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IMPROVED AVERAGING METHOD FOR TURBULENT FLOW SIMULATION

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IMPROVED AVERAGING METHOD
FOR
TURBULENT FLOW SIMULATION

DISSERTATION

Presented in Partial Fulfillment of the Requirements for
the Degree Doctor of Philosophy in the Graduate
School of The Ohio State University

By

Youssef Michel Dakhoul, B.Sc., M.S.

* * * *

The Ohio State University
1983

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LIST OF SYMBOLS

Latin Letters

- $c$  scalar concentration
- $\bar{c}$  large-scale component of $c$
- $c'$  SGS component of $c$
- $c_r$  residual field coefficient
- $c_1, \ldots, c_5$  constants
- $D$  eddy viscosity coefficient
- $E$  general spectrum value
- $F$  Fourier transform
- $f$  frequency
- $f_c$  cut-off frequency
- $G(x,t)$  general filter function
- $G_t(t)$  temporal component of $G(x,t)$
- $G_{\xi}(x_{\xi})$  component of $G(x,t)$ in the $x_\xi$ direction
- $I$  complex number $\sqrt{-1}$
i subscript denoting spatial direction or node number

j subscript for direction or superscript for time step

$K_{i,j}$ eddy viscosity coefficients

$k$ turbulent kinetic energy per unit mass

$L$ total length of flow domain

$L_s$ significant length scale

$l$ length scale or subscript for spatial direction

$l_m$ Prandtl mixing length

$M$ total number of time steps

$m$ mean of spatial velocity distribution

$m_{i}$ ratio of spatial filter width to spatial grid spacing

$m_{i}$ ratio of temporal filter width to temporal grid spacing

$N$ total number of spatial nodes

$n$ total number of spatial direction

$P$ total pressure
\[ \bar{P} \quad \text{large-scale component of } P \]
\[ p \quad \text{kinematic pressure} \]
\[ \bar{p} \quad \text{large-scale component of } p \]
\[ R_e \quad \text{Reynolds number} \]
\[ S_m \quad \text{molecular Schmidt number} \]
\[ S_t \quad \text{turbulent Schmidt number} \]
\[ T \quad \text{total time of calculation} \]
\[ t \quad \text{time} \]
\[ u \quad \text{one-dimensional velocity} \]
\[ \bar{u} \quad \text{large-scale components of } u \]
\[ u' \quad \text{SGS component of } u \]
\[ u_i, u_j \quad \text{velocity components in } x_i, x_j \text{ directions} \]
\[ \bar{u}_i, \bar{u}_j \quad \text{large-scale components of } u_i, u_j \]
\[ u'_i, u'_j \quad \text{SGS components of } u_i, u_j \]
\[ V_o \quad \text{significant velocity scale} \]
\[ v \quad \text{deviation of } u \text{ from its spatial mean } m \]
\[ \bar{v} \quad \text{large-scale component of } v \]
\[ w \quad \text{averaging length for Smagorinsky's } K \]
$x$ positional vector

$x, y, z$ cartesian coordinates

$x_i, x_j$ cartesian coordinates in tensor notation

Greek Letters

$\alpha$ general turbulent variable or molecular diffusivity

$\tilde{\alpha}$ large scale component of

$\alpha'$ SGS component of

$\alpha_1, \alpha_2, \ldots$ general turbulent variables

$\alpha(x, t)$ general 3D transient turbulent variable

$\tilde{\alpha}(x, t)$ large-scale component of $\alpha(x, t)$

$\alpha'(x, t)$ SGS component of $\alpha(x, t)$

$\gamma$ filter constant

$\Delta$ representative filtering scale

$\Delta_i$ filter width in the $x_i$ direction

$\Delta_t$ temporal filter width

$\Delta_x$ spatial filter width
\[ \delta_{ij} \quad \text{kronencker delta} \]

\[ \delta_i \quad \text{grid spacing in } x_i \text{ direction} \]

\[ \delta_t \quad \text{temporal grid spacing} \]

\[ \delta_x \quad \text{spatial grid spacing} \]

\[ \varepsilon \quad \text{dissipation rate} \]

\[ \lambda \quad \text{wave number} \]

\[ \nu \quad \text{molecular kinematic viscosity} \]

\[ \xi \quad \text{enstropy (vorticity squared)} \]

\[ \rho \quad \text{fluid density} \]

\[ \chi \quad \text{rate of destruction of thermal variance} \]

\[ \omega \quad \text{wave number} \]

\[ \omega_i \quad \text{wave number in } x_i \text{ direction} \]

\[ \omega_{IC} \quad \text{cut-off wave number in } x_i \text{ direction} \]
Chapter I
INTRODUCTION

1.1 DEFINITION OF TURBULENCE MODELING
Whenever a system of equations describing turbulent fluctuations is to be solved numerically, the equations must be "prepared" commensurate with the grid spacings. That is because any numerical grid is capable of resolving only a certain portion of a rapidly fluctuating variable. This portion, being a function of the grid spacings, is called the large-scale component. The remaining portion is called the subgrid-scale (SGS) component. Although not calculable, the SGS's have an important impact on the calculated large-scales since they are responsible for receiving and dissipating the energy contained in the large-scale motion.

The term "preparing" the equations (Turbulence Modeling) then means replacing the total variables by their large-scale equivalents, and modeling the SGS effects in terms of the large-scale components. After turbulence modeling, the equations can be solved on relatively coarser grids since the large-scales vary less rapidly than the total variables.
1.2 IMPORTANCE OF TURBULENCE MODELING

Any turbulent quantity contains fluctuations (eddies, or Fourier components) ranging in size from a few micrometers and microseconds to large spatial and temporal scales governed by the size of the problem. Therefore, only a very dense grid is capable of fully describing the equations of highly turbulent flows. Implementation of such dense grids is, and may always be, impossible with regards to the available computing machines. According to Rodi (1980), the spatial domain of a typical turbulent flow has to be divided into a minimum of 10 intervals, in each direction, in order for the original equations to yield a reliable and stable solution. This means that, for a three-dimensional flow, a minimum of 10 spatial nodes are necessary. Note that the upper limit on this number of nodes is open and depends on the intensity of turbulence which determines the steepness of the spatial and temporal gradients of the turbulent variables. Present computers, and those projected for the next 20 years, cannot offer large enough memory space nor can they economically handle the required number of calculations.

It is, therefore, necessary to use a numerical grid with much larger spacings than that required to resolve all the turbulent motion in the original equations. This is the importance of turbulence modeling which simply prepares the governing equations for solution on coarser grids. This preparation involves difficult mathematical and conceptual
problems, and the success of a given modeling approach depends on how these problems are treated.

1.3 METHODS AND AREAS OF IMPROVEMENT IN TURBULENCE MODELING

Turbulence modeling is accomplished by decomposing each variable into the sum of its large-scale and SGS components. The large-scale is defined by an "averaging operation." The SGS is defined as the difference between the total variable and its large-scale component. After the decomposition, the whole equation is averaged by the same averaging operation used to define the large-scales. This yields a governing equation containing both the large-scale and the SGS components of the variables. The terms containing the SGS's are separated and modeled in terms of the large-scales through a "closure" procedure. In summary, turbulence modeling is done in two main steps: averaging and closure. The final result is an equation, or a system of equations, containing only the large-scale components of the variables. Such equations can be discretized by the coarser grids. After numerically solving the equations, the results should of course be thoroughly checked and verified. This "Verification" of the results constitutes the third and final step in turbulence modeling.

The importance of averaging was first realized by Reynolds (1883) who introduced the temporal averaging procedure, and the rules of averaging which are still the most
commonly used in turbulence modeling. The Reynolds method averages turbulent variables in time. In other words, the large-scale component is a temporal average of the total variable. The averaging is done with a constant weight function which has uniform values within a certain averaging period. This averaging period is large enough to smooth out the SGS fluctuations, unresolvable by the grid, and small enough not to suppress the smooth variations of the large-scales (see Brodkey, 1967). The Reynolds method is based on the assumption that the time average is the true average of the total variable. In other words, averaging in time is capable of removing SGS fluctuations from the spatial distributions as well. It is also assumed that averaged quantities may be considered constants in subsequent averaging. This results in the important rule of averaging \( \bar{u}_i \bar{u}_j = \bar{u}_i \bar{u}_j \) (where \( \bar{u}_i \) and \( \bar{u}_j \) are large-scale velocity components in \( x_i \) and \( x_j \) directions) which has been used by most modelers until the present time.

The first conceptual improvement on Reynolds method was the realization of the importance of averaging in space, and the importance of relating the averaging intervals to the spatial grid spacings. Researchers such as Smagorinsky (1963); Lilly (1967); and Deardorff (1972b) define the large-scale component as the spatial, uniformly weighted average of the total variable within the spatial grid cell. The Reynolds approximation \( \bar{u}_i \bar{u}_j = \bar{u}_i \bar{u}_j \) is now believed to be a source of error.
The second improvement is due to Leonard (1974) who introduced the Gaussian averaging or "filtering" concept. Leonard's averaging (weight or filter) function has \( n \) spatial components where \( n \) is the total number of spatial directions in which averaging is desired. These components are Gaussian (rather than uniform) functions over the averaging space intervals. A simple Fourier analysis (see Chapter III) shows that the Gaussian averaging or "filtering" is superior to the uniform or "box" averaging regarding the success with which the SGS (high frequency or high wave number) components are smoothed out. Moreover, Leonard realizes the error in the Reynolds approximation \( \overline{u_i u_j} = \overline{u_i} \overline{u_j} \). Instead, Leonard applies his spatial Gaussian filtering operation on \( \overline{u_i u_j} \) to obtain a better approximation for \( \overline{u_i} \overline{u_j} \). The Leonard's method assumes that the spatial average is the true average of the total turbulent variable, i.e. averaging in space removes SGS fluctuations from the temporal distribution as well.

The logical extension of the above methods is Gaussian averaging in both space and time. In other words, to employ a Gaussian weight or filter function having \( n \) spatial components as well as a temporal component. The new filtering operation can be applied on \( \overline{u_i u_j} \) to obtain a new approximation for \( \overline{u_i} \overline{u_j} \) which is filtered in both space and time. Since turbulent variables fluctuate rapidly in all spatial directions and in time, the new idea of spatial-temporal filter-
ing (STF) seems to conform with the physics of the problem better than the temporal or spatial averaging methods. The STF idea takes advantage of the superiority of the Gaussian filters over the uniform ones, and avoids the assumption that either temporal or spatial averaging alone is sufficient. One of the main objectives of this research is to develop the STF idea of averaging and to prove its advantages both theoretically and in terms of actual numerical predictions.

No effort is made in this research to improve the present state of the closure methods. The available methods of closure are reviewed and assessed in Chapter II. Based on the assessment, some closure models are chosen for application in conjunction with the existing and newly suggested averaging procedures.

Concerning the verification phase of turbulence modeling, a special attention in this research is devoted to establishing a proper and systematic technique for verification. So far, the commonly used procedure is to compare the gross-averaged features of the model results with field data collected at the nodes of a monitoring network. Since turbulent variables are stochastic in nature, it has been recognized that, for surface water models, verification should most importantly involve statistical and spectral comparisons between the model results and the theoretically and empirically known properties (Bedford 1981). An important ob-
jective of the present research is to implement these statistical principles in a complete, step-by-step method of verification suitable for the kind of flow investigated in this report.

1.4 OBJECTIVES OF THE PRESENT RESEARCH

The objectives of the present research are:

1. To review the available methods of averaging and to suggest a new method involving spatial-temporal filtering (STF).

2. To theoretically analyze and integrate the new method into the existing theory of mathematical averaging.

3. To review the available closure models and to choose simple ones for use in this research.

4. To develop a rigorous and direct method of verification based on the statistical and spectral properties of the results.

5. To perform numerical applications on one-dimensional, transient flow equations under a range of input conditions. The suggested verification method is to be used in judging the performance of the new and the existing averaging methods when used in different combinations with the chosen closure models.

1.5 RESEARCH PLAN AND ORGANIZATION

Chapter II is devoted to reviewing the available conceptual theory of turbulence, and the existing methods of averaging and closing the turbulent flow equations. Based on a general assessment of the reviewed closure methods, particular closures are chosen for application in this research.

In Chapter III, the new STF method of averaging is developed based on a mathematical analysis of the previous aver-
aging techniques. The rules of averaging for the new procedure are derived and, as a demonstration, applied to model the three-dimensional Navier-Stokes equation for turbulence.

Chapter IV is a presentation of the one-dimensional, transient equations upon which the new and existing techniques of averaging are applied in this research. The similarities between the one-dimensional equations and the corresponding three-dimensional equations of hydrodynamics are studied.

In Chapter V, one-dimensional analogues of the three-dimensional averaging and closure methods are derived. These analogues are applied to model the one-dimensional equations presented in Chapter IV.

Chapter VI gives the details of the finite difference discretization for both the original and the modeled one-dimensional equations.

Chapter VII presents the suggested verification method which is based on statistical and spectral analysis of the results. Also, the input data and a plan for numerical experiments are presented in Chapter VII.

In Chapter VIII, the results of solving the one-dimensional equations are presented and processed according to the verification method.

Finally, Chapter IX includes a discussion of the results presented in the preceding chapter. The conclusions drawn from the discussion are also listed in Chapter IX.
Chapter II
LITERATURE REVIEW AND BACKGROUND

2.1 INTRODUCTION
Understanding the concepts of turbulence is vital to any modeller concerned with solving turbulent flow equations on coarse grids. Therefore, this chapter includes a description of the "Energy Cascade" conceptual picture of turbulence which should be preserved in the results of turbulence models. Also given in this chapter is a brief review of the existing methods of averaging. For demonstration, these methods are applied to the three-dimensional, time dependent Navier-Stokes equation. The chapter is concluded by a review of the available methods of closure and a general assessment of these methods. Based on the assessment, particular closure methods are chosen for application in this research.

2.2 TURBULENCE
According to Tennekes and Lumly (1972); and Monin and Yaglom (1975), a turbulent quantity (such as velocity or scalar concentration) is traditionally viewed as a totally random variable. The random variable is thought of as a superposition of eddies (fluctuations, or Fourier components). These have a wide spectrum of length scales ranging from a few mi-
crometers to the length scales of the flow domain, and a corresponding spectrum of time scales. The largest eddies, which are associated with the long length and time scales (low wave numbers and low frequencies), are determined by the boundary conditions and the geometry of the flow domain. The smallest eddies, associated with high frequencies and wave numbers, are independent of the flow domain and are determined by the viscous forces. The large eddies, having length and time scales similar to those of the flow domain, interact with and extract energy from the mean motion and pass it on to the ever smaller eddies, until the viscous forces become active and dissipate the energy at the smallest of eddies. This process is called the energy cascade. The range of eddy sizes between the largest and the smallest is called the inertial subrange. The eddies in the inertial subrange are the media through which the energy is passed from the large eddies to the small eddies where dissipation occurs.

The energy cascade process is best demonstrated by the spectral plots of the turbulent signal in question. That is because the spectral distribution is a direct measure of the energy contained at the different levels of wave numbers or frequencies (Frost, 1978). From theoretical arguments, supported by experimental observation, considerable information is known about the wave number spectra of turbulent variables. For surface water flows, Bedford (1981) summarised
this information in Figures 2.1 and 2.2. In the inertial subrange, the wave number spectrum of a three-dimensional turbulence is described by:

\[ E(\lambda) = c_1 \varepsilon^{2/3} \lambda^{-5/3} \]  \hspace{1cm} (2.1)

\( c_1 \) is a constant, \( \lambda \) is the wave number, and \( \varepsilon \) is the viscous dissipation rate. For accelerated or two-dimensional turbulence, the wave number spectrum in the inertial subrange is given by:

\[ E(\lambda) = c_2 \xi^{2/3} \lambda^{-3} \]  \hspace{1cm} (2.2)

where \( c_2 \) is a constant and \( \xi \) is the enstrophy (vorticity squared) dissipation. For temperature or passive scalar, the spectrum is:

\[ E(\lambda) = c_3 \chi \varepsilon^{-1/3} \lambda^{-5/3} \]  \hspace{1cm} (2.3)

where \( c_3 \) is a coefficient, \( \chi \) is the rate of destruction of thermal variance. The general shape of the wave number spectra for active contaminants is given in Figure 2.2(c).

Since the spectral plots describe the energy cascade which should be preserved in the calculated turbulent variables, they are becoming a powerful tool for verifying the modeling techniques which are reviewed below.
Figure 2.1: General Energy Spectrum, Frost (1978).
Figure 2.2: General Spectral Distributions, Bedford (1981).
2.3 AVERAGING

The equation that governs general fluid flow is the three-dimensional Navier-Stokes equation. For incompressible, Newtonian flow in the absence of external forces, the equation reads (see Brodkey 1967 for derivation):

$$\frac{\partial u_i}{\partial t} + \frac{\partial u_j}{\partial x_j} = \frac{-1}{\rho} \left( \frac{\partial p}{\partial x_i} \right) + \nu \left( \frac{\partial^2 u_i}{\partial x_j \partial x_j} \right).$$  (2.4)

Where $x_i$ denotes cartesian coordinate directions; $t$ is time; $u_i$ denotes velocity in the $x_i$ direction; $\rho$ is the fluid's density; $p$ is kinematic pressure; and $\nu$ is the molecular kinematic viscosity. The tensor notation is used to write (2.4); the repetition of an index in a certain term implies the summation of that term over the three spatial directions.

As mentioned in Chapter I, the above equation cannot be solved for highly turbulent flow unless the grid spacings are very small. In order to solve Equation (2.4) on coarse grids, averaging must be done. In other words the total variables must be replaced by their large-scale components which can be handled by the coarse grid. According to Reynolds (1883), a general three-dimensional transient variable, $\alpha(x,t)$, is decomposed into two parts:

$$\alpha(x,t) = \bar{\alpha}(x,t) + \alpha'(x,t).$$  (2.5)
Where $\mathcal{R}(x,t)$ represents the superposition of all eddies or Fourier components to be resolved by the coarse grid. The remaining portion $\alpha'(x,t)$ denotes all eddies or Fourier components unresolvable by the grid. $x$ denotes the spatial position vector and $t$ is the time coordinate.

