}_3,t)_{t=t_o} \qquad \text{(AIII-13)}$$

Y_{3ao} denotes the initial condition of Y_{3a} in the transformed space. The original function Y_a at $t = t_o$ is given by Eq. (L-III-7), as,

$$(Y_a)_{t=t_o} = \delta(\vec{x}_1 - \vec{x}_{1o})\delta(\vec{x}_2 - \vec{x}_{2o})\delta(\vec{x}_3 - \vec{x}_{3o}) \qquad \text{(L-III-7)}$$

where $\vec{x}_1$, $\vec{x}_{1o}$, etc., are vectors.

By the same transformation of (III-10), Eq. (L-III-7) becomes

$$Y_{3ao} = e^{-(\xi_{1,j}x_{1o,j}+\xi_{2,j}x_{2o,j}+\xi_{3,j}x_{3o,j})} \qquad \text{(AIII-14)}$$

By substituting Eq. (AIII-14) into Eq. (AIII-12) and by taking an inverse integral transform of the resulting equation, we obtain

$$Y_{3a}(\vec{x}_1,\vec{x}_2,\vec{x}_3,t/\vec{x}_{1o},\vec{x}_{2o},\vec{x}_{3o},t_o)$$

$$= \frac{1}{(2\pi)^9} \iiint_{-\infty}^{\infty} \exp\Big\{ - [M_{11}\xi_{1,j}\xi_{1,j} + M_{22}\xi_{2,j}\xi_{2,j} + M_{33}\xi_{3,j}\xi_{3,j}$$

$$+ 2\xi_{1,j}\xi_{2,j}M_{12} + 2M_{13}\xi_{1,j}\xi_{3,j} + 2M_{23}\xi_{2,j}\xi_{3,j}]\Big\}$$

$$\exp\Big\{- i[\xi_{1,j}(x_{1,j} - x_{1o,j}) + \xi_{2,j}(x_{2,j} - x_{2o,j})$$

$$+ \xi_{3,j}(x_{3,j} - x_{3o,j})]\Big\} \; d\vec{\xi}_1 d\vec{\xi}_2 d\vec{\xi}_3 \qquad \text{(AIII-15)}$$

$j = 1, 2, 3$. Since M_{ij}'s are a function of t only we may write (the repeated tensor summation rule, jj, has been expanded and written out)

$$Y_{3a} = (\vec{x}_1, \vec{x}_2, \vec{x}_3, t/\vec{x}_{1o}, \vec{x}_{2o}, \vec{x}_{3o}, t_o)$$

$$= \left\{ \frac{1}{(2\pi)^3} \iiint_{-\infty}^{\infty} \exp\left\{-[M_{11}\xi_{1,1}^2 + M_{22}\xi_{2,1}^2 + M_{33}\xi_{3,1}^2 + 2M_{12}\xi_{1,1}\xi_{1,2} \right.\right.$$

$$\left. + 2M_{13}\xi_{1,1}\xi_{3,1} + 2M_{23}\xi_{2,1}\xi_{3,1}]\right\}$$

$$\exp\left\{- i[\xi_{1,1}(x_{1,1} - x_{1o,1}) + \xi_{2,1}(x_{2,1} - x_{2o,1}) \right.$$

$$\left. + \xi_{3,1}(x_{3,1} - x_{3o,1})]\right\} \; d\xi_{1,1}d\xi_{2,1}d\xi_{3,1} \Bigg\}$$

$$\left\{ \frac{1}{(2\pi)^3} \iiint_{-\infty}^{\infty} \exp\left\{- [M_{11}\xi_{1,2}^2 + M_{22}\xi_{2,2}^2 + M_{33}\xi_{3,2}^2 + 2M_{12}\xi_{1,2}\xi_{2,2} \right.\right.$$

$$\left. + 2M_{13}\xi_{1,2}\xi_{3,2} + 2M_{23}\xi_{2,2}\xi_{3,2}]\right\}$$

$$\exp\left\{- i[\xi_{1,2}(x_{1,2} - x_{1o,2}) + \xi_{2,2}(x_{2,2} - x_{2o,2}) \right.$$