The mathematical definition of $\mathcal{R}(x,t)$ differs from one method of averaging to another, however, all methods obviously imply smoothing. In other words, $\mathcal{R}(x,t)$ must be obtained from $\alpha(x,t)$ by removing the high wave number and high frequency components. Therefore, a general definition covering all possible methods of averaging can be written as:

$$\mathcal{R}(x,t) = \int_{-\infty}^{\infty} G(x-x',t-t') \alpha(x',t') \, dx' dt'. \quad (2.6)$$

This is a convolution integral in which $G(x,t)$ is a weight, average, or filter function defined as:

$$G(x,t) = G(t) \prod_{i=1}^{n} G_i(x_i), \quad (2.7)$$

where $G_i(x_i)$ is the component of $G(x,t)$ in the $x_i$ direction; $G_t(t)$ is the temporal component; and $n$ is the total number of spatial directions in which averaging is desired. The function $G(x,t)$ must satisfy the condition:

$$\int_{-\infty}^{\infty} G(x-x',t-t') \, dx' dt' = 1, \quad (2.8)$$

such that the large-scale component of a constant becomes the same constant. The averaging operation (2.6) is obtained by adding the time dimension to the spatial averaging operation given in Leonard (1974).
The expression (2.5) is used to decompose the velocity components \( u_i \) and \( u_j \) in the nonlinear inertial term of equation (2.4). This gives:

\[
\frac{\partial u_i}{\partial t} + \frac{\partial}{\partial x_j} \left( \bar{u}_i \bar{u}_j + \bar{u}_i u_j + u_i \bar{u}_j + u_i u_j \right)/\partial x_j =
\]

\[
(-1/\rho) \left( \frac{\partial p}{\partial x_i} \right) + \nu \frac{\partial^2 u_i}{\partial x_j \partial x_j}. \tag{2.9}
\]

Equation (2.9) is then averaged using the averaging operation (2.6). The available averaging methods use different special cases of (2.6), and different shapes of the weight function (2.7). These are reviewed in the following subsections.

2.3.1 Reynolds Temporal Averaging

Reynolds (1883) introduced the temporal averaging procedure which has been used by literally hundreds of researchers in solving practical hydraulic problems. For excellent lists of references see Rodi (1980) and Brodkey (1967). The averaging function has only one temporal component and no spatial components. Therefore, the following special case of equation (2.6) applies:

\[
\bar{\alpha}(x,t) = \int_{-\infty}^{\infty} G_t(t-t') \alpha(x,t') \, dt', \tag{2.10}
\]

where the temporal averaging function, \( G_t(t) \), is defined as:

\[
G_t(t) = 1/\Delta_t \quad (\text{for } -\Delta_t/2 \leq t \leq \Delta_t/2), \tag{2.11}
\]
where $\Delta_t$ is a temporal averaging scale. This averaging period should be large enough to suppress the SGS fluctuations, unresolvable by the grid, and small enough not to average out the variations of the large scales. Equation (2.11) obviously satisfies the condition (2.8). Substituting (2.11) into (2.10) yields:

$$\bar{\alpha}(x,t) = \frac{1}{\Delta_t} \int_{-\Delta_t/2}^{\Delta_t/2} \alpha(x,t') \, dt'.$$  \hspace{1cm} (2.12)

Now, Equation (2.9) is to be averaged according to (2.12) and thereof the following Reynolds Axioms (see Brodkey, 1967):

$$\alpha_1 + \alpha_2 + \ldots = \bar{\alpha}_1 + \bar{\alpha}_2 + \ldots,$$ \hspace{1cm} (2.13)

$$\frac{\partial \alpha}{\partial t} = \frac{\partial \bar{\alpha}}{\partial t},$$ \hspace{1cm} (2.14)

$$\frac{\partial \alpha}{\partial x_i} = \frac{\partial \bar{\alpha}}{\partial x_i},$$ \hspace{1cm} (2.15)

$$\bar{\alpha} \alpha' = 0.$$ \hspace{1cm} (2.16)

The overbars denote averaging as defined by (2.12). Equation (2.9) thus becomes:

$$\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial (\bar{u}_i \bar{u}_j)}{\partial x_j} = \frac{-1}{\rho} \left( \frac{\partial \bar{p}}{\partial x_i} \right)$$

$$+ \nu \left( \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} \right) - \frac{\partial (u_i' u_j')}{\partial x_j}.$$ \hspace{1cm} (2.17)

Reynolds further assumes that

$$\bar{u}_i \bar{u}_j = \bar{u}_i \bar{u}_j$$ \hspace{1cm} (2.18)

which modifies Equation (2.17) to give:
\[ \frac{\partial \bar{u}_i}{\partial t} + \frac{\partial (\bar{u}_i \bar{u}_j)}{\partial x_j} = \frac{(-1)}{\rho} \frac{\partial p}{\partial x_i} \]

\[ + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} - \frac{\partial \bar{u}_i}{\partial x_j} \frac{\partial \bar{u}_j}{\partial x_j}. \]  

(2.19)

Equation (2.19) now contains the large-scale components of the variables and can be solved on coarse grid after closure, i.e. expressing \( \bar{u}_i \bar{u}_j \) in terms of the large-scales.

The Reynolds approach is based on the assumption that temporal averaging of a turbulent variable produces its true large-scale component. In other words, the resulting large-scale has no high wave number components with respect to the spatial grid spacings.

2.3.2 Uniform Spatial Averaging

In this approach, the Reynolds definition of the large-scale is modified into a spatial rather than temporal average. The importance of averaging in space is linked to the requirement that the large-scale be free of eddies smaller in size than the spatial grid cell. Researchers such as Smagorinsky (1963); Deardorff (1972b, 1973, 1974a, 1974b); Lilly (1967); Bedford and Rai (1978); and Bedford and Shah (1977) adopt the following special case of the general averaging procedure (2.6):

\[ \bar{\alpha}(\bar{x}, t) = \int_{-\infty}^{\infty} G(\bar{x} - \bar{x}') \alpha(\bar{x}', t) \, d\bar{x}'. \]  

(2.20)

The spatial averaging function is defined as:

\[ G(\bar{x}) = \prod_{i=1}^{n} G_i(x_i) \]
where \( \Delta_i \) is the grid spacing in the \( x_i \) direction (see Lilly, 1967). Combining (2.21) and (2.20) yields:

\[
\overline{\alpha}(x,t) = \left( \prod_{i=1}^{n} 1/\Delta_i \right) \int \ldots \int (x', \ldots, x'_n, t) \, dx'_1 \ldots dx'_n \tag{2.22}
\]

The Reynolds axioms (2.13) through (2.16) are still derived from (2.22), thus Equation (2.17) is unchanged. The Reynolds approximation (2.18) is believed inaccurate, and the difference between \( \overline{u_i u_j} \) and \( \overline{u_i} \overline{u_j} \) is absorbed into the last term in Equation (2.17) as in Lilly (1967). The result is:

\[
\frac{\partial \overline{u_i}}{\partial t} + \overline{u_j} \frac{\partial \overline{u_i}}{\partial x_j} + \nu \frac{\partial^2 \overline{u_i}}{\partial x_j \partial x_j} - \nu \frac{\partial \overline{\tau_{ij}}}{\partial x_j} = \frac{-1}{\rho} \frac{\partial \overline{p}}{\partial x_i} \tag{2.23}
\]

where \( \overline{\tau_{ij}} \) is equal to \( \overline{u_i' u_j'} \) plus the difference between \( \overline{u_i} \overline{u_j} \) and \( \overline{u_i} \overline{u_j} \). The evaluation of \( \overline{\tau_{ij}} \), in terms of the large-scale velocities, is a closure problem. The operation (2.20) is important as a historical development in defining the large-scales. Here, temporal averaging is no longer acknowledged as sufficient in removing spatial SGS's. Also, at this point of development, researchers began to doubt the validity of the Reynolds approximation (2.18).
2.3.3 Leonard's Spatial Filtering

According to the Leonard's filtering method (Leonard 1974), averaging is done in space with Gaussian rather than "box" or uniform averaging function. Leonard also abandoned the approximation (2.18) and applied his averaging procedure on \( \bar{u}_i \bar{u}_j \) to obtain a better approximation of \( \bar{u}_i \bar{u}_j \). Important applications of the Leonard's filtering in practical problems are due to Babajimopoulos and Bedford (1980); Bedford et al. (1978); Bedford and Babajimopoulos (1980); Bedford (1981); Cosier (1979); Kwak et al. (1975); Mansour et al. (1978); Clark et al. (1977); Findikakis and Street (1979); and Antonopoulos-Domis (1981).

The following special case of Equation (2.6) is used:

\[
\alpha(x,t) = \int_{-\infty}^{\infty} G(x-x') \alpha(x',t) \, dx',
\]  

(2.24)

where the spatial averaging or filter function is defined as:

\[
G(x) = \prod_{i=1}^{n} G_i(x_i)
\]

\[
= \prod_{i=1}^{n} \sqrt{\frac{\gamma}{\pi}} \left( \frac{1}{\Delta_i} \right) \exp\left(-\gamma x_i^2 / \Delta_i^2 \right) \text{ (for all } x_i \text{).} \tag{2.25}
\]

\( \gamma \) is a constant and \( \Delta_i \) is an averaging scale in the \( x_i \) direction. This filter function satisfies the condition (2.8). Substituting (2.25) into (2.24) gives:

\[
\bar{\alpha}(x,t) = (\sqrt{\gamma/n})^n \left\{ \prod_{i=1}^{n} \left( \frac{1}{\Delta_i} \right) \right\} \int_{-\infty}^{\infty} \alpha(x',t) \left\{ \prod_{i=1}^{n} \exp\left[-\gamma (x_i - x_i')^2 / \Delta_i^2 \right] \right\} \, dx'.
\]  

(2.26)
Equation (2.9) is now to be averaged according to the averaging operation (2.26). The Reynolds' axioms (2.13), (2.14), and (2.15) can be proved by working with Equation (2.26). See for example Leonard (1974), and Kwak et al. (1975). Axioms (2.16) cannot be mathematically proved but is usually assumed true as an approximation. Equation (2.9) thus transforms to the same averaged form (2.17).

The most important difference between the Leonard's method of averaging and the previous methods is in dealing with the term \( \overline{u_i} \overline{u_j} \). While the previous methods approximate \( \overline{u_i} \overline{u_j} \) by \( \overline{u_i} \overline{u_j} \) or absorb the difference into the closure term, Leonard applies (2.26) on the variable \( \overline{u_i} \overline{u_j} \) to obtain:

\[
\overline{u_i} \overline{u_j} = \left( \frac{1}{\tau} \right)^n \left[ \prod_{i=1}^{n} \left( 1/\Delta_i \right) \right] \int_{-\infty}^{\infty} \overline{u_i} \overline{u_j} (x_1, \ldots, x_n, t) \exp \left[ -y(x_1 - x_1')^2 / \Delta_1^2 \right] dx_1 \ldots dx_n. \tag{2.27}
\]

Now, \( \overline{u_i} \overline{u_j} (x_1', \ldots, x_n', t) \) is expressed in terms of \( \overline{u_i} \overline{u_j} (x_1, \ldots, x_n, t) \) through a Taylor series expansion. The integration is carried out, as in Kwak et al. (1975) and Bedford et al. (1978), to yield:

\[
\overline{u_i} \overline{u_j} = \overline{u_i} \overline{u_j} + \sum_{i=1}^{n} (\Delta_i^2 / 4y) \frac{\partial^2 (\overline{u_i} \overline{u_j})}{\partial x_i^2} + \text{H.O.T.} \tag{2.28}
\]

The higher order terms (H.O.T) are neglected. The final averaged equation is obtained by combining (2.28) with (2.17). In tensor notation, the equation is:

\[
\frac{\partial \overline{u_i}}{\partial t} + \partial \left[ \overline{u_i} \overline{u_j} + (\Delta_2^2 / 4y) \frac{\partial^2 (\overline{u_i} \overline{u_j})}{\partial x_i^2} \right] / \partial x_j = (-1/\rho)
\]
(\partial \bar{p} / \partial x_j) + \nu \left( \partial^2 \bar{u}_i / \partial x_j \partial x_j \right) - \partial \bar{(u_i^e u_j^e)} / \partial x_j \right). \quad (2.29)

The implications of both uniform and Gaussian averaging operations are shown in Figure 2.3(a) and 2.3(b). Mathematically, the result of the Reynolds' integration (2.12) is a constant \( \bar{a}(x,t) \) through the averaging scale \( \Delta_x \). But the result of the Leonard's integration (2.26) is a variable \( \bar{a}(x,t) \) over the averaging scale \( \Delta_x \). Thus one is forced, in case of box averaging, to deal with a SGS component larger than that produced by the Gaussian averaging. Therefore, the Reynolds' scheme attaches more importance to the ambiguous closure procedures than does the Leonard's method.

2.4 CLOSURE

Averaging the three-dimensional Navier-Stokes Equation (2.4) by the above mentioned averaging schemes yields Equation (2.19), (2.23) or (2.29). The two equations (2.19) and (2.29) are used below to demonstrate the closure problem:

\[
\begin{align*}
\partial \bar{u}_i / \partial t + \partial (\bar{u}_i \bar{u}_j) / \partial x_j &= (-1/\rho) \left( \partial \bar{p} / \partial x_i \right) \\
+ \nu \left( \partial^2 \bar{u}_i / \partial x_j \partial x_j \right), \quad (2.4) \\
\partial \bar{u}_i / \partial t + \partial (\bar{u}_i \bar{u}_j) / \partial x_j &= (-1/\rho) \left( \partial \bar{p} / \partial x_i \right) \\
+ \nu \left( \partial^2 \bar{u}_i / \partial x_j \partial x_j \right) - \partial \bar{(u_i^e u_j^e)} / \partial x_j, \quad (2.19) \\
\partial \bar{u}_i / \partial t + \partial [\bar{u}_i \bar{u}_j] + (\Delta x^2 / 4\nu) \partial (\bar{u}_i \bar{u}_j) / \partial x_j &= (-1/\rho) \\
(\partial \bar{p} / \partial x_i) + \nu \left( \partial^2 \bar{u}_i / \partial x_j \partial x_j \right) - \partial \bar{(u_i^e u_j^e)} / \partial x_j. \quad (2.29)
\end{align*}
\]
Figure 2.3: Averaging Operations (Leonard 1974).
Both Equations (2.19) and (2.29) have to be closed, i.e. the term $u_i^i u_j^j$ must be replaced by the large-scale quantities $\bar{u}_i$ and $\bar{u}_j$.

In order to close the equations one might derive a new set of transport equations relating the SGS components to the large-scale components. It has become customary to classify the closure models according to the number of transport equations used for the SGS quantities. Following Rodi (1980), the following closure models are summarized below:

1. Zero-Equation Models;
2. One-Equation Models;
3. Two-Equation Models; and

2.4.1 Zero-Equation Models

The Zero-Equation Models do not employ any additional exact transport equations for the SGS's; but, rather, make use of the Boussinesq eddy viscosity concept (Boussinesq, 1877). This concept assumes, in analogy to Newton's law of molecular viscosity, that the turbulent stresses are proportional to the spatial gradients of the large-scale variables. In mathematical terms:

$$u_i^i u_j^j = -K_{ij} (\delta \bar{u}_i / \delta x_j) + 2k \delta_{ij}/3,$$

where $K_{ij}$ is called the eddy viscosity coefficient; $\delta_{ij}$ is the kronecker delta; and $k$ is the turbulent kinetic energy defined as the summation of the normal stresses (Tennekes and Lumly, 1972):
In Equation (2.30) no summation over the spatial directions is implied. For example:

\[ u_x' u_y' = -K_{xy} (\partial \tilde{u}_x / \partial y), \]  

\[ u_y' u_y' = -K_{yy} (\partial \tilde{u}_y / \partial y) + 2k/3. \]  

It follows that the summation of the three normal stress \( u_x' u_x' \), \( u_y' u_y' \), and \( u_z' u_z' \) is:

\[ u_x' u_x' + u_y' u_y' + u_z' u_z' = -K_{xx} (\partial \tilde{u}_x / \partial x) - K_{yy} (\partial \tilde{u}_y / \partial y) - K_{zz} (\partial \tilde{u}_z / \partial z) + 2k. \]  

By continuity, the first three terms in the right hand side add up to zero if the three eddy viscosity coefficients are assumed equal. Thus the definition of the turbulent kinetic energy (2.31) is satisfied.

Equation (2.30) is now used to eliminate \( u_i' u_j' \) from the averaged but not yet closed Equations (2.19) and (2.29). Using Equation (2.19):

\[ \partial \tilde{u}_i / \partial t + \partial (\tilde{u}_i \tilde{u}_j )/ \partial x_j = (-1/\rho) (\partial p / \partial x_i ) + \nu (\partial^2 \tilde{u}_i / \partial x_j ^2 \partial x_j ) \]

\[ + \partial [ K_{i,j} (\partial \tilde{u}_i / \partial x_j ) / \partial x_j ] - \partial (2k/3) / \partial x_i. \]  

The last term in the right hand side is absorbed by the pressure gradient term. The result is \((-1/\rho) \partial (\tilde{p} + 2k\rho/3) / \partial x_i\). The quantity \( \tilde{p} + 2k\rho/3 \) is considered as a total pressure, \( \tilde{p} \).
The molecular viscosity term is often neglected with respect to the eddy viscosity term. Equation (2.19) and (2.29) finally reduce to the following closed forms:

\[
\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial (\bar{u}_i \bar{u}_j)}{\partial x_j} = \left(\frac{1}{\rho}\right) \left(\frac{\partial \bar{p}}{\partial x_i}\right) - \frac{1}{\rho} \left(\frac{\partial \bar{p}}{\partial x_i}\right) + \partial \left[K_{ij} \frac{\partial \bar{u}_i}{\partial x_j}\right]\frac{\partial x_j}{\partial x_j},
\]  

(2.36)

\[
\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial (\bar{u}_i \bar{u}_j)}{\partial x_j} + \left(\frac{\Delta t}{4\gamma}\right) \frac{\partial^2 (\bar{u}_i \bar{u}_j)}{\partial x_j^2} = \left(\frac{1}{\rho}\right) \left(\frac{\partial \bar{p}}{\partial x_i}\right) + \partial \left[K_{ij} \frac{\partial \bar{u}_i}{\partial x_j}\right]\frac{\partial x_j}{\partial x_j}.
\]  

(2.37)

The equations are now closed and the problem is shifted to the determination of the eddy viscosity coefficients. Zero-Equation Models can be properly subdivided according to the method by which these coefficients are determined. For example, the most frequently used form is constant eddy coefficients determined by experiment or numerical tuning. A "mixing length model" employs the Prandtl mixing length hypothesis (Prandtl, 1933) to evaluate the eddy viscosity. In its most general form, the hypothesis is written as:

\[
K_{ij} = \ell_m^2 \left[(\partial \bar{u}_i/\partial x_j)(\partial \bar{u}_i/\partial x_j + \partial \bar{u}_j/\partial x_i)\right]^{1/2}
\]  

(2.38)

The determination of the mixing length, \(\ell_m\), remains an empirical problem whose difficulty depends on the complexity of the flow.

The Smagorinsky's closure model (Smagorinsky 1963) is a direct application of the Prandtl mixing length concept.
This model is often used in conjunction with the Leonard's method of averaging, i.e. to close Equation (2.29). Smagorinsky uses Equation (2.38) with the following expression for the mixing length \( l_m \):

\[
l_m = c_r \Delta ,
\]

where \( \Delta \) is a representative filtering scale defined, as in Deardorff (1970, 1972a), by:

\[
\Delta = \left( \prod_{i=1}^{n} \Delta_i \right)^{1/n},
\]

and \( c_r \) is a constant called the residual field coefficient. This coefficient is usually determined by numerical tuning. See for example Spraggs and Street (1975), and Cosier (1979).

2.4.2 One-Equation Models

The One-Equation Models also employ the Boussinesq eddy viscosity concept to derive the closed equations (2.36) and (2.37). But instead of using constant or functional forms of \( K_{ij} \) (as do the Zero-Equation Models) the One-Equation Models employ an additional transport equation for the distribution of \( K_{ij} \). All the coefficients \( K_{ij} \) are assumed equal and represented by the symbol \( K \). The Kolmogoroff-Prandtl expression (Kolmogoroff, 1941) is used to write \( K \) as proportional to a velocity scale, \( k \), and a length scale, \( \ell \):

\[
K = c_s \sqrt{k} \ell ,
\]
A transport equation for the distribution of the kinetic energy, $k$, is needed to be used in conjunction with Equation (2.41). The equation is derived from the original and the averaged forms of the Navier-Stokes equation (Rodi 1980). The equation reads:

$$\frac{\partial k}{\partial t} + \vec{u}_i \frac{\partial k}{\partial x_i} = \partial \left[ \left( \frac{K}{c_z} \right) \frac{\partial k}{\partial x_i} \right] \frac{\partial x_i}{\partial x_i} + K \left( \frac{\partial \vec{u}_i}{\partial x_j} + \frac{\partial \vec{u}_j}{\partial x_i} \right) \left( \frac{\partial \vec{u}_i}{\partial x_j} \right) - c_3 k^{2/3} \ell. \quad (2.42)$$

The constants $c_1$, $c_2$, $c_3$ and the length scale, $\ell$, are to be determined empirically.

2.4.3 Two-Equation Models

The Two-Equation Models again recognize the Boussinesq eddy viscosity concept, and assume the equality of all the coefficients $K_{ij}$. The eddy viscosity $K$ is then determined by (see Tennekes and Lumly, 1972):

$$K = c_4 k^2 / \varepsilon, \quad (2.43)$$

where $c_4$ is a constant, and $\varepsilon$ is the dissipation rate. The most widely used $k-\varepsilon$ model employs the following two transport equations for the distribution of $k$ and $\varepsilon$:

$$\frac{\partial k}{\partial t} + \vec{u}_i \frac{\partial k}{\partial x_i} = \partial \left[ \left( \frac{K}{c_z} \right) \frac{\partial k}{\partial x_i} \right] \frac{\partial x_i}{\partial x_i} + K \left( \frac{\partial \vec{u}_i}{\partial x_j} + \frac{\partial \vec{u}_j}{\partial x_i} \right) \left( \frac{\partial \vec{u}_i}{\partial x_j} \right) - \varepsilon, \quad (2.44)$$
\[
\frac{\partial \varepsilon}{\partial t} + \bar{u}_i \left( \frac{\partial \varepsilon}{\partial x_i} \right) = \varepsilon \left[ \left( \frac{K}{c_3} \right) \left( \frac{\partial \varepsilon}{\partial x_i} \right) \right] / \partial x_i \\
+ c_4 \left( \frac{\varepsilon}{k} \right) (PR) - c_5 \left( \frac{\varepsilon^2}{k} \right).
\]

The constants \(c_1, c_2, c_3, c_4\) and \(c_5\) are to be determined empirically. Launder and Spalding (1974) recommend the values 0.09, 1.0, 1.3, 1.44 and 1.92 for these constants respectively.

2.4.4 Turbulent Stress-Equation Models

The starting step in all the above closure methods is the Boussinesq assumption which substitutes for the turbulent stresses by eddy coefficients and spatial gradients of the large-scale velocities. The different models then estimate the eddy coefficients using zero, one, or two additional transport equations.

The Turbulent Stress-Equation Models, on the other hand, do not employ the Boussinesq concept. Rather, they provide an exact transport equation for each of the nine turbulent stresses \(u_i^j u_j^i\).

Chow (1945), based on suggestions by Keller and Friedmann in 1924, derived an exact differential equation for the Reynolds stresses, \(u_i^j u_j^i\). The derivation is done by subtracting the Reynolds averaged Navier-Stokes equation from the original equation for both \(x_i\) and \(x_j\) directions. The resulting equation is then multiplied by \(u_j^i\), and the resulting \(j\) equation is multiplied by \(u_i^i\). Summation of the two equations and
subsequent Reynolds averaging yields the desired equation for $\overline{u_i'u_j'}$. After some approximations (see Rotta 1972; Launder et al. 1975; Naot et al. 1970; and Reynolds 1970) the final form of the turbulent stress equation may be written as:

$$\partial (\overline{u_i'u_j'}) / \partial t + \overline{u_i'} \partial (\overline{u_i'u_j'}) / \partial \mathbf{x}_j = - (\overline{u_i'u_j'}) (\partial \overline{u_j'}/\partial \mathbf{x}_i)$$

$$- \overline{u_j'u_j'} (\partial \overline{u_i'}/\partial \mathbf{x}_i) - c_1 (\mathcal{E}/k) (\overline{u_i'u_j'} - 2 \delta_{ij} k/3)$$

$$- c_2 \left[ P_{ij} - (2 \delta_{ij}/3) \left( \overline{u_i'u_j'} \right) (\partial \overline{u_i'}/\partial \mathbf{x}_j) \right]$$

$$- c_3 \partial [(\mathcal{E}/k) (\overline{u_i'u_j'}) (\partial \overline{u_i'u_j'}/\partial \mathbf{x}_k)] / \partial \mathbf{x}_k$$

$$- 2 \mathcal{E} \delta_{ij}/3.$$  \hspace{1cm} (2.46)

Here $c_1$, $c_2$, and $c_3$ are constants; $P_{ij}$ is the sum of the first two terms in the right hand side; $\delta_{ij}$ is the kronecker delta; and $k$ and $\mathcal{E}$ are to be determined by the $k-\mathcal{E}$ model given by Equations (2.44) and (2.45).

2.5 GENERAL ASSESSMENT OF CLOSURE METHODS

The Boussinesq concept is the foundation of most closure models presented in section 2.4. The concept implies analogy between molecular motion and the motion of turbulent eddies. This analogy is at least questionable since, unlike molecules, turbulent eddies are not rigid bodies that retain their identity. Also, the large eddies and their paths are not small compared to the dimensions of the flow domain, e.g., Corrison (1957); and Bradshaw (1969). Nevertheless,
these models are very heavily used in solving practical problems with varied levels of success.

The Zero-Equation Model with constant eddy coefficients is commonly used for simulating geophysical flows of large bodies of water. Usually, it is combined with the Reynolds' averaging procedure. This combination is attractive because of its simplicity and its reasonable success in cases of low-level turbulence. In some cases, constant eddy viscosity models were used merely to improve the numerical stability of the simulation (see Leendertse 1967). On the other hand, when turbulence is important, Zero-Equation Models with constant eddy coefficients fail to produce statistically correct results. Even with careful tuning of the eddy coefficients the performance of such models could not be improved (see Bedford and Babajimopoulos 1980).

Zero-Equation Models with variable eddy coefficients, such as the Smagorinsky's model, proved to be more successful than the constant coefficient models. The Smagorinsky's model is used usually in conjunction with the Leonard's spatial averaging method. For example, Love (1980); Clark et al. (1977); and Babajimopoulos and Bedford (1980) predict turbulent fields statistically superior to those obtained from constant eddy coefficient models. Note, however, that at least a part of the improvement may be due to the higher order averaging method rather than the variable eddy coefficients. One of the objectives of the present research is to investigate this point.
The One-Equation, Two-Equation and Turbulent Stress-Equation Models are out of the scope of this research. These models are associated with three-dimensional flows while the present investigation is one-dimensional. Also, these models are derived using the Reynolds averaged and the original hydrodynamic equations. Thus, the models are used only in conjunction with the traditional Reynolds method of averaging.

For the purposes of this research, Zero-Equation Models with constant or Smagorinsky's eddy coefficients are chosen for application. The reason for this choice is that the Zero-Equation Models are simple and economic. Also, they can be used in conjunction with all the existing and the newly suggested averaging methods. One-dimensional analogues of these models are available and already in use (see Chapter V).
Chapter III
DEVELOPMENT OF IMPROVED AVERAGING METHOD

3.1 INTRODUCTION
This chapter includes a mathematical analysis of the averaging methods reviewed in Chapter II. Based on this analysis, a new procedure involving spatial-temporal filtering (STF) is suggested. The new procedure is mathematically developed and analyzed in comparison to the existing methods. "Rules of averaging" are then derived for the new procedure and applied to average the three-dimensional Navier-Stokes Equation.

3.2 FOURIER ANALYSIS OF AVERAGING OPERATIONS
The general definition representing all possible averaging procedures is given in section 2.3. This definition is rewritten below for convenience:

$$\bar{\omega}(x,t) = \int_{-\infty}^{\infty} G(x-x',t-t') \alpha(x',t') \, dx' \, dt', \quad (3.1)$$

where the weight, average, or filter function, $G(x,t)$, is defined as:

$$G(x,t) = G_t(t) \prod_{i=1}^{n} G_i(x_i). \quad (3.2)$$
If $\tilde{c}(x,t)$ is really the large-scale component (the component that can be calculated by a coarse grid), its Fourier transform should vanish at wave lengths and wave periods equal to or smaller than twice the corresponding grid spacing. This can be easily examined by applying the Convolution (Fultang) Theorem which states that if (3.1) is true then:

$$F\{\tilde{c}(x,t)\} = F\{G(x,t)\} F\{c(x,t)\},$$  \hspace{1cm} (3.3)

where $F$ denotes the Fourier transform. Equation (3.3) shows that the Fourier transform of $\tilde{c}(x,t)$ is directly proportional to the Fourier transform of the filter function. Therefore, we need a filter function whose Fourier transform is zero for wave periods and wave lengths equal to or smaller than twice the corresponding grid spacings.

In Reynolds' temporal averaging (see section 2.3.1), the following special cases of Equations (3.1), (3.2), and (3.3) apply:

$$\tilde{c}(x,t)) = \int_{-\infty}^{\infty} G(t - t') c(x,t') dt', \hspace{1cm} (3.4)$$

$$G_t(t) = 1/\Delta_t \hspace{1cm} \text{(for } -\Delta_t/2 \leq t \leq \Delta_t/2), \hspace{1cm} (3.5)$$

$$F\{\tilde{c}(x,t)\} = F\{G_t(t)\} F\{c(x,t)\}. \hspace{1cm} (3.6)$$

The Fourier transform of the averaging function, $F G_t(t)$, is given by:

$$F\{G_t(t)\} = \int_{-\infty}^{\infty} G_t(t) \exp(-i ft) dt$$

$$= \int_{-\Delta_t/2}^{\Delta_t/2} (1/\Delta_t) \exp(-i ft) dt$$
$$= \frac{\sin(f \Delta t/2)}{(f \Delta t/2)}.$$  \hspace{1cm} (3.7)$$

Here, \( f \) stands for frequencies and \( i \) is the complex number \( -1 \). The function \( G_t(t) \) and its Fourier transform are plotted in Figure 3.1. It is clear that \( F\{G_t(t)\} \) has appreciable values at high frequencies which inflicts an undesirable feature upon the large-scale component \( \alpha(x,t) \). Note also that no averaging is done in the spatial domain which means that \( F\{\alpha(x,t)\} \) is non-zero for all wave numbers.

In case of uniform spatial averaging (see section 2.3.2), the following special cases of Equations (3.1), (3.2) and (3.3) are used:

\[
\bar{\alpha}(x,t) = \int \limits_{-\infty}^{\infty} G(x-x') \alpha(x',t) \, dx', \hspace{1cm} (3.8)
\]

\[
G(x) = \prod_{i=1}^{n} G_i(x_i) = \prod_{i=1}^{n} \left(1/\Delta_i\right) \quad \text{(for } -\Delta/2 < x_i < \Delta/2\text{)}, \hspace{1cm} (3.9)
\]

\[
F\{\bar{\alpha}(x,t)\} = F\{G(x)\} \cdot F\{\alpha(x,t)\}. \hspace{1cm} (3.10)
\]

The Fourier transform of the averaging function, \( F\{G(x)\} \), is given by:

\[
F\{G(x)\} = F \left\{ \prod_{i=1}^{n} G_i(x_i) \right\}
\]

\[
= \prod_{i=1}^{n} F\{G_i(x_i)\}
\]

\[
= \prod_{i=1}^{n} \int \limits_{-\Delta_i}^{\Delta_i} G_i(x_i) \exp(-i \omega_i x_i) \, dx_i
\]

\[
= \prod_{i=1}^{n} \left(1/\Delta_i\right) \int \limits_{-\Delta}^{\Delta} \exp(-i \omega_i x_i) \, dx_i
\]

\[
= \prod_{i=1}^{n} \{\sin(\omega_i \Delta_i/2) \} / (\omega_i \Delta_i/2). \hspace{1cm} (3.11)
\]
Figure 3.1: Reynolds Temporal Filter and its Fourier Transform.
Here, $\omega_i$ is wave number in the $x_i$ direction. The filter component $G_i(x_i)$ and its Fourier transform are plotted in Figure 3.2. Note that $F\{G_i(x_i)\}$ has appreciable values at high wave numbers which inflicts the same property on the large-scale $\tilde{\alpha}(x,t)$. Note also that, since the filter function has no temporal component, the Fourier transform $F\{\tilde{\alpha}(x,t)\}$ is non-zero for all frequencies.

In case of Leonard's spatial filtering (see section 2.3.3), the following special cases of Equations (3.1), (3.2), and (3.3) apply:

\[
\tilde{\alpha}(x,t) = \int_{-\infty}^{\infty} G(x-x') \alpha(x',t) \, dx', \quad (3.12)
\]

\[
G(x) = \prod_{i=1}^{n} G_i(x_i)
\]

\[
= \prod_{i=1}^{n} \frac{1}{\sqrt{\pi}} \left( \frac{1}{\Delta_i} \right) \exp\left( -\frac{\gamma x_i^2}{\Delta_i^2} \right), \quad (3.13)
\]

\[
F\{\tilde{\alpha}(x,t)\} = F\{G(x)\} \cdot F\{\alpha(x,t)\}. \quad (3.14)
\]

The Fourier transform of the averaging function, $F\{G(x)\}$, is given by:

\[
F\{G(x)\} = F \left\{ \prod_{i=1}^{n} G_i(x_i) \right\}
\]

\[
= \prod_{i=1}^{n} F\{G_i(x_i)\}
\]

\[
= \prod_{i=1}^{n} \int_{-\infty}^{\infty} G_i(x_i) \exp(-I \omega_i x_i) \, dx_i
\]

\[
= \prod_{i=1}^{n} \int_{-\infty}^{\infty} \frac{1}{\sqrt{\pi}} \left( \frac{1}{\Delta_i} \right) \exp\left( -\frac{\gamma x_i^2}{\Delta_i^2} \right)
\]

\[
\exp(-I \omega_i x_i) \, dx_i
\]

\[
= \prod_{i=1}^{n} \exp(-\omega_i^2 \Delta_i^2/4\gamma). \quad (3.15)
\]
Figure 3.2: Uniform Spatial Filter and its Fourier Transform.
The filter component $G_i(x_i)$ and its Fourier transform are plotted in Figure 3.3. It is clear that the high wave number components are successfully eliminated. The cut-off wave number, $\omega_{ic}$, is obviously a function of the filter width and the nondimensional constant $\gamma$. It is, therefore, the primary function of $\Delta_i$ and $\gamma$ to bring the value of $\omega_{ic}$ as close as possible to $2\pi/2\delta_i$ (rad./unit of length), where $\delta_i$ is the grid spacing in the $x_i$ direction. The constant $\gamma$ is usually set equal to 6, and $\Delta_i$ is usually a multiple of $\delta_i$. Note that no averaging is done in the temporal domain which means that $F\{\tilde{\omega}(x,t)\}$ has non-zero values at high frequencies.

3.3 THE NEW STF METHOD OF AVERAGING

It is now clear that Gaussian filtering possesses two important advantages over box filtering. First, the Gaussian filter defines a variable $\tilde{\omega}(x,t)$ over the averaging scales while the box filter implies a constant $\tilde{\omega}(x,t)$. The resulting SGS component (see Figure 2.3) is larger in case of box filtering. This means more importance attached to the ambiguous closure models. The second advantage is that Gaussian filters perform better in eliminating high wave number or high frequency components than do box filters. This is easily seen by comparing the two Fourier transforms (3.7) and (3.15).
Figure 3.3: Leonard's Spatial Filter and its Fourier Transform.
Curiously however, none of the above methods takes full advantage of the general averaging operation (3.1). Reynolds' method employs a filter function having only a temporal component. The Fourier transform of this filter component is small at high frequencies but does not depend on the wave number. Therefore, according to Equation (3.6), the Fourier transform of $\mathcal{A}(x,t)$ may vanish at high frequencies but not at high wave numbers. In case of uniform or Leonard's spatial filtering, the filter function has $n$ spatial components and no temporal components. Thus, according to Equations (3.10) and (3.14), the Fourier transform of $\mathcal{A}(x,t)$ vanishes at high wave numbers but not at high frequencies.

The ultimate goal of any averaging operation is to achieve a large-scale component whose Fourier transform is zero for frequencies greater than $2\pi/2 \delta_t$ (rad./unit of time) and for wave numbers greater than $2\pi/2 \delta_i$ (rad./unit of length).

Based on the above discussion, a new averaging scheme which filters in both time and space, with Gaussian filter components, is suggested. The complete scheme is given below with application to the three-dimensional Navier-Stokes Equation (2.4). Using the most general averaging operator:

$$\mathcal{A}(x,t) = \int_{-\infty}^{\infty} G(x-x',t-t') \alpha(x',t') \, dx' \, dt', \quad (3.16)$$

and the most general filter function:

$$G(x,t) = G_t(t) \prod_{i=1}^{n} G_i(x_i). \quad (3.17)$$

The temporal component, $G_t(t)$, is:
\[ G_t(t) = \frac{\sqrt{m}}{A_t} \exp(-\gamma t^2/A_t^2) \quad (\text{for all } t), \quad (3.18) \]

and the \( x_i \) spatial component, \( G_i(x_i) \), is:

\[ G_i(x_i) = \frac{\sqrt{y/n}}{A_i} \exp(-\gamma x_i^2/A_i^2) \quad (\text{for all } x_i). \quad (3.19) \]

All symbols are as defined previously. The Fourier transform of the large-scale component is obtained by transforming both sides of Equation (3.16). According to the convolution theorem, this gives:

\[ F\{\mathbb{P}(x,t)\} = F\{G(x,t)\} F\{\alpha(x,t)\}. \quad (3.20) \]

The Fourier transform of the filter function, \( F(G(x,t)) \), is given by:

\[
F\{G(x,t)\} = F\{G_t(t) \prod_{i=1}^{n} G_i(x_i)\} \\
= F\{G_t(t)\} \prod_{i=1}^{n} F\{G_i(x_i)\} \\
= \int_{-\infty}^{\infty} G_t(t) \exp(-I \omega t) \, dt \\
\prod_{i=1}^{n} \int_{-\infty}^{\infty} G_i(x_i) \exp(-I \omega_i x_i) \, dx_i \\
= \int_{-\infty}^{\infty} \left[\frac{\sqrt{y/n}}{A_i} \exp(-\gamma x_i^2/A_i^2) \right] \exp(-I \omega_i x_i) \, dx_i \\
= \exp\left(-\frac{\omega^2 A_i^2}{4y}\right) \prod_{i=1}^{n} \exp\left(-\frac{\omega_i^2 A_i^2}{4y}\right). \quad (3.21) \]

Figure 3.4 shows the filter components \( G_t(t) \) and \( G_i(x_i) \) along with their respective Fourier transforms.
Figure 3.4: STF Filter Components and Their Fourier Transforms.
Table 3.1 summarizes all the methods of averaging presented above. The advantage of the newly suggested STF is realized by examining the Fourier transform of the large-scale component. This Fourier transform, $F[\tilde{\alpha}(x,t)]$, is always equal to the Fourier transform of the total variable, which is non-zero for all frequencies and wave numbers, multiplied by the Fourier transform of the filter function.