$$\left. + \xi_{3,2}(x_{3,2} - x_{3o,2})]\right\} \; d\xi_{1,2}d\xi_{2,2}d\xi_{3,2} \Bigg\}$$

$$\left\{ \frac{1}{(2\pi)^3} \iiint_{-\infty}^{\infty} \exp\left\{- [M_{11}\xi_{1,3}^2 + M_{22}\xi_{2,3}^2 + M_{33}\xi_{3,3}^2 + 2M_{12}\xi_{1,3}\xi_{2,3} \right.\right.$$

$$\left. + 2M_{13}\xi_{1,3}\xi_{3,3} + 2M_{23}\xi_{2,3}\xi_{3,3}]\right\}$$

$$\exp\left\{- i[\xi_{1,3}(x_{1,3} - x_{1o,3}) + \xi_{2,3}(x_{2,3} - x_{2o,3}) \right.$$

$$\left. + \xi_{3,3}(x_{3,3} - x_{3o,3})]\right\} \; d\xi_{1,3}d\xi_{2,3}d\xi_{3,3} \Bigg\}$$

(AIII-16)

Each parenthesis on the right hand side of Eq. (AIII-16) is identical in form to that of Eq. (AIII-7). After going through the integration in each parenthesis, { }, on the right hand side of Eq. (AIII-16), each one of the sets of parentheses becomes functions of $(x_{1,1}, x_{2,1}, x_{3,1}, t | x_{1o,1}, x_{2o,2}, x_{3o,3}, t_o)$, $(x_{1,2}, x_{2,2}, x_{3,2}, t | x_{1o,2}, x_{2o,2}, x_{3o,2}, t_o)$, and $(x_{1,3}, x_{2,3}, x_{3,3}, t | x_{1o,3}, x_{2o,3}, x_{3o,3}, t_o)$, respectively. Therefore, Y_{3a} can be expressed in the following manner

$$Y_{3a} = Y_{3a1}(x_{1,1}, x_{2,1}, x_{3,1}, t | x_{1o,1}, x_{2o,1}, x_{3o,1}, t_o)$$

$$Y_{3a2}(x_{1,2}, x_{2,2}, x_{3,x}, t | x_{1o,1}, x_{2o,1}, x_{3o,1}, t_o)$$

$$Y_{3a3}(x_{1,3}, x_{2,3}, x_{3,3}, t | x_{1o,3}, x_{2o,3}, x_{3o,3}, t_o) \qquad \text{(AIII-17)}$$

The above equation, Eq. (AIII-17), shows that in the solution of Eq. (L-III-6), its variables can be separated into three parts. If we let $\vec{x}_3 = 0$ in Eq. (L-III-6), then the equation is reduced to the type similar to Eq. (IV-14)--that is, three-directional with two-coupled diffusion equation--and its solution can be expressed by setting $\vec{x}_3 = 0$ and $\vec{x}_{3o} = 0$ in Eq. (AIII-17), as

$$Y_{2a} = Y_{2a1}(x_{1,1}, x_{2,1}, t | x_{1o,1}, x_{2o,1}, t_o) Y_{2a2}(x_{1,2}, x_{2,2}, t | x_{1o,2}, x_{2o,2}, t_o)$$

$$Y_{2a3}(x_{1,3}, x_{2,3}, t | x_{1o,3}, x_{20,3}, t_o) \qquad \text{(AIII-17a)}$$

Equation (A-III-17a) gives the explanation of the expression given by Eq. (IV-16).

By comparing Eq. (A-III-16) and Eq. (A-III-7) we notice that each function, Y_{3a1}, Y_{3a2}, and Y_{3a3}, in Eq. (A-III-17) stands for the solution as given in Lemma III. Therefore, with the aid of Eqs. (AIII-7), (AIII-8), (A-III-16) and (A-III-17), the solution of Eq. (A-III-6) is readily obtained as given in Eq. (L-III-9).

VITA

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