Each of these three transforms is an $(n+1)$-dimensional function of $\omega_1, \ldots, \omega_n$ and $f$. In case of Reynolds' averaging, the multiplication of $F[\alpha(x,t)]$ by $[\sin(f \Delta t/2)]/(f \Delta t/2)$ results in $F[\tilde{\alpha}(x,t)]$ that is small at high frequencies but does not vanish at large values of $\omega_i (i=1,\ldots,n)$. In case of uniform or Leonard's spatial filtering, the multiplication of $F[\alpha(x,t)]$ by $F[\delta(x)]$ results in $F[\tilde{\alpha}(x,t)]$ that vanishes for $\omega_i > \omega_{ic} (i=1,\ldots,n)$ but does not vanish at high frequencies. When the newly suggested method is used, $F[\alpha(x,t)]$ is multiplied by $\exp(-f^2 \Delta_t^2/4Y) \prod_{i=1}^{n} \exp(-\omega_i^2 \Delta_t^2/4Y)$. This yields $F[\tilde{\alpha}(x,t)]$ that reduces to zero at $\omega_i > \omega_{ic} (i=1,\ldots,n)$ and at $f > f_c$. It is seen clearly that the newly suggested method is the only one capable of eliminating both high frequencies and high wave numbers from $\alpha(x,t)$. The resulting $\tilde{\alpha}(x,t)$, therefore, closely satisfies the requirements for being the large-scale component of $\alpha(x,t)$.

The cut-off values $\omega_{ic}$ and $f_c$ are functions of $Y$, and $\Delta_t$. These cut-off values must be brought as close as possible to $2\pi/2 \delta_t$ (rad./unit of length) and $2\pi/2 \delta_t$. 
TABLE 3.1 History of the Averaging Procedure.

<table>
<thead>
<tr>
<th>Definition of the Large-scale component</th>
<th>Reynolds Temporal Averaging 1982 to Present</th>
<th>Uniform Spatial Averaging 1950 to Present</th>
<th>Leonard's Spatial Filtering 1971 to Present</th>
<th>UFO suggested by the Author</th>
</tr>
</thead>
<tbody>
<tr>
<td>Definition of the filter function</td>
<td>$\phi(x,t) = \frac{1}{A} \text{ for } \frac{y}{A} \leq 0$</td>
<td>$G(x) = \sum G_{k}(t)$</td>
<td>$G_{k}(t) = \frac{1}{\sqrt{\pi}} e^{-y_{k}^{2}/A}$</td>
<td>$G_{k}(t) = \frac{1}{\sqrt{\pi}} e^{-y_{k}^{2}/A}$</td>
</tr>
<tr>
<td></td>
<td>$= 0$ Otherwise</td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

Fourier transform of the large-scale component

where $\phi(x,t) = \frac{\sin(\omega_{o}t/2)}{\omega_{o}}$
(rad./unit of time) respectively. In order to accomplish this, set \( Y=6 \), \( \Delta_i=m_i \delta_i \), and \( \Delta_i=m_i \delta_i \). Here \( m_i \) and \( m_i \) are positive numbers signifying the ratio between a filter component's width and its corresponding grid spacing. These ratios are usually chosen through numerical experiments.

3.4 **STF RULES OF AVERAGING**

The averaging operation (3.16) obviously satisfies the distributive law:

\[
\alpha_1 + \alpha_2 + \ldots = \bar{\alpha}_1 + \bar{\alpha}_2 + \ldots
\]  

(3.22)

Applying the averaging procedure (3.16) to \( (\partial \alpha/\partial t) \) yields:

\[
\bar{\partial \alpha}/\bar{\partial t} = \int_{-\infty}^{\infty} G(x-x', t-t') \left[ \partial \alpha(x', t')/\partial t' \right] dx' dt', \quad (3.23)
\]

which, after integration by parts with respect to \( t' \), yields:

\[
\bar{\partial \alpha}/\bar{\partial t} = \int_{-\infty}^{\infty} \left\{ \alpha(x', t') \ G(x-x', t-t') \right\} dx' \\
- \int_{-\infty}^{\infty} \alpha(x', t') \left[ \partial G(x-x', t-t')/\partial t' \right] dx' dt'. \quad (3.24)
\]

The first term in the right hand side is zero since \( G(x-x', t-t') \) rapidly approaches zero. It is easily seen by differentiating the filter function (3.17) that

\[
\partial G(x-x', t-t')/\partial t' = -\partial G(x-x', t-t')/\partial t. \quad (3.25)
\]

Thus Equation (3.24) becomes:

\[
\bar{\partial \alpha}/\bar{\partial t} = \int_{-\infty}^{\infty} \alpha(x', t') \left[ \partial G(x-x', t-t')/\partial t \right] dx' dt'
\]
Similarly, the following can be easily proved:
\[
\frac{\partial \alpha}{\partial x} = \frac{\partial \bar{\alpha}}{\partial x_i}.
\]  
(3.27)

3.5 APPLYING STF TO THE THREE-DIMENSIONAL NAVIER-STOKES EQUATION

To average the three-dimensional Navier-Stokes equation (2.4), according to the new procedure, first decompose \( u_i \) and \( u_j \) in the nonlinear inertial term using expression (2.5). This gives Equation (2.9) which is then averaged according to the three rules (3.22), (3.26), and (3.27). The averaging rule (2.16) is assumed true as an approximation. The result is:

\[
\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial (\bar{u}_i \bar{u}_j)}{\partial x_j} = \left( -\frac{1}{\rho} \right) \frac{\partial p}{\partial x_i} + \nu \left( \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} - \frac{\partial (\bar{u}_i \bar{u}_j)}{\partial x_j} \right). 
\]  
(3.28)

Now evaluate \( \bar{u}_i \bar{u}_j \) by applying the STF operation (3.16) to \( \bar{u}_i \bar{u}_j \):

\[
\bar{u}_i \bar{u}_j (x,t) = \int_{-\infty}^{\infty} G(x-x',t-t') \bar{u}_i \bar{u}_j (x',t') \, dx' \, dt'. 
\]  
(3.29)

Expressing \( \bar{u}_i \bar{u}_j (x',t') \) in terms of \( \bar{u}_i \bar{u}_j (x,t) \) through a Taylor series expansion gives:

\[
\bar{u}_i \bar{u}_j (x,t) = \int_{-\infty}^{\infty} G(x-x',t-t') \left\{ \bar{u}_i \bar{u}_j (x,t) \right\} + (t'-t) \frac{\partial \bar{u}_i \bar{u}_j (x,t)}{\partial t} 
\]
\[ + \sum_{k=1}^{n} (x_k - x_j) \frac{\partial \bar{u}_i \bar{u}_j (x,t)}{\partial x_k} \]
\[ + \left( \frac{1}{2} \right) (t' - t)^2 \frac{\partial^2 \bar{u}_i \bar{u}_j (x,t)}{\partial t^2} \]
\[ + \sum_{k=1}^{n} \left( \frac{1}{2} \right) (x_k - x_j)^2 \frac{\partial \bar{u}_i \bar{u}_j (x,t)}{\partial x_k^2} \]
\[ + \text{H.O.T.} \int dx^i \int dt^i. \]  

(3.30)

Neglecting the higher order terms (H.O.T.), the above equation is rearranged to:

\[ \bar{u}_i \bar{u}_j = \bar{u}_i \bar{u}_j \int_{-\infty}^{\infty} G(x-x',t-t') \, dx' \, dt' \]
\[ + \left( \frac{\partial \bar{u}_i \bar{u}_j}{\partial t} \right) \int_{-\infty}^{\infty} (t'-t) \, G(x-x',t-t') \, dx' \, dt' \]
\[ + \sum_{k=1}^{n} \left( \frac{\partial \bar{u}_i \bar{u}_j}{\partial x_k} \right) \int_{-\infty}^{\infty} (x_k - x_j) \, G(x-x',t-t') \, dx' \, dt' \]
\[ + 0.5 \left( \frac{\partial^2 \bar{u}_i \bar{u}_j}{\partial t^2} \right) \int_{-\infty}^{\infty} (t'-t)^2 \, G(x-x',t-t') \, dx' \, dt' \]
\[ + 0.5 \sum_{k=1}^{n} \left( \frac{\partial^2 \bar{u}_i \bar{u}_j}{\partial x_k^2} \right) \int_{-\infty}^{\infty} (x_k - x_j)^2 \, G(x-x',t-t') \, dx' \, dt'. \]  

(3.31)

The components of \( G(x,t) \) are defined in Equations (3.18) and (3.19). Note that each of these components is a Gaussian probability distribution with a zero mean; a variance equal to \( \Delta^2/2\gamma \) or \( \Delta^2/2\gamma; \) and a unit area under the curve. Therefore, Equation (3.31) reduces to:

\[ \bar{u}_i \bar{u}_j = \bar{u}_i \bar{u}_j + (\Delta_i^2/4\gamma) \frac{\partial^2 \bar{u}_i \bar{u}_j}{\partial t^2} \]
\[ + \sum_{k=1}^{n} (\Delta_k^2/4\gamma) \frac{\partial^2 \bar{u}_i \bar{u}_j}{\partial x_k^2}. \]  

(3.32)
Substituting (3.32) into (3.28) gives the final averaged equation which, in tensor notation, reads:

\[
\begin{align*}
\frac{\partial \tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j} \left[ \tilde{u}_i \tilde{u}_j + (\Delta_i^2/4\gamma) \frac{\partial^2 (\tilde{u}_i \tilde{u}_j)}{\partial t^2} \right] \\
+ (\Delta_i^2/4\gamma) \frac{\partial^2 (\tilde{u}_i \tilde{u}_j)}{\partial x_i^2} \frac{1}{\partial x_j} = (-1/\rho) \left( \frac{\partial \tilde{p}}{\partial x_i} \right) \\
+ \nabla (\tilde{u}_i \tilde{u}_j/\partial x_j \partial x_j) - \tilde{\sigma}(u_i^i u_j^j)/\partial x_j.
\end{align*}
\] (3.33)

Table 3.2 summarizes the different forms of the averaged Navier-Stokes equation. By induction from Table 3.2, the averaged forms of the three-dimensional scalar transport equation are obtained and listed in Table 3.3. Note that the original equations contain the total variables which contain components of high wave numbers and frequencies. Therefore, the original equations must be solved on a very fine grid. The averaged equations, on the other hand, contain the large-scale components of the variables. These large-scale components contain only those wave numbers and frequencies lower than certain cut-off values (see table 3.1). Therefore, the averaged equations can be solved on coarser grids.

The price paid for averaging is the appearance of the subgrid-scale terms (last terms in the right hand sides of the averaged equations). These terms must be replaced by the large-scale components through a closure model (see section 2.4). Another price paid for averaging is the appearance of the nonlinear filter terms. In the Leonard's averaged equations their exist n filter terms where n is the number of
**TABLE 3.2: Averaged Navier-Stokes Equation.**

<table>
<thead>
<tr>
<th>Method</th>
<th>The Three-Dimensional Navier-Stokes Equation</th>
</tr>
</thead>
</table>
| Unaveraged                    | \[
\begin{align*}
\frac{\partial \tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j} \left[ \tilde{u}_i \tilde{u}_j \right] = & \frac{-1}{\rho} \frac{\partial p}{\partial x_i} + \nu \frac{\partial^2 \tilde{u}_i}{\partial x_j \partial x_j}
\end{align*}
\] |
| Reynolds Averaging            | \[
\begin{align*}
\frac{\partial \tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j} \left[ \tilde{u}_i \tilde{u}_j \right] = & \frac{-1}{\rho} \frac{\partial \tilde{p}}{\partial x_i} + \nu \frac{\partial^2 \tilde{u}_i}{\partial x_j \partial x_j} - \frac{\partial u_i^j u_i^j}{\partial x_j}
\end{align*}
\] |
| Leonard's Averaging           | \[
\begin{align*}
\frac{\partial \tilde{u}_i}{\partial t} + \frac{\partial}{\partial x_j} \left[ \tilde{u}_i \tilde{u}_j + \frac{\Delta^2 \tilde{u}_i \tilde{u}_j}{4 \gamma} \right] = & \frac{-1}{\rho} \frac{\partial \tilde{p}}{\partial x_i} + \nu \frac{\partial^2 \tilde{u}_i}{\partial x_j \partial x_j} - \frac{\partial u_i^j u_i^j}{\partial x_j}
\end{align*}
\] |
| STF                           | \[
\begin{align*}
\frac{\partial \bar{u}_i}{\partial t} + \frac{\partial}{\partial x_j} \left[ \bar{u}_i \bar{u}_j + \frac{\Delta^2 \bar{u}_i \bar{u}_j}{4 \gamma} \right] + \frac{\Delta^2 \bar{u}_i \bar{u}_j}{4 \gamma} = & \frac{-1}{\rho} \frac{\partial \bar{p}}{\partial x_i} + \nu \frac{\partial^2 \bar{u}_i}{\partial x_j \partial x_j} - \frac{\partial \bar{u}_i^j \bar{u}_i^j}{\partial x_j}
\end{align*}
\] |
TABLE 3.3: Averaged Scalar Transport Equation

<table>
<thead>
<tr>
<th></th>
<th>The Three-Dimensional Scalar Transport Equation</th>
</tr>
</thead>
</table>
| Unaveraged     | \[
\frac{\partial c}{\partial t} + \frac{\partial}{\partial x_1} \left[ u \frac{\partial c}{\partial x_1} \right] = \alpha \frac{\partial^2 c}{\partial x_1^2} \]

| Reynolds Averaging | \[
\frac{\partial \bar{c}}{\partial t} + \frac{\partial}{\partial x_1} \left[ u \frac{\partial \bar{c}}{\partial x_1} \right] = \alpha \frac{\partial^2 \bar{c}}{\partial x_1^2} - \frac{2u'c'}{\partial x_1} \]

| Leonard's Averaging | \[
\frac{\partial \bar{c}}{\partial t} + \frac{\partial}{\partial x_1} \left[ u \frac{\partial \bar{c}}{\partial x_1} + \frac{\partial^2 \bar{u} \frac{\partial c}{\partial x_1}}{2x_1} \right] = \alpha \frac{\partial^2 \bar{c}}{\partial x_1^2} - \frac{2u'c'}{\partial x_1} \]

| STF             | \[
\frac{\partial \bar{c}}{\partial t} + \frac{\partial}{\partial x_1} \left[ u \frac{\partial \bar{c}}{\partial x_1} + \frac{\partial^2 \bar{u} \frac{\partial c}{\partial x_1}}{4x_1} + \frac{\partial \bar{u} \frac{\partial^2 c}{\partial x_1^2}}{4x_1} + \frac{\partial^3 \bar{u} \frac{\partial c}{\partial x_1^3}}{4x_1} \right] = \alpha \frac{\partial^2 \bar{c}}{\partial x_1^2} - \frac{2u'c'}{\partial x_1} \]
spatial directions in which averaging is desired. The new STF equations contain n+1 filter terms. The extra term results from filtering in the time domain. Naturally, all these extra terms require a long computation time. But the formidable problem of having to employ a huge number of nodes, to simulate a highly turbulent flow, is solved.
Chapter IV
THE ONE-DIMENSIONAL, TRANSIENT EQUATIONS

4.1 INTRODUCTION
The three-dimensional Navier-Stokes equation is extremely
cumbersome and expensive as far as its numerical solution is
concerned. The same is true about the three-dimensional sca­
lar transport equation. So much care and effort must be de­
voted to the numerical solution that, in many cases, impor­
tant physics have to be sacrificed through simplifying
assumptions.

For highly turbulent flows, the number of nodes required
to solve the three-dimensional equations is large even after
averaging the equations. With any attempt to reduce this
number of nodes, the intensity of resolved turbulence must
be reduced or a certain amount of instability and error must
be tolerated. The three-dimensional equations are therefore
unsuitable for testing and experimenting with new ideas in
modeling highly turbulent flows.

Many researchers resort to one-dimensional momentum and
transport equations to investigate certain problems in tur­
bulence modeling. The simplicity of such equations permits
modelers to concentrate their attention on the physics that
should be preserved in the averaging and closure schemes.
The numerical solution is so simplified that the interference from numerical errors and noise is at a minimum level.

This chapter is devoted to introducing the one-dimensional transient equations used in the present research. The original or unaveraged forms of the equations are presented here. Note that, for high Reynolds numbers, these equations must be solved on very dense grids. A sample solution of this kind is included below in order to highlight the similarities to the three-dimensional hydrodynamic equations. In the next chapter, these one-dimensional equations will be modeled (i.e. prepared for solution on coarser grids) according to the newly suggested and the existing methods of averaging and closure.

4.2 BURGERS EQUATION

Burgers (1939,1948) was the first to suggest a one-dimensional momentum equation as a model equation for real turbulence. Burgers used the equation in an attempt to investigate the role of the viscous and nonlinear terms in the Navier-Stokes equation. Burgers equation was later extensively used to examine the different characteristics of turbulence, and to test the different averaging and SGS models. See for example Burgers (1964); Meecham and Siegel (1964); Kraichnan (1968); Saffman (1968); Jeng(1969); Lee (1970); Jeng and Meecham (1971); Roache (1972); Murray (1973); Hosokawa and Yamamoto (1975); and Love (1980).
The Burgers equation is a nonlinear partial differential equation describing the behavior of a variable, \( u \), which is a function of time, \( t \), and a single coordinate, \( x \). The equation reads:

\[
\frac{\partial u}{\partial t} + \frac{1}{2} \frac{\partial u^2}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2}. \tag{4.1}
\]

If the values of \( u \) are given for all \( x \) at \( t=0 \), the above equation can be solved for the behavior of \( u \) as a function of \( x \) and \( t \) for \( t>0 \). At first glance, the Burgers equation is seen to retain both the advective and the dissipative natures of the Navier-Stokes Equation (2.4). Therefore, it is logically possible to gain some insight into these properties of turbulence from the Burgers equation. The Burgers equation also describes the formation and decay of weak shock waves in compressible fluids. Thus, the equation is important in its own right, as well as being a one-dimensional vehicle for testing approximations designed for Navier-Stokes turbulence.

The Burgers equation has a well known closed form solution when an initial distribution \( u(x,0) \) is given. The solution is:

\[
u(x,t) = -2\nu (\partial \ln \theta / \partial x), \tag{4.2}
\]

where \( \theta \), a function of the initial condition, is defined as:

\[
\theta(x,t) = \frac{1}{4\pi \nu t} \int_{-\infty}^{\infty} \exp\left[-\frac{1}{2\nu} \int u(x'',0) \, dx'' \right]
\]
$$\exp[-(x-x')/4\nu t] \, dx'. \quad (4.3)$$

An "exact" solution can also be obtained simply by discretizing and solving (4.1) on a very dense x-t grid. This approach is appropriate when $u(x,0)$ is random and therefore does not follow any mathematical expression.

The most important behavioral aspect of the solution $u(x,t)$ is that, due to the nonlinear term, the value of $|\partial u/\partial x|$ grows larger with time in regions where $(\partial u/\partial x)$ was initially negative. On the other hand, in regions of initially positive $(\partial u/\partial x)$, the values of this gradient becomes smaller with time. This means gradual development of shock fronts connected by regions of mildly sloping velocity. Also, the magnitude of the velocity values, $u(x,t)$, gradually decays with time as a result of the dissipative term. Figure 4.1 demonstrates the behavior just described. The existence of the shocks in the spatial distribution of $u$ is what makes the Burgers equation a "model equation for turbulence." These shocks are nothing but a variable which changes so rapidly with space that a coarse grid is not capable of handling the solution. That is exactly the definition of turbulence from a purely numerical point of
Figure 4.1: An Exact Solution Of Burgers Equation.
view. When the Burgers equation is averaged and closed, the variable \( u(x,t) \) is replaced by its large-scale component \( \bar{u}(x,t) \). This large-scale component is expected to vary less rapidly with space so that a coarser grid becomes capable of handling the numerical solution. In other words, the effect of averaging the Burgers equation is to spread out the thin shock fronts over longer distances.

It is known that the Burgers equation is capable of propagating the spatial distribution of velocity, through the flow domain, with a speed equal to the spatial mean of \( u(x,t) \) which remains constant with time. Thus, point B in Figure 4.1 feels the shocks passing through it from left to right. Therefore, a time history of velocity at point B (Figure 4.2) shows the shocks developing in time, as well as the gradual decay due to viscous dissipation. The rapid variations of \( u \), in both the spatial and temporal domains, are of special importance to this research since a new averaging procedure which filters in both space and time is being tested.
Figure 4.2: Time History of Velocity at Point B (Figure 4.1).
4.3 **ENERGY EQUATION**

An important aspect of the solution of Burgers equation is the temporal variation of the total energy contained in the flow domain. This total energy (per unit mass) is measured by \(<v^2/2>\), where \(v\) is the velocity \(u\) minus its spatial mean \(m\); and \(< >\) denotes an ensemble average. Ensemble averaging means integration over a long spatial distance; then averaging the result over a large number of realizations (see Meecham and Siegel 1964).

An "Energy Equation" describing the temporal variation of \(<v^2/2>\) can be obtained from (4.1) by decomposing \(u\) into \(v+m\):

\[
\frac{\partial (v+m)}{\partial t} = -\frac{1}{2} \frac{\partial (v+m)^2}{\partial x} + \nu \frac{\partial^2 (v+m)}{\partial x^2}. \tag{4.4}
\]

Since \(\frac{\partial m}{\partial x}\) is zero by definition, the above equation reduces to:

\[
\frac{\partial v}{\partial t} = -\frac{\partial m}{\partial t} - \frac{1}{2} \frac{\partial v^2}{\partial x} - m \frac{\partial v}{\partial x} + \nu \frac{\partial^2 v}{\partial x^2}. \tag{4.5}
\]

Multiplying through by \(v\) yields:

\[
\frac{\partial (v^2/2)}{\partial t} = -v \frac{\partial m}{\partial t} - \frac{1}{2} \frac{\partial v^3}{\partial x} - (1/2) m \frac{\partial v^2}{\partial x} + \nu v \frac{\partial^2 v}{\partial x^2}. \tag{4.6}
\]
To ensemble average the above equation, first integrate over a large spatial distance, say from $x_1$ to $x_2$:

$$\frac{1}{2} \left[ \int_{x_1}^{x_2} (v^2/2) \, dx \right] / \partial t = -m(\partial m/\partial t) - (1/3) [v^3(x_2,t)] - v^3(x_1,t) - (1/2) m \left[ v^2(x_2,t) - v^2(x_1,t) \right] + \int_{x_1}^{x_2} \left( \frac{\partial^2 v}{\partial x^2} \right) \, dx. \quad (4.7)$$

To complete the ensemble averaging, each term in the above equation is averaged over a large number of realizations. Since $v(x,t)$ is statistically homogeneous in $x$, then the average of $v^3(x_2,t)$, over a large number of realizations, is equal to that of $v^3(x_1,t)$. Also, the average of $v^2(x_2,t)$ is equal to that of $v^2(x_1,t)$. Figure 4.1 shows that the mean $m$ remains constant with time. In fact, the initial value of $m$ is 3.0 (units of length/unit of time), and the final value, after 2000 time steps, is 2.9935 (units of length/unit of time). This means a change of 0.2% compared to the huge reduction in $v$ at point B as observed in Figure 4.2. Thus, $\partial m/\partial t$ is zero and Equation (4.7) is reduced to:

$$\partial <v^2/2>/\partial t = \nabla \cdot \nabla^2 v/\partial x^2. \quad (4.8)$$

The inertial term $(1/2)\partial u^2/\partial x$ is, therefore, energy conservative because it does not contribute to the energy balance equation (4.8). The time rate of change of total ener-
gy is caused solely by viscous dissipation. For all practical purposes, Equation (4.8) can be derived by simply replacing $u$ by $v$ in Equation (4.1); multiplying by $v$ and taking ensemble average:

$$\frac{\partial \langle v^2/2 \rangle}{\partial t} = -\frac{1}{2} \langle v \frac{\partial v}{\partial x} \rangle + \nu \langle \frac{\partial^2 v}{\partial x^2} \rangle.$$  \hspace{1cm} (4.9)

The importance of the energy equation (4.9) is the insight gained into the process of energy change and dissipation. If the Burgers equation is to be averaged and closed, the appearance of filter terms and eddy viscosity or turbulent dissipation terms is expected. An energy analysis, in the above fashion, should prove very useful in studying the role of each of the new terms in the production, transfer, and dissipation of energy.

4.4 SCALAR TRANSPORT EQUATION

The three-dimensional scalar transport equation, in tensor notation, reads:

$$\frac{\partial c}{\partial t} + \frac{\partial u_i c}{\partial x_i} = \alpha \frac{\partial^2 c}{\partial x_i \partial x_i},$$  \hspace{1cm} (4.10)

where $c$ is the scalar concentration; and $\alpha$ is the molecular diffusivity. By averaging over a constant cross-sectional area in the $y$-$z$ plane, one may obtain the following one-dimensional equation (see Pritchard 1958, and Okubo 1964):

$$\frac{\partial c}{\partial t} + \frac{\partial u c}{\partial x} = \alpha \frac{\partial^2 c}{\partial x^2}.$$  \hspace{1cm} (4.11)
The above equation has been extensively used by researchers interested in one-dimensional convection and diffusion of pollutants. See for example Holley and Harleman (1965); Holley (1969); and Fischer (1967, 1968, 1969).

Figure 4.3 shows a sample exact solution of (4.11). The concentration field is convected by the same velocity field shown in Figure 4.1. Figure 4.4 shows a time history of concentration at the same point B shown in Figure 4.1. The most important aspect of the solution $c(x,t)$ is the existence of regions and periods in which the slopes $\partial c/\partial x$ and $\partial c/\partial t$ are very steep. Because of such steep slopes, very dense grid must be used or a very potent turbulence model must be implemented to prepare the equation for solution on coarser grids.
Figure 4.3: An Exact Solution of the Transport Equation.
Figure 4.4: Time Histories of $u$ and $c$ at Point B.
Chapter V
IMPROVED ONE-DIMENSIONAL, TRANSIENT MODELING

5.1 INTRODUCTION

Chapters II and III present all the averaging and closure methods applied in this research. In summary, the different averaging methods are distinguished by the way they handle the expanded nonlinear terms:

\[
\bar{u_i} u_j = (\bar{u_i} + u_i^\prime) (\bar{u_j} + u_j^\prime)
\]

\[
= \bar{u_i} u_j + \bar{u_i} u_j^\prime + u_i^\prime \bar{u_j} + u_i^\prime u_j^\prime, \quad \text{(all methods)} \quad (5.1)
\]

The term \(\bar{u_i} u_j\) is approximated as:

\[
\bar{u_i} u_j = \bar{u_i} \bar{u_j}, \quad \text{(Reynolds)} \quad (5.2)
\]

\[
\bar{u_i} u_j = \bar{u_i} \bar{u_j} + \frac{n}{2} (\Delta^2/4\gamma) \frac{\partial^2 \bar{u_i} \bar{u_j}}{\partial x_k^2}, \quad \text{(Leonard's)} \quad (5.3)
\]

\[
\bar{u_i} \bar{u_j} = \bar{u_i} \bar{u_j} + (\Delta^2/4\gamma) \frac{\partial^2 \bar{u_i} \bar{u_j}}{\partial t^2}
+ \frac{n}{2} (\Delta^2/4\gamma) \frac{\partial^2 \bar{u_i} \bar{u_j}}{\partial x_k^2}. \quad \text{(STF)} \quad (5.4)
\]

The above three expressions are obtained by averaging \(\bar{u_i} \bar{u_j}\) according to the operations (2.10), (2.24) and (3.16) respectively. The cross terms are usually neglected (or modeled as in section 5.3):

\[
\bar{u_i} u_j^\prime + u_i^\prime \bar{u_j} = 0, \quad \text{(5.5)}
\]
and the closure methods, applied in this research, use the Boussinesq concept to evaluate $u_i^j u_j^i$:

$$u_i^j u_j^i = -K_{i,j} \frac{\partial u_i}{\partial x_j} + 2k \delta_{i,j}/3,$$  \hspace{1cm} (5.6)

where $k$ is the summation of the normal stresses:

$$2k = \sum_{l=1}^{n} u_i^l u_j^l.$$  \hspace{1cm} (5.7)

For the eddy viscosities, $K_{i,j}$, this research employs either constant values:

$$K_{i,j} = \text{constant},$$  \hspace{1cm} (5.8)

or the Smagorinsky's model:

$$K_{i,j} = (c_r \Delta)^2 \left[ \frac{\partial u_i}{\partial x_j} \frac{\partial u_j}{\partial x_i} + \frac{\partial u_i}{\partial x_i} \frac{\partial u_j}{\partial x_j} \right].$$  \hspace{1cm} (5.9)

In this chapter, the above methods are applied to the one-dimensional equations presented in Chapter IV. Therefore, a one-dimensional analogue of the above methods is needed. This is presented in the following sections. Complete details of the finite difference discretization, for the original and the modeled one-dimensional equations, are presented in the next chapter.
5.2 **ONE-DIMENSIONAL MOMENTUM ANALOGY**

A one-dimensional analogue to Equations (5.1) through (5.9) can be obtained simply by setting \( i = j = 1 \) and \( n = 1 \). The direction \( x_i \) is called \( x \) and the velocity \( u_i \) is called \( u \). Thus, the expanded nonlinear terms are treated by the different averaging methods as follows:

\[
\overline{uu} = (\overline{u+u'})(\overline{u+u'})
\]

\[
= \overline{uu} + 2\overline{uu'} + u'u'. \quad \text{(all methods) (5.10)}
\]

The term \( \overline{uu} \) is approximated as:

\[
\overline{uu} = \overline{uu}, \quad \text{(Reynolds) (5.11)}
\]

\[
\overline{uu} = \overline{uu} + (\Delta_x^2/4\nu) \overline{\partial^2 u/\partial x^2}, \quad \text{(Leonard's) (5.12)}
\]

\[
\overline{uu} = \overline{uu} + (\Delta_t^2/4\nu) \overline{\partial^2 u/\partial t^2}
+ (\Delta_x^2/4\nu) \overline{\partial^2 u/\partial x^2}. \quad \text{(STF) (5.13)}
\]

The cross terms may be neglected:

\[
2\overline{uu'} = 0, \quad \text{(5.14)}
\]

and the Boussinesq concept, for evaluating \( u'u' \), is:

\[
\overline{u'u'} = -K(\partial\overline{u}/\partial x), \quad \text{(5.15)}
\]

where \( K \) is either constant or given by the Smagorinsky's model:

\[
K = (c_r \Delta^3_x) [2(\partial\overline{u}/\partial x)^2]^{1/2}. \quad \text{(5.16)}
\]
For the purpose of this research, Equation (5.16) is rearranged in the following form:

\[ K = c_r \frac{\delta^2}{\delta x^2} |\partial \overline{u}/\partial x|, \tag{5.17} \]

where \( |\partial \overline{u}/\partial x| \) denotes the average over a length \( w \) of the quantity \( |\partial \overline{u}/\partial x| \). When \( w = 0 \), Equation (5.17) is a one-dimensional analogue of the Smagorinsky's model (5.9). See Smagorinsky (1963); and Lilly (1966), (1967). In the limit \( w = L \), where \( L \) is the total length of the flow domain, Equation (5.17) is the "Direct-Interaction" closure used by Leslie and Quarini (1979); and Love and Leslie (1977).

5.3 CLARK'S REDUCTION

The filter terms in Equations (5.12) and (5.13) are second order derivatives. When inserted into the averaged momentum equation, these terms are differentiated once more with respect to space. The result is third order derivatives which are troublesome with regards to their numerical discretization (see table 3.2). Clark et al. present a method to reduce the order of these derivatives. In a one-dimensional case, instead of neglecting the cross term \( 2\overline{uu}' \), the Leonard's spatial filtering operation (2.24), with \( n = 1 \), is applied to the variable \( u \). The result can be obtained simply by induction from (5.3):

\[ \overline{u} = u + (\Delta^2/4 \nu) \overline{\partial u/\partial x^2}. \tag{5.18} \]

Since \( \overline{u} \) is also equal to \( u - u' \) then:
\[ u' = -(\Delta_x^2/4Y) \frac{\delta^2 u}{\delta x^2}. \quad (5.19) \]

Multiplying both sides by \( \bar{u} \), and using \( u = \bar{u} + u' \) gives:

\[ \bar{u} u' = -(\Delta_x^2/4Y) \{ \bar{u} \frac{\delta^2 \bar{u}}{\delta x^2} + \bar{u} \frac{\delta^2 u'}{\delta x^2} \}. \quad (5.20) \]

Applying the averaging rule (2.13) on the above equation yields:

\[ \bar{u} u' = -(\Delta_x^2/4Y) \{ \bar{u} \frac{\delta^2 \bar{u}}{\delta x^2} + \bar{u} \frac{\delta^2 u'}{\delta x^2} \}. \quad (5.21) \]

Since \( u' \) is of an order of magnitude much smaller than \( \bar{u} \), and since \( u' \) fluctuates rapidly within the averaging scale and has a mean value of approximately zero, the last term of Equation (5.21) can be neglected. The lowest order approximation of \( \bar{u} \frac{\delta^2 \bar{u}}{\delta x^2} \) is just \( \bar{u} \frac{\delta^2 \bar{u}}{\delta x^2} \). Thus, Equation (5.21) reduces to:

\[ \bar{u} u' = -(\Delta_x^2/4Y) \bar{u} \frac{\delta^2 \bar{u}}{\delta x^2}. \quad (5.22) \]

The approximation of the cross term by the expression (5.22), instead of simply neglecting it, may seem to further complicate the averaged equation. The opposite however becomes true when (5.22) and (5.12) are inserted into (5.10):

\[ \bar{u} u = \bar{u} u + (\Delta_x^2/4Y) \frac{\delta^2 \bar{u} u}{\delta x^2} - (\Delta_x^2/2Y) \bar{u} \frac{\delta \bar{u} u}{\delta x} + u' u' \]

\[ = \bar{u} u + (\Delta_x^2/4Y) \frac{\delta^2 \bar{u} u}{\delta x^2} \]

\[ - (\Delta_x^2/2Y) \{ (1/2) \frac{\delta^2 \bar{u} u}{\delta x^2} - (\delta \bar{u} u)^2 \} + u' u' \]

\[ = \bar{u} u + (\Delta_x^2/2Y) \{ (\delta \bar{u} u)^2 \} + u' u'. \quad (5.23) \]
The filter term is now a first order derivative. This obviously ensures simpler numerical discretization and less complicated treatment of the boundary conditions.

5.4 Extension of Clark's Reduction to the New Averaging Procedure

The Clark's method for reducing the order of the filter terms can be easily extended to cover the newly suggested STF scheme. The new filtering operation (3.16), with \( n=1 \), is applied to the variable \( u \). By induction from (5.4), the result is:

\[
\bar{u} = u + \left( \frac{\Delta t^2}{4Y} \right) \frac{\partial u}{\partial t} + \left( \frac{\Delta \gamma^2}{4Y} \right) \frac{\partial^2 u}{\partial x^2}.
\]  

(5.24)

Since \( \bar{u} \) is also equal to \( u - u' \), then:

\[
u' = -\left( \frac{\Delta t^2}{4Y} \right) \frac{\partial u}{\partial t} - \left( \frac{\Delta \gamma^2}{4Y} \right) \frac{\partial^2 u}{\partial x^2}.
\]  

(5.25)

Multiplying both sides by \( \bar{u} \), and using \( u=\bar{u}+u' \), gives:

\[
\overline{uu'} = -\left( \frac{\Delta t^2}{4Y} \right) \left\{ \bar{u} \left( \frac{\partial \bar{u}}{\partial t} \right)^2 + \bar{u} \left( \frac{\partial u'}{\partial t} \right)^2 \right\} \\
\quad -\left( \frac{\Delta \gamma^2}{4Y} \right) \left\{ \bar{u} \left( \frac{\partial \bar{u}}{\partial x} \right)^2 + \bar{u} \left( \frac{\partial u'}{\partial x} \right)^2 \right\}.
\]  

(5.26)

Applying the averaging rule (2.13) to the above equation yields:

\[
\overline{uu'} = -\left( \frac{\Delta t^2}{4Y} \right) \left\{ \bar{u} \left( \frac{\partial \bar{u}}{\partial t} \right)^2 + \bar{u} \left( \frac{\partial \bar{u}'}{\partial t} \right)^2 \right\} \\
\quad -\left( \frac{\Delta \gamma^2}{4Y} \right) \left\{ \bar{u} \left( \frac{\partial \bar{u}}{\partial x} \right)^2 + \bar{u} \left( \frac{\partial \bar{u}'}{\partial x} \right)^2 \right\}.
\]  

(5.27)
The same arguments used to derive (5.22) are invoked to reduce Equation (5.27) into:

\[
\bar{u}u' = \left(\frac{\Delta_i^2}{4Y}\right) \bar{u} \frac{\partial \bar{u}}{\partial t} - \left(\frac{\Delta_x^2}{4Y}\right) \bar{u} \frac{\partial^2 \bar{u}}{\partial x^2}. \tag{5.28}
\]

The Clark's reduction is achieved by inserting (5.28) and (5.13) into Equation (5.10):

\[
\bar{u}u = \bar{u} \bar{u} + \left(\frac{\Delta_i^2}{4Y}\right) \bar{u} \frac{\partial \bar{u}}{\partial t} + \left(\frac{\Delta_x^2}{4Y}\right) \bar{u} \frac{\partial^2 \bar{u}}{\partial x^2} - \left(\frac{\Delta_i^2}{2Y}\right) \bar{u} \frac{\partial \bar{u}}{\partial t} - \left(\frac{\Delta_x^2}{2Y}\right) \bar{u} \frac{\partial^2 \bar{u}}{\partial x^2} + \bar{u}'u' \tag{5.29}
\]

Both the spatial and temporal filter terms are now first order derivatives. This simplifies the numerical solution and the treatment the boundary conditions.

### 5.5 One-Dimensional Scalar Transport Analogy

In a one-dimensional scalar transport equation, the averaged nonlinear quantity takes the form \(\bar{u}c\) where \(c\) is the concentration. The decomposition of \(u\) and \(c\) into \(\bar{u}+u'\) and \(\bar{c}+c'\) yields:

\[
\bar{u}c = \left(\bar{u}+u'\right)\left(\bar{c}+c'\right)
\]

\[
= \bar{u}\bar{c} + \bar{u}c' + u'\bar{c} + u'c'. \tag{5.30}
\]

In analogy to the momentum transport case, the different averaging approaches treat the terms in (5.30) as follows:

\[
\bar{u}\bar{c} = \bar{u}\bar{c}, \tag{Reynolds} (5.31)
\]
\[
\overline{\dot{u}c} = \overline{\dot{u}c} + (\Delta_x^2/4Y) \frac{\partial^2 \overline{\dot{u}c}}{\partial x^2} , \quad \text{(Leonard's) (5.32)}
\]
\[
\overline{\dot{u}c} = \overline{\dot{u}c} + (\Delta_t^2/4Y) \frac{\partial^2 \overline{\dot{u}c}}{\partial t^2}
\]
\[
+ (\Delta_x^2/4Y) \frac{\partial^2 \overline{\dot{u}c}}{\partial x^2} . \quad \text{(STF) (5.33)}
\]

The above equations are obtained simply by induction from (5.11), (5.12) and (5.13) or by applying the averaging operations (2.10), (2.24) and (3.16), with \( n=1 \), to the variable \( \overline{\dot{u}c} \). The cross terms are usually neglected:

\[
\overline{\dot{u}c} + u'c = 0 , \quad \text{(5.34)}
\]

and the closure methods, used in this research, employ the Boussinesq eddy diffusivity concept to evaluate \( \overline{u'c'} \):

\[
\overline{u'c'} = -D(\partial \overline{\dot{c}}/\partial x) . \quad \text{(5.35)}
\]

Here \( D \) is the eddy diffusivity which is related to the eddy viscosity through the turbulent Schmidt number \( S_t \):

\[
D = K/S_t . \quad \text{(5.36)}
\]

The eddy viscosity, \( K \), is either constant or as given by Equation (5.17).
5.6 **EXTENSION OF CLARK'S REDUCTION TO SCALAR TRANSPORT**

Again, the filter terms in Equation (5.32) and (5.33) are second order derivatives. In a fashion similar to Clark's method (section 5.3) the order of these derivatives can be reduced. Instead of neglecting the cross terms, the filtering operation (3.16) with n=1 is applied to the variable c. By induction from (5.4), the result is:

$$\bar{c} = c + (\Delta_t^2/4\gamma) \frac{\partial^2 c}{\partial t^2} + (\Delta_x^2/4\gamma) \frac{\partial^2 c}{\partial x^2}. \quad (5.37)$$

Since $\bar{c}$ is also equal to $c-c'$, then:

$$c' = -(\Delta_t^2/4\gamma) \frac{\partial^2 c}{\partial t^2} - (\Delta_x^2/4\gamma) \frac{\partial^2 c}{\partial x^2}. \quad (5.38)$$

Multiplying both sides by $\bar{u}$, and using $c=\bar{c}+c'$ gives:

$$\bar{u}c' = -(\Delta_t^2/4\gamma) \left\{ \bar{u} \frac{\partial^2 \bar{c}}{\partial t^2} + \bar{u} \frac{\partial^2 c'}{\partial t^2} \right\}
- (\Delta_x^2/4\gamma) \left\{ \bar{u} \frac{\partial^2 \bar{c}}{\partial x^2} + \bar{u} \frac{\partial^2 c'}{\partial x^2} \right\}. \quad (5.39)$$

Applying the averaging rule (2.13) to the above equation yields:

$$\overline{uc'} = -(\Delta_t^2/4\gamma) \left\{ \overline{\bar{u} \frac{\partial^2 \bar{c}}{\partial t^2}} + \overline{\bar{u} \frac{\partial^2 c'}{\partial t^2}} \right\}
- (\Delta_x^2/4\gamma) \left\{ \overline{\bar{u} \frac{\partial^2 \bar{c}}{\partial x^2}} + \overline{\bar{u} \frac{\partial^2 c'}{\partial x^2}} \right\}. \quad (5.40)$$

The same arguments used to derive (5.22) are invoked to reduce Equation (5.40) into:

$$\overline{uc'} = -(\Delta_t^2/4\gamma) \bar{u} \frac{\partial^2 \bar{c}}{\partial t^2} - (\Delta_x^2/4\gamma) \bar{u} \frac{\partial^2 \bar{c}}{\partial x^2}. \quad (5.41)$$

A similar derivation can be carried out to obtain:
\[
\overline{u'c} = -(\Delta_s^2/4Y) \overline{c} \overline{\delta u/\delta t}^2 - (\Delta_s^2/4Y) \overline{c} \overline{\delta^2 u/\delta x^2}. \quad (5.42)
\]

The order of the filter terms is reduced when Equations (5.42), (5.41) and (5.33) are inserted into (5.30):

\[
\overline{u'c} = \overline{uc} + (\Delta_s^2/4Y) \overline{\delta u_c/\delta t}^2 + (\Delta_s^2/4Y) \overline{\delta^2 u_c/\delta x^2} - (\Delta_s^2/4Y) \overline{\delta u_c/\delta t}^2 - (\Delta_s^2/4Y) \overline{\delta^2 u_c/\delta x^2} - (\Delta_s^2/4Y) \overline{\delta u_c/\delta t}^2 - (\Delta_s^2/4Y) \overline{\delta^2 u_c/\delta x^2} + \overline{uc}'. \quad (5.43)
\]

Separating the time derivatives from the space derivatives, Equation (5.43) is rearranged as follows:

\[
\overline{u'c} = \overline{uc} + (\Delta_s^2/4Y) \{\overline{\delta^2 u_c/\delta t}^2 - \overline{\delta u_c/\delta t}^2 - \overline{\delta^2 u_c/\delta x^2}\} + (\Delta_s^2/4Y) \{\overline{\delta^2 u_c/\delta x^2} - \overline{\delta u_c/\delta x}^2 - \overline{\delta^2 u_c/\delta x^2}\} + \overline{uc}'. \quad (5.44)
\]

After some algebra, and without approximating or neglecting any of the terms, the above equation reduces to:

\[
\overline{u'c} = \overline{uc} + (\Delta_s^2/2Y) \{\overline{\delta u/\delta t})(\overline{\delta c/\delta t}) \}
+ (\Delta_s^2/2Y) \{\overline{\delta u/\delta x})(\overline{\delta c/\delta x}) \} + \overline{uc}'. \quad (5.45)
\]

The filter terms are now reduced to first order derivatives.
5.7 SUMMARY OF ONE-DIMENSIONAL ANALOGUES

The one-dimensional transient methods, presented in the preceding sections, are summarized in table 5.1. The averaging operations (2.10), (2.24) and (3.16) are reduced to one spatial dimension and listed in the table. The treatment of the averaged nonlinear terms and their components (large-scale, cross and SGS terms) is also tabulated. The table facilitates comparison between the different averaging methods, with and without the Clark's reduction. Column 6 in table 5.1 indicates whether or not a particular averaging method is applied in the present research. The two closure methods (constant or Smagorinsky's K) will be used in different combinations with the averaging methods marked 'yes' in column 6.

5.8 THE MODELED ONE-DIMENSIONAL EQUATIONS

The above methods are applied here to prepare the one-dimensional equations (Chapter IV) for solution on coarse grids. The two equations are rewritten below for convenience:

\[
\frac{\partial u}{\partial t} + \left(\frac{1}{2}\right) \frac{\partial u^2}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2}, \quad (5.46)
\]

\[
\frac{\partial c}{\partial t} + \frac{\partial uc}{\partial x} = \alpha \frac{\partial^2 c}{\partial x^2}. \quad (5.47)
\]

In the nonlinear terms, decompose \( u \) into \( \bar{u} + u' \) and \( c \) into \( \bar{c} + c' \):

\[
\frac{\partial u}{\partial t} + \left(\frac{1}{2}\right) \frac{\partial [\bar{u}u + 2\bar{u}u' + u'u']}{\partial x} = \nu \frac{\partial^2 u}{\partial x^2} , \quad (5.48)
\]

\[
\frac{\partial c}{\partial t} + \frac{\partial [\bar{u}c + \bar{u}c' + u'\bar{c} + u'c']}{\partial x} = \alpha \frac{\partial^2 c}{\partial x^2} . \quad (5.49)
\]
Table 5.1 One-Dimensional Averaging and Closure.
(Continued Next Page).

<table>
<thead>
<tr>
<th>AVERAGING METHODS</th>
<th>ONE-DIMENSIONAL AVERAGING OPERATION</th>
<th>AVERAGING OF THE NONLINEAR TERMS</th>
<th>APPLIED ZERO-EQUATION IN CLOSURE MODELS</th>
</tr>
</thead>
<tbody>
<tr>
<td>REYNOLDS' TEMPORAL AVERAGING</td>
<td>$G(x,t) = \int G(x-t')G(t-t')dt'$ where $G(t) = -\frac{1}{t}$ for $\frac{x}{2} \leq t \leq \frac{x}{2}$</td>
<td>$\overline{uu} = \overline{uc} = \overline{uc'} = 0$</td>
<td>YES</td>
</tr>
<tr>
<td>LEONARD'S SPATIAL FILTERING</td>
<td>$G(x) = \frac{1}{\lambda} e^{-x^2/\lambda^2}$</td>
<td>$\overline{uu} = \overline{uc} = \overline{uc'} = 0$</td>
<td>NO $k = \text{constant}$ or $k = c_r \frac{\lambda}{\lambda_{\text{ref}}}$</td>
</tr>
<tr>
<td>LEONARD'S SPATIAL FILTERING WITH CLARK'S REDUCTION</td>
<td>Same as above</td>
<td>$\overline{uu'} = \frac{\partial}{\partial x} \left( \frac{\lambda^2}{\lambda_{\text{ref}}^2} \right) + \frac{\partial}{\partial x} \left( \frac{\lambda^2}{\lambda_{\text{ref}}^2} \right)$</td>
<td>YES</td>
</tr>
</tbody>
</table>

Note: $\overline{uu} = \overline{uc} = \overline{uc'} = 0$ implies zero cross terms for the closure models.
Table 5.1 (Continued).

<table>
<thead>
<tr>
<th>AVERAGING METHODS</th>
<th>ONE-DIMENSIONAL AVERAGING OPERATION</th>
<th>LARGE-SCALE TERMS</th>
<th>CROSS TERMS</th>
<th>APPLIED ZERO-EQUATION CLOSURE IN THIS RESEARCH</th>
</tr>
</thead>
<tbody>
<tr>
<td>STF G(x,t) = G(x-t) * G(x-t') * o(x',t')dx'dt'</td>
<td>2uu' = 0</td>
<td>2uu' = 0</td>
<td>NO</td>
<td></td>
</tr>
<tr>
<td>[ G(x,t) = G(x) * G(t) ] G(x-t) * ( \frac{1}{\Lambda} ) e^{-2x^2/\Lambda}</td>
<td>2uu' = 0</td>
<td>2uu' = 0</td>
<td>k = constant</td>
<td></td>
</tr>
<tr>
<td>[ G(\Lambda) = \frac{1}{\sqrt{\pi}} e^{-x^2/\Lambda} ]</td>
<td>uc = 0</td>
<td>uc = 0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>[ u'c = 0 ]</td>
<td>uc' = 0</td>
<td>uc' = 0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>[ k = constant ]</td>
<td>uc = ( \frac{\Lambda}{4\pi} ) uc</td>
<td>uc = ( \frac{\Lambda}{4\pi} ) uc</td>
<td></td>
<td></td>
</tr>
<tr>
<td>[ k = constant ]</td>
<td>uc' = ( \frac{\Lambda}{4\pi} ) uc</td>
<td>uc' = ( \frac{\Lambda}{4\pi} ) uc</td>
<td></td>
<td></td>
</tr>
<tr>
<td>STF WITH CLARK'S REDUCTION</td>
<td>Same as above</td>
<td>Same as above</td>
<td>YES</td>
<td></td>
</tr>
<tr>
<td>[ u = u' - k \frac{\partial u}{\partial x} ]</td>
<td>2uu' = 0</td>
<td>2uu' = 0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>[ u = u' - k \frac{\partial u}{\partial x} ]</td>
<td>uc = 0</td>
<td>uc = 0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>[ u'c = 0 ]</td>
<td>uc' = 0</td>
<td>uc' = 0</td>
<td></td>
<td></td>
</tr>
<tr>
<td>[ k = c_r \frac{\partial u}{\partial x} ]</td>
<td>uc = ( \frac{\Lambda}{4\pi} ) uc</td>
<td>uc = ( \frac{\Lambda}{4\pi} ) uc</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
As seen in Chapters II and III, the following averaging rules are valid for the three averaging methods applied in this research:

\[
\alpha_1 + \alpha_2 + \ldots = \bar{\alpha}_1 + \bar{\alpha}_2 + \ldots, \quad (5.50)
\]

\[
\frac{\partial \alpha}{\partial x} = \frac{\partial \bar{\alpha}}{\partial x}, \quad (5.51)
\]

\[
\frac{\partial \alpha}{\partial t} = \frac{\partial \bar{\alpha}}{\partial t}. \quad (5.52)
\]

Thus, averaging (5.48) and (5.49), according to all averaging procedures gives:

\[
\frac{\partial \bar{\alpha}}{\partial t} + \frac{1}{2} \varepsilon \left[ \bar{\alpha} \bar{u} + 2 \bar{u} \bar{u}' + \bar{u}' \bar{u}' \right] / \partial x = \gamma \frac{\partial^2 \bar{\alpha}}{\partial x^2}, \quad (5.53)
\]

\[
\frac{\partial \tilde{c}}{\partial t} + \delta \left[ \bar{c} \bar{c} + \bar{c}' \bar{c}' + \bar{u}' \bar{c} + \bar{u}' \bar{c}' \right] / \partial x = \delta \frac{\partial^2 \tilde{c}}{\partial x^2}. \quad (5.54)
\]

According to Table 5.1, the newly suggested STF with Clark's reduction gives:

\[
\bar{u} \bar{u}' + 2 \bar{u} \bar{u}' + \bar{u}' \bar{u}' = \bar{u} \bar{u}' + \left( \Delta_x^2 / 2Y \right) \bar{u} \bar{u}'^2 + \left( \Delta_x^2 / 2Y \right) \left( \bar{u} \bar{u}' / \partial t \right)^2 + \frac{1}{2} \bar{u}' \bar{u}'^2, \quad (5.55)
\]

\[
\bar{u} \bar{c} + \bar{u} \bar{c}' + \bar{u}' \bar{c} + \bar{u}' \bar{c}' = \bar{u} \bar{c} + \left( \Delta_x^2 / 2Y \right) \bar{u} \bar{u}' / \partial t \left( \bar{u} \bar{u}' / \partial t \right) + \left( \Delta_x^2 / 2Y \right) \left( \bar{u} \bar{u}' / \partial x \right) \left( \bar{u} \bar{u}' / \partial x \right) + \bar{u}' \bar{c}' \quad (5.56)
\]

The Boussinesq concepts \( \bar{u} \bar{u}' = -K(\bar{u} \bar{u}' / \partial x) \) and \( \bar{u}' \bar{c}' = -D(\bar{u} \bar{c}' / \partial x) \) are substituted into (5.55) and (5.56) which, in turn, are inserted into (5.53) and (5.54) to yield the final equations:
\[
\frac{\partial \ddot{u}}{\partial t} + \frac{1}{2} \left[ u \ddot{u} + \left( \frac{\Delta_x^2}{2Y} \right) \left( \dddot{u} \right)^2 + \left( \frac{\Delta_t^2}{2Y} \right) \left( \dddot{u} \right)^2 \right] \frac{1}{\partial x} \\
= \nu \frac{\partial^2 \ddot{u}}{\partial x^2} + \frac{1}{2} k \frac{\partial^2 (\ddot{u})}{\partial x^2} \frac{1}{\partial x}, \quad (5.57)
\]

\[
\frac{\partial \ddot{c}}{\partial t} + \ddot{c} \left[ \frac{u \dddot{u} + \left( \frac{\Delta_x^2}{2Y} \right) \left( \dddot{u} \right) \left( \frac{\partial u}{\partial x} \right) + \left( \frac{\Delta_t^2}{2Y} \right) \left( \dddot{u} \right) \left( \frac{\partial c}{\partial x} \right)}{\partial x} \right] \\
= \alpha \frac{\partial^2 \ddot{c}}{\partial x^2} + \partial \left[ \frac{\partial D (\ddot{c} \dddot{c})}{\partial x} \right] \frac{1}{\partial x}. \quad (5.58)
\]

The three averaging approaches applied in this research are: (1) Reynolds scheme for which Equations (5.57) and (5.58) are solved with \( \Delta_x = \Delta_t = 0 \); (2) Leonard's spatial filtering scheme with Clark's reduction. Equations (5.57) and (5.58) are solved with \( \Delta_t = 0 \); and (3) The suggested STF method with Clark's reduction. Here, the equations are solved in their complete form.

The molecular diffusivity is related to the molecular viscosity through a molecular Schmidt number:

\[
\alpha = \nu / \mu_m. \quad (5.59)
\]

Also, the turbulent diffusivity is related to the turbulent viscosity through a turbulent Schmidt number:

\[
D = K / \mu_t. \quad (5.60)
\]

And the eddy viscosity is either constant, or given by the Smagorinsky's model (see section 5.2):

\[
K = c_r \delta z^2 \left| \frac{\partial \ddot{u}}{\partial x} \right|. \quad (5.61)
\]
The total energy contained in the large-scale motion is defined as \( \langle \tilde{v}^2/2 \rangle \) where \( v = u - m \), and \( \langle \rangle \) means ensemble averaging as defined in section 4.3. In order to derive an equation for the temporal behavior of the total energy, insert \( \tilde{u} = \tilde{v} + m \) into (5.57) and set \( \partial m/\partial x \) and \( \partial m/\partial t \) both equal to zero. The result is:

\[
\frac{\partial \tilde{v}}{\partial t} = -(1/2) \frac{\partial \tilde{v}}{\partial x} - m \frac{\partial \tilde{v}}{\partial x} - \left( \frac{\Delta^2}{4\gamma} \right) \frac{\partial (\partial \tilde{v}/\partial t)}{\partial x}
- \left( \frac{\Delta^2}{4\gamma} \right) \frac{\partial (\partial \tilde{v}/\partial x)^2}{\partial x} + \nu \frac{\partial^2 \tilde{v}}{\partial x^2}
+ (1/2) \frac{\partial [K(\partial \tilde{v}/\partial x)]}{\partial x}.
\] (5.62)

Multiplying the above equation by \( \tilde{v} \), and taking ensemble average yields:

\[
\frac{\partial \langle \tilde{v}^2/2 \rangle}{\partial t} = -(1/2) \langle \tilde{v} \partial (\partial \tilde{v}/\partial x) \rangle - (1/2) m \langle \partial \tilde{v}/\partial x \rangle
- \left( \frac{\Delta^2}{4\gamma} \right) \langle \tilde{v} \partial (\partial \tilde{v}/\partial t) \rangle /\partial x
- \left( \frac{\Delta^2}{4\gamma} \right) \langle \tilde{v} \partial (\partial \tilde{v}/\partial x)^2 \rangle /\partial x
+ \nu \langle \partial^2 \tilde{v}/\partial x^2 \rangle
+ (1/2) \langle \tilde{v} \partial [K(\partial \tilde{v}/\partial x)]/\partial x \rangle.
\] (5.63)

As shown in section 4.3, the first two terms in the right hand side of the above equation are zero. However, the first term is kept as a tool for checking the calculation; its actual value should be zero at all time steps. The above equation is used in studying the role of the filter terms and
the viscosity terms in distributing and dissipating the energy.
Chapter VI
NUMERICAL SOLUTION

6.1 SUMMARY OF EQUATIONS

The modeled equations, derived in Chapter V, are rearranged and written below without the overbars:

Momentum:

\[
\frac{\partial u}{\partial t} = -(1/2) \frac{\partial uu}{\partial x} - \left( \frac{A^2}{4Y} \right) \frac{\partial (\partial u/\partial t)^2}{\partial x} \\
- \left( \frac{A^2}{4Y} \right) \frac{\partial (\partial u/\partial x)^2}{\partial x} + \nu \frac{\partial u}{\partial x^2} \\
+ (1/2) \frac{\partial [K(\partial u/\partial x)]}{\partial x}.
\]  (6.1)

Scalar Transport:

\[
\frac{\partial c}{\partial t} = -\frac{\partial uc}{\partial x} - \left( \frac{A^2}{2Y} \right) \frac{\partial [(\partial u/\partial t)(\partial c/\partial t)]}{\partial x} \\
- \left( \frac{A^2}{2Y} \right) \frac{\partial [(\partial u/\partial x)(\partial c/\partial x)]}{\partial x} \\
+ \alpha \frac{\partial^2 c}{\partial x^2} + \frac{\partial [D(\partial c/\partial x)]}{\partial x}.
\]  (6.2)
Energy:

\[
\frac{\partial \langle v^2 / 2 \rangle}{\partial t} = -\frac{1}{2} \langle v (\partial v / \partial x)^2 \rangle
\]

L.H.S.

\[
-\frac{(\Delta_t^2 / 4\gamma)}{\langle v (\partial v / \partial t)^2 / \partial x \rangle}
\]

2

\[
-\frac{(\Delta_x^2 / 4\gamma)}{\langle v (\partial v / \partial x)^2 / \partial x \rangle}
\]

3

\[
+ v \langle v \partial^2 v / \partial x^2 \rangle
\]

4

\[
+ \frac{1}{2} \langle v \partial (K \partial v / \partial x) / \partial x \rangle.
\]

R.H.S.

These equations are obtained from the original equations through the spatial-temporal filtering (STF) scheme. Setting \( \Delta_t = 0 \) invokes Leonards spatial filtering. With \( \Delta_x = \Delta_t = 0 \), the Reynolds averaging approach is implemented. And with \( \Delta_x = \Delta_t = K = 0 \), the original unaveraged equations which must be solved on very dense grids are obtained. Closure is achieved through the Boussinesq concept in which \( K \) is either constant or given by the Smagorinsky's model:

\[
K = c_r \frac{\varepsilon^2}{\delta_x} |\partial u / \partial x| \quad (6.4)
\]

where \( \alpha \) and \( D \) are related to \( \nu \) and \( K \) as in Equations (5.59) and (5.60).

Equation (6.1) is solved first for the velocity field \( u(x,t) \). This velocity field is used as an input for Equation (6.2) which is solved for the concentration field \( c(x,t) \).
The energy equation (6.3) does not introduce any new unknowns and need not be solved separately. The velocity field obtained from Equation (6.1) is used to calculate \( v(x,t) \) by the simple subtraction \( v = u - m \) at each time step and each node. The resulting \( v(x,t) \) field is then used to calculate a time history of each term in Equation (6.3). The ensemble averaging procedure, denoted by \( \langle \rangle \), is hereafter approximated by a simple arithmetic averaging over all spatial nodes.

6.2 **FINITE DIFFERENCE DISCRETIZATION**

An explicit finite difference scheme is given below for solving Equations (6.1), (6.2) and (6.3). For the nonlinear and filter terms, maximum obtainable accuracy is required since these terms are responsible for creating and averaging the rapid changes in the turbulent variables. To maintain a simple calculation procedure, the Adam-Bashforth explicit method is used for time marching.

6.2.1 **Spatial Discretization**

The nonlinear terms are discretized by a fourth order accurate scheme as in Bedford et al. (1978) and Kwak et al. (1975):

\[
\frac{\partial uu}{\partial x} \bigg|_i^j = \frac{1}{3} \delta_x \left[ \left( \frac{uu}{\delta x} \right)_{i+1}^j - \left( \frac{uu}{\delta x} \right)_{i-1}^j 
+ 2u_i^j \left( \frac{uu}{\delta x} \right)_{i+1}^j - \left( \frac{uu}{\delta x} \right)_{i-1}^j \right] 
- \frac{1}{24} \delta_x \left[ \left( \frac{uu}{\delta x} \right)_{i+2}^j - \left( \frac{uu}{\delta x} \right)_{i-2}^j \right]
\]
where the subscripts denote spatial node numbers, and the superscripts denote time levels. The spatial filter terms are discretized by two successive second order accurate schemes as follows:

\[
\begin{align*}
[\partial u/\partial x]_i^j &= (1/2 \delta_x) (u_{{i+1}}^j - u_{{i-1}}^j), \\
[\partial (\partial u/\partial x)/\partial x]_i^j &= (1/2 \delta_x) \left\{ \left[ (\partial u/\partial x)^2 \right]_i^j - \left[ (\partial u/\partial x) \right]_i^j \right\}_i^j \\
&= (1/8 \delta_x) \left[ \left( u_{{i+2}}^j - u_{{i-2}}^j \right) \\
&- \left( u_{{i+1}}^j - u_{{i-1}}^j \right) \right], \\
[\partial u/\partial x] (\partial c/\partial x)_i^j &= (1/2 \delta_x) (u_{{i+1}}^j - u_{{i-1}}^j) \\
&\quad \quad \left( c_{{i+1}}^j - c_{{i-1}}^j \right), \\
\{ \partial \left[ \partial (\partial u/\partial x)(\partial c/\partial x)/\partial x \right]_i^j &= (1/2 \delta_x) \left\{ \left[ (\partial u/\partial x) \right]_i^j \right\} \\
&\quad \quad \left[ (\partial u/\partial x)(\partial c/\partial x) \right]_i^j \\
&\quad \quad \left[ (\partial u/\partial x) \right]_i^j \left( c_{{i+1}}^j - c_{{i-1}}^j \right) \\
&= (1/8 \delta_x) \left( u_{{i+2}}^j - u_{{i-2}}^j \right) \left( c_{{i+2}}^j - c_{{i-2}}^j \right) \\
&\quad \quad \left( u_{{i+1}}^j - u_{{i-1}}^j \right) \left( c_{{i+1}}^j - c_{{i-1}}^j \right). 
\end{align*}
\]
To maintain an explicit solution, the time derivatives in the temporal filter terms are discretized by a first order backward formula. The successive spatial derivatives are fourth order accurate:

\[
[(\partial u/\partial t)^2]_i^j = (1/\delta_t)^2 (u_i^j - u_{i-1}^j)^2,
\]  

(6.11)

\[
[\partial(\partial u/\partial t)^2/\partial x]_i^j = (1/12 \delta_x) \left\{ [(\partial u/\partial t)^2]_{i-2}^j - 8[(\partial u/\partial t)^2]_{i-1}^j + 8[(\partial u/\partial t)^2]_{i+1}^j - [(\partial u/\partial t)^2]_{i+2}^j \right\}
\]

\[
= (1/12 \delta_x \delta_t^2) \left\{ (u_{i-2}^j - u_{i-1}^j)^2 - 8(u_{i-1}^j - u_{i-1}^{j-1})^2 + 8(u_{i+1}^j - u_{i+1}^{j-1})^2 - (u_{i+2}^j - u_{i+2}^{j-1})^2 \right\},
\]  

(6.12)

\[
[(\partial u/\partial t)(\partial c/\partial t)]_i^j = (1/\delta_t)^2 (u_i^j - u_i^{j-1})(c_i^j - c_i^{j-1}),
\]  

(6.13)

\[
[\partial (\partial u/\partial t)(\partial c/\partial t)/\partial x]_i^j = (1/12 \delta_x) \left\{ [(\partial u/\partial t)(\partial c/\partial t)]_{i-2}^j - 8[(\partial u/\partial t)(\partial c/\partial t)]_{i-1}^j + 8[(\partial u/\partial t)(\partial c/\partial t)]_{i+1}^j - [(\partial u/\partial t)(\partial c/\partial t)]_{i+2}^j \right\}
\]

\[
= (1/12 \delta_x \delta_t^2) \left\{ (u_{i-2}^j - u_{i-1}^j)(c_{i-2}^j - c_{i-2}^{j-1}) - 8(u_{i-1}^j - u_{i-1}^{j-1})(c_{i-1}^j - c_{i-1}^{j-1}) + 8(u_{i+1}^j - u_{i+1}^{j-1})(c_{i+1}^j - c_{i+1}^{j-1}) - (u_{i+2}^j - u_{i+2}^{j-1})(c_{i+2}^j - c_{i+2}^{j-1}) \right\}.
\]  

(6.14)
The molecular viscosity and diffusivity terms are described by the usual second order accurate central scheme:

\[
(\delta^2 u/\delta x^2)_i^j = \left(1/\delta_x^2\right) (u_{i+1}^j - 2u_i^j + u_{i-1}^j), \quad (6.15)
\]

\[
(\delta^2 c/\delta x^2)_i^j = \left(1/\delta_x^2\right) (c_{i+1}^j - 2c_i^j + c_{i-1}^j), \quad (6.16)
\]

And the eddy viscosity and diffusivity terms are discretized as follows:

\[
\left[ \partial (K \partial u/\partial x)/\partial x \right]_i^j = \left(1/\delta_x^2\right) \left[ (K \partial u/\partial x)_{i+1}^j - (K \partial u/\partial x)_{i-1}^j \right]
= \left(1/4 \delta_x^2\right) \left[ K_{i+1}^j (u_{i+2}^j - u_i^j)
- K_{i-1}^j (u_i^j - u_{i-2}^j) \right], \quad (6.17)
\]

\[
\left[ \partial (D \partial c/\partial x)/\partial x \right]_i^j = \left(1/\delta_x^2\right) \left[ (D \partial c/\partial x)_{i+1}^j - (D \partial c/\partial x)_{i-1}^j \right]
= \left(1/4 \delta_x^2\right) \left[ D_{i+1}^j (c_{i+2}^j - c_i^j)
- D_{i-1}^j (c_i^j - c_{i-2}^j) \right], \quad (6.18)
\]

where \( K \) and \( D \) are given by:

\[
K = c_r \delta_x^2 |\partial u/\partial x|, \quad (6.19)
\]

\[
K_i^j = c_r \delta_x^2 \left(1/2 \delta_x\right) |u_{i+1}^j - u_{i-1}^j|
= \left(c_r \delta_x /2\right) |u_{i+1}^j - u_{i-1}^j|, \quad (6.20)
\]

\[
D_i^j = K_i^j / S_t. \quad (6.21)
\]
Substituting (6.5) through (6.21) into (6.1) and (6.2) gives the corresponding finite difference equations in the following form:

\[
\frac{\partial u}{\partial t} = S_i, \quad (6.22)
\]

\[
\frac{\partial c}{\partial t} = Q_i. \quad (6.23)
\]

6.2.2 Time Marching

The numerical solution is kept purely explicit by using the Adam-Bashforth time marching method. This method is derived by writing a Taylor expansion for \( u^j \) in terms of \( u^{j-1} \):

\[
u^j = u^{j-1} + \delta_t (\partial u / \partial t)^{j-1} + (\delta_t^2/2)(\partial^2 u / \partial t^2)^{j-1} + \ldots (6.24)
\]

The second derivative is evaluated as follows:

\[
(\partial^2 u / \partial t^2)^{j-1} = \delta_t [(\partial u / \partial t)^{j-1}] / \delta t = (1/\delta_t) [(\partial u / \partial t)^{j-1} - (\partial u / \partial t)^{j-2}] . \quad (6.25)
\]

Combining (6.25) and (6.24) gives:

\[
u^j = u^{j-1} + \delta_t (\partial u / \partial t)^{j-1} + (\delta_t^2/2)[(\partial u / \partial t)^{j-1} - (\partial u / \partial t)^{j-2}] \\
= u^{j-1} + (3\delta_t/2)(\partial u / \partial t)^{j-1} - (\delta_t/2) (\partial u / \partial t)^{j-2} , \quad (6.26)
\]

which, using (6.22), is rewritten as:

\[
u^j = u^{j-1} + (3\delta_t/2) S_i^{j-1} - (\delta_t/2) S_i^{j-2} . \quad (6.27)
\]
A similar equation can be easily obtained for the scalar transport:

\[ c_i^j = c_i^{j-1} + (3\delta t/2) Q_i^{j-1} - (\delta t/2) Q_i^{j-2}. \]  

Equations (6.27) and (6.28) are completely explicit. At a certain time level, \( j \), evaluate \( u_i^j \) at \( i=1,2,...,N \) where \( N \) is the total number of nodes. The velocity field \( u_i^j \) is stored and used in the evaluation of \( c \) by Equation (6.28).

The Adam-Bashforth explicit method is known to be second order accurate in time. It is, however, weakly unstable (see Roach 1972). Because it uses information in three time levels, it may develop computational modes the severity of which depends on the grid spacings. This problem is alleviated by keeping the grid spacings reasonably small so that the computational modes become unappreciable.
Chapter VII
SUGGESTED VERIFICATION AND EXPERIMENTAL PROCEDURES

7.1 INTRODUCTION
This chapter presents a verification procedure suggested for one-dimensional, transient flow situations. The procedure is based on statistical and spectral analysis of the results of Equations (6.1) and (6.2). The necessary input parameters, and a program for numerical experiments are also given in this chapter. In the next chapter, the results are presented and processed according to the verification procedure.

7.2 VERIFICATION METHOD
Logically, the verification scheme should depend on the nature of the problem in hand. However, in cases of highly turbulent flows, some general guidelines are obvious. The most important point to consider is that turbulence is a stochastic phenomenon. In other words, the values assumed by any turbulent variable, at a certain location, are random and un-reproducible. Any slight change in the surrounding boundaries or the initial conditions results in totally different values of the parameters measured at a certain location. Therefore, point-to-point comparison between model
results and measured data is not a valid method of verification. The only logical procedure is to compare the statistical properties of the model results to the theoretically or experimentally known statistics of the real world variables. Another important point is that turbulence models calculate the large-scale components of the variables. Therefore, the field data must be similarly averaged to extract the large-scales from the total measured variables. Only after this averaging can the field data be compared to the model results.

Unfortunately, these simple considerations have been overlooked by most engineers while solving their practical hydraulic problems. The common procedure is to measure field or laboratory data at certain points in the flow domain. The data is often measured by the available low-frequency devices missing the most part of the important turbulent activities. Measurement stations are often chosen haphazardly and with little or no consultation with the modeler. The measured data is then used to verify the corresponding results by calculating correlation coefficients.

Not until recently that the need for proper methods of verification has been recognized. See for example Clark et al. (1977); Kwak et al. (1975); Bedford (1981); Cosier (1979); and Babajimopoulos and Bedford (1975). The authors of these publications recognized the importance of comparing the statistical features of the model results to those of
the exact solution whenever possible. In many cases where an exact solution is not possible, sufficient information on these statistical features is available through theoretical and dimensional arguments.

Most important of all the statistics is the spectral properties of the turbulent variables. As mentioned in section 2.2, the spectral distribution of a turbulent velocity is a direct measure of the energy contained at the different levels of frequencies or wave numbers. Therefore, the spectral plots describe the energy cascade process which is nothing but the distribution of energy between the different eddy sizes. It is, therefore, essential to require that the model be able to calculate turbulent variables with the correct spectral properties. Fortunately, a great deal of information is available on the spectral distributions of multi-dimensional turbulence and scalar contaminants. This information, a sample of which is presented in section 2.2, is obtainable through theoretical and dimensional arguments as well as accumulated empirical work. The enormous amount of dense and high-speed measurements required to obtain this information from the field is therefore not necessary. The implication is that, by resorting to statistical properties for verification purposes, a great deal of effort and expense can be saved.

In this research, turbulence modeling is applied to one-dimensional, transient, momentum and scalar transport equa-
tions. Thus, an "exact" solution of the original equations on very dense grid is possible. A verification procedure, based on the above discussion, is suggested as follows:

1. Obtain an exact solution of the original (unaveraged) equations on a very dense grid. The solution is represented by the one-dimensional, transient velocity and concentration arrays \( u(x,t) \) and \( c(x,t) \).

2. From the exact variable fields, extract the large-scale components, \( \bar{u}(x,t) \) and \( \bar{c}(x,t) \), commensurate with each coarse grid planned for solving the modeled equations.

3. For the large-scale components of the exact variables obtain the following:
   a) Time histories of the mean, variance, skewness, and kurtosis of the spatial distributions. These statistics completely describe the probability structure of the variables.
   b) Wave number spectra of the spatial distributions at different time steps.
   c) Frequency spectra of the time signals at different locations.

4. Apply turbulence modeling and solve the modeled equations on the coarse grid. The resulting variables, \( \bar{u}(x,t) \) and \( \bar{c}(x,t) \), are large-scales commensurate with the coarse grid, and comparable to the large-scales obtained in point 2 above.

5. For the model results obtain the same statistics listed in point 3.

6. Compare 5 against 3 to judge the performance of the different turbulence models used to prepare the equations for the coarse grid.

For a given Reynolds number and a given set of initial and boundary conditions, point 1 in the above list needs to be done only once on a grid dense enough to resolve all the scales of motion. But the rest of the points must be repeated every time a different averaging or closure method is
applied. They must also be repeated at any change in the grid spacings; filter widths; empirical coefficients; or any other input parameter.

In point 2, the exact fields $u(x,t)$ and $c(x,t)$ are averaged to extract the large-scale components commensurate with a particular coarse grid on which the modeled equations will be solved. Ideally, the extraction of $\bar{u}$ and $\bar{c}$ from the exact fields should be done with the same averaging operation used to derive the modeled equations. The modeled equations, however, will be solved repeatedly using three different averaging methods with a wide range of filter widths. It would be neither practical nor economic to average the exact fields for such a large number of times.

As an approximation, point 2 will be done only once for each coarse grid. This gives representative large-scale components that are commensurate with that particular coarse grid. Figure 7.1 shows how a large-scale component is extracted from the exact field calculated by the dense grid. For example, the large-scale component of a certain variable at point "A" is simply an average of the exact values at the circled nodes on the exact grid. A similar procedure was used by Clark et al. (1977) to prepare an "exact-averaged" three-dimensional velocity field at low Reynolds numbers.

If $\omega_i$ stands for a general signal consisting of $N$ points ($i=1,2,\ldots,N$) with a spacing between the points, then the statistics listed in point 3 above are calculated as follows:
Figure 7.1: Averaging the Exact Fields.
\[ \text{Mean} = (1/N) \sum_{i=1}^{N} \alpha_i, \quad \text{(7.1)} \]

\[ \text{Variance} = (1/N) \sum_{i=1}^{N} (\alpha_i - \text{Mean})^2, \quad \text{(7.2)} \]

\[ \text{Skewness} = \left[ \frac{\sum_{i=1}^{N} (\alpha_i - \text{Mean})^3}{N\text{Variance}^{3/2}} \right], \quad \text{(7.3)} \]

\[ \text{Kurtosis} = \left[ \frac{\sum_{i=1}^{N} (\alpha_i - \text{Mean})^4}{N\text{Variance}^2} \right], \quad \text{(7.4)} \]

\[ \text{Spectrum} = \frac{2\delta/\pi}{\sum_{k=1}^{NS} \mathcal{E}_k R_k \cos[(j-1)(k-1)\pi/(NS-1)]}, \quad \text{(7.5)} \]

\[ \text{Wave number} j \text{ or frequency} j = (j-1)/(2\delta(NS-1)), \quad \text{(7.6)} \]

where

\[ \mathcal{E}_k = \frac{1}{2} \quad \text{(for } k=1,\text{NS)} \]

\[ = 1 \quad \text{(for } k=2,3,\ldots,\text{NS-1)}, \quad \text{(7.7)} \]

and \( R_k \) stands for the autocorrelations:

\[ R_k = \frac{1}{N-k+1} \sum_{l=1}^{N-K+1} (\alpha_l - \text{Mean})(\alpha_{l+k-1} - \text{Mean}). \quad \text{(7.8)} \]

The index \( j \) takes the values \( 1,2,\ldots,\text{NS} \) where \( \text{NS} \) is the required number of points in the computed spectrum. \( \text{NS} \) is usually chosen within the range \( 0.15N \) to \( 0.25N \). The wave numbers or frequencies, calculated by Equation (7.6), are in cycle/unit of length or cycle/unit of time depending on the nature of the spacing \( \delta \).

The mean, variance, skewness and kurtosis are calculated, for the spatial distributions of \( u \) and \( c \) and plotted against
The skewness is calculated by Equation (7.3) only for the concentration fields. For velocity fields, the following formula (see Clark et al. 1977) is used instead:

\[
\text{Skewness} = \left[ \frac{1}{N} \sum_{i=1}^{N} \frac{\text{slope}_i^3}{\left( \frac{1}{N} \sum_{i=1}^{N} \text{slope}_i^2 \right)^{3/2}} \right] / \left( \frac{\alpha_i - \alpha_{i-1}}{2\delta} \right),
\]

where

\[
\text{slope}_i = \frac{\alpha_{i+1} - \alpha_{i-1}}{2\delta},
\]

Equation (7.10)

The reason is that the skewness as defined in Equation (7.9) bears a special physical meaning with regards to the one-dimensional equations solved in this research. The details are given in section 8.1. The kurtosis, in Equation (7.4), is divided by the square of the variance to obtain the nondimensional "coefficient of kurtosis" which, hereafter, will be referred to as simply the kurtosis. Also the skewness, in Equation (7.3), is divided by the variance raised to the 3/2 power to give the nondimensional "coefficient of skewness".

The FORTRAN computer program for solving the Burgers equation is listed in Appendix A. The program computes the velocity field, on any chosen grid, along with its spectral distributions and statistics as recommended above. All terms of the energy equation (6.3) are also calculated and plotted against time. Appendix B includes the FORTRAN program for solving the scalar transport equation. The program calculates the concentration field using the velocities obtained from solving the Burgers equation. The program also calcu-
lates the spectral distributions and the statistics of the concentration field according to the verification procedure.

7.3 EXPERIMENTAL RATIONALE
The following sections present the input data and the initial and boundary conditions needed for solving (6.1), (6.2) and (6.3). The input parameters are divided into "fixed" and "variable" parts. The fixed input parameters are constant for all subsequent runs. The variable input parameters are mainly the averaging procedure; closure procedure; Reynolds number and; the grid spacings. The calculations are carried out in groups of runs; each group is designed to investigate the effect of a certain variable input parameter. The runs are summarized and tabulated following the input data listings.

7.4 INPUT PARAMETERS
In order to solve Equations (6.1), (6.2) and (6.3) the following input information is needed:

1. Total length of flow domain, $L$, and total time of calculation, $T$.
2. Grid spacings for exact or dense grid calculations.
3. Initial distributions of velocity and concentration.
4. Boundary conditions.
5. Molecular and turbulent Schmidt numbers.
6. Spatial filter width, $\Delta_x$.
7. Residual field coefficient in Smagorinsky's model, $c_r$. 
8. Averaging method (Reynolds, Leonard's or STF).
10. closure method (constant or Smagorinsky's K).
11. The value of the constant $K$.
12. The averaging length $w$ in Smagorinsky's model for $K$.
13. The molecular viscosity (as a function of $Re$).

Table 7.1 shows the units in which all input parameters and results are measured.

7.4.1 Fixed Input Parameters

$L$, $T$ and Dense Grid Spacings:

In all the following calculations, the total length of the flow domain, $L$, is kept constant at 12 arbitrary units of length. And the total time of simulation, $T$, is kept constant at 1.0 arbitrary unit of time. For solving the original unaveraged equations, the total length is divided into 4026 intervals (4027 nodes) and the total time is divided into 2013 intervals (2014 time steps). This division is dense enough to place about 100 nodes within each wave in the initial velocity distribution shown in Figure 7.2. Thus, the steep slopes in the expected shock fronts can be accurately resolved.
Table 7.1  Units of Input Data and Results.

<table>
<thead>
<tr>
<th>Quantity</th>
<th>Symbol</th>
<th>Units</th>
</tr>
</thead>
<tbody>
<tr>
<td>total length of flow domain</td>
<td>L</td>
<td>arbitrary unit of length &quot;L&quot;</td>
</tr>
<tr>
<td>spatial grid interval</td>
<td>δₓ</td>
<td></td>
</tr>
<tr>
<td>spatial filter width</td>
<td>δₓ</td>
<td></td>
</tr>
<tr>
<td>significant length scale</td>
<td>L₀</td>
<td></td>
</tr>
<tr>
<td>averaging length in Smag. model</td>
<td>w</td>
<td></td>
</tr>
<tr>
<td>total time of calculation</td>
<td>T</td>
<td>arbitrary unit of time &quot;T&quot;</td>
</tr>
<tr>
<td>temporal grid spacing</td>
<td>δ₉</td>
<td></td>
</tr>
<tr>
<td>temporal filter width</td>
<td>δ₉</td>
<td></td>
</tr>
<tr>
<td>total velocity</td>
<td>u, ū</td>
<td></td>
</tr>
<tr>
<td>deviation of velocity from its mean</td>
<td>v, v̅</td>
<td>L/T</td>
</tr>
<tr>
<td>significant velocity scale</td>
<td>V₀</td>
<td></td>
</tr>
<tr>
<td>concentration</td>
<td>c, ċ</td>
<td>arbitrary unit of concentration &quot;G&quot;</td>
</tr>
<tr>
<td>viscosity and diffusivity coefficients</td>
<td>v, k, α, D</td>
<td>L²/T</td>
</tr>
<tr>
<td>wave number</td>
<td>ω</td>
<td>cycle/L</td>
</tr>
<tr>
<td>frequency</td>
<td>f</td>
<td>cycle/T</td>
</tr>
</tbody>
</table>
Initial Distributions:

The initial distribution of velocity, for the exact solutions, is a random signal consisting of 4027 equally spaced points with a mean of 3.0 units of length/unit of time and a target wave number spectrum as shown in Figure 7.2. The signal is generated, according to the method suggested by Shinnozuka and Jan (1972), as follows:

\[ u(x,0) = v(x,0) + 3.0, \quad (7.11) \]

\[ v(x,0) = \frac{1}{\sqrt{2}} \sum_{i=1}^{NS} \sqrt{E_j(\Delta \omega)} \cos(\omega_j x + \phi_j), \quad (7.12) \]

where \( E_j(j=1,2,\ldots,NS) \) is the target spectrum, consisting of \( NS \) points, which is assumed to have insignificant values outside the region \( 0 < \text{wave number} < \omega_m \). The wave number interval, \( \Delta \omega \), is equal to \( \omega_m/NS \), and \( \omega_j \) is defined as:

\[ \omega_j = \omega_j + \delta_\omega, \quad (7.13) \]

where \( \omega_j \) is the wave number at which the target spectrum is equal to \( E_j \), and \( \delta_\omega \) is a random wave number with a uniform probability distribution over the interval \( (-\Delta \omega/40, \Delta \omega/40) \). The independent phase, \( \phi_j \), is a random number uniformly distributed over the interval \( (0, 2\pi) \). The target spectrum \( E_j(\omega_j) \) is chosen such that the area under the spectrum is equal to the required variance of \( u(x,0) \) which is set equal to 0.02 (units of length/unit of time).
Figure 7.2 shows the generated signal, which consists of 4027 points, along with its target and actual wave number spectra. The spectrum has a very accentuated maximum at \( \log \omega_{\text{max}} = 0.5235 \). Thus, the most significant length scale, \( L_0 \), is calculated as:

\[
\omega_{\text{max}} = \log 0.5235 = 3.3383 = 1/L_0
\]

\[
L_0 = 1/3.3383 = 0.299 \text{ units of length.} \tag{7.15}
\]

The most significant velocity scale, \( V_0 \), is the mean of \( u(x,0) \) which is equal to 3.0 units of length/unit of time.

The molecular viscosity is a function of the constant \( L_0 \) and \( V_0 \), and the variable Reynolds number:

\[
\nu = L_0 V_0 / R_e = (0.299)(3.0) / R_e
\]

\[
= 0.897 / R_e \text{ (units of length /unit of time).} \tag{7.16}
\]

The inertial subrange in the initial wave number spectrum is void of any significant spectrum values. This makes it possible to observe the gradual development, at later time steps, of an inertial subrange with the expected \( \omega^2 \) dependency.

The initial \( u(x,0) \) distribution mentioned above consists of 4027 equally spaced points, and is used for solving the unaveraged equations on the dense grid. For solving the modeled equations on coarser grids, initial velocity distribution \( \bar{u}(x,0) \) consisting of much fewer points is needed. This
Figure 7.2: Initial Velocity and its Wave Number Spectrum.
is obtained as shown in Figure 7.3; \( \bar{u}(x,0) \) at point "A" on the coarse grid is the Gaussian-weighted average of \( u(x,0) \) at the circled points on the dense grid.

The initial concentration distribution, for all exact and coarse grid solutions, is kept constant throughout the flow domain and set equal to 1 arbitrary unit of concentration. This makes it possible to observe the gradual convection of the contaminant by the velocity field; the concentration should diminish in high velocity regions, and accumulate in regions of low velocity.

**Boundary Conditions:**

The boundary conditions for both velocity and concentration are periodic with a period equals to the total length of the flow domain:

\[
\begin{align*}
    u(x,t) &= u(x+L,t), \\
    c(x,t) &= c(x+L,t).
\end{align*}
\]

(7.17) (7.18)

With this kind of boundary condition, the finite difference approximation of derivatives close to the boundaries becomes very simple. For example, in Figure 7.4, the values of \( u \) and \( c \) at point "B" (needed to calculate derivatives at point "A") are replaced by the values of \( u \) and \( c \) at point "2" which is inside the flow domain.
Figure 7.3: Initial Velocities for Dense and Coarse Grids.
Figure 7.4: The Periodic Boundary Condition.
Schmidt Numbers, $\Delta_m$ and $c_r$:

The molecular and turbulent Schmidt numbers, $S_m$ and $S_t$, are set equal to 1.0 in all subsequent calculations. Thus, the molecular diffusivity is equal to the molecular viscosity, and the turbulent or eddy diffusivity is equal to the eddy viscosity. The spatial filter width, $\Delta_x$, is fixed at twice the spatial grid spacing for all coarse grid calculations. This ratio of filter width to grid spacing is found optimum by all modelers who used the Leonard's spatial filtering method. Also, the residual field coefficient $c_r$ is fixed at a value of 4.0 which was tuned by Love (1980) who used the Leonard's spatial filtering scheme.

7.4.2 Variable Input Parameters
The input parameters 8 through 14 (listed in the beginning of section 7.4) are variables. For dense grid calculations, the condition $\Delta_x = \Delta_t = K = D = 0$ reduces the modeled equations back to their original forms for which $Re$ is the only needed variable input parameter (see table 7.2). For coarse grid calculations, the variable input parameters are listed in tables 7.3 through 7.6.
7.5 SUMMARY OF DENSE GRID EXPERIMENTS

Table 7.2 is a list of the dense grid runs and their respective Reynolds number values. The calculated $u$ and $c$ fields are processed according to the verification method, and the results are plotted in Figures 8.1 through 8.9. In these figures, the curves marked "E" are the exact statistics, and the curves marked "EA" are the exact-averaged equivalents.

7.6 SUMMARY OF COARSE GRID EXPERIMENTS

Table 7.3 is a listing of the first group of coarse grid runs. This group is designed to study the effect of the averaging method on the results, and to compare the performances of the different averaging methods. The variable input parameters are listed in the table along with the numbers of the figures containing the results. The statistics and spectral distributions of $\bar{u}$ and $\bar{c}$ are calculated, according to the verification procedure, and compared to the corresponding exact-averaged statistics in Figures 8.10 through 8.19.

The second group of coarse grid runs is listed in table 7.4. This group shows the effect of the closure method on the results. The constant $K$ and the Smagorinsky's $K$ closures are implemented in different combinations with the averaging methods of Table 7.3. Again the spectra and statistics of the calculated $\bar{u}$ and $\bar{c}$ are compared to their exact-averaged counterparts in Figures 8.20 through 8.52.
The third group of coarse grid calculations is intended to study the effect of an increasing Reynolds number on the model results. The averaging method is STF and the closure is Smagorinsky's. A complete list of the input data is given in Table 7.5, and the results are presented in Figures 8.53 through 8.62.

Table 7.6 presents the fourth and the last group of coarse grid calculations. In this group, different grid spacings in both space and time are implemented. The effects of increasing grid spacings on the results are shown in Figures 8.63 to 8.67.
Table 7.2  Dense-Grid Runs. Effect of Reynolds Number.

<table>
<thead>
<tr>
<th>Run #</th>
<th>Reynolds No.</th>
<th>Number of Nodes N</th>
<th>Number of Time Steps M</th>
<th>Figures</th>
</tr>
</thead>
<tbody>
<tr>
<td>E1</td>
<td>300</td>
<td>4027</td>
<td>2014</td>
<td>8.1 through 8.9</td>
</tr>
<tr>
<td>E2</td>
<td>500</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>E3</td>
<td>700</td>
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<td></td>
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</tr>
</tbody>
</table>
Table 7.3  First Group of Coarse-Grid Runs. Effect of Averaging Method.

<table>
<thead>
<tr>
<th>Run #</th>
<th>Averaging Method</th>
<th>$\Delta_t$</th>
<th>$\Delta_x$</th>
<th>Closure Method</th>
<th>Constant K Value</th>
<th>$w$</th>
<th>$R_e$</th>
<th>$N$</th>
<th>$M$</th>
<th>Figures</th>
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<tbody>
<tr>
<td>A1</td>
<td>None</td>
<td>0</td>
<td>0</td>
<td>None</td>
<td>-</td>
<td>-</td>
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</tr>
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<td>A2</td>
<td>Reynolds</td>
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<td>0</td>
<td>None</td>
<td>-</td>
<td>-</td>
<td></td>
<td></td>
<td></td>
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</tr>
<tr>
<td>A3</td>
<td>Leonard's</td>
<td>0</td>
<td>0</td>
<td></td>
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<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A4</td>
<td>STF</td>
<td>$4\delta_t$</td>
<td>$2\delta_x$</td>
<td>Smagorinsky</td>
<td>$14\delta_x$</td>
<td>500</td>
<td>806</td>
<td>470</td>
<td></td>
<td>8.10 through 8.19</td>
</tr>
<tr>
<td>A5</td>
<td>STF</td>
<td>$8\delta_t$</td>
<td>$26\delta_x$</td>
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<td></td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>A6</td>
<td>STF</td>
<td>$10\delta_t$</td>
<td>$26\delta_x$</td>
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</table>

Variable Input Parameters
Table 7.4  Second Group of Coarse-Grid Runs. Effect of Closure Method.

<table>
<thead>
<tr>
<th>Run #</th>
<th>Averaging Method</th>
<th>$\Delta t$</th>
<th>$\Delta x$</th>
<th>Closure Method</th>
<th>Constant K Value</th>
<th>$w$</th>
<th>$R_e$</th>
<th>N</th>
<th>M</th>
<th>Figures</th>
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<td>B1</td>
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<td>0</td>
<td>Constant K</td>
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<td>806</td>
<td>470</td>
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<td>8.20 through 8.27</td>
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<td>B2</td>
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<td>0</td>
<td>0</td>
<td>Constant K</td>
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<td>146x</td>
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<tr>
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<td>Leonard's</td>
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<td>26x</td>
<td>Const. K</td>
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<td>500</td>
<td>806</td>
<td>470</td>
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<td>8.28 through 8.34</td>
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<td>Const. K</td>
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<td>146x</td>
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<td>26x</td>
<td>Smag. K</td>
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</tr>
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<td>A9</td>
<td>STF</td>
<td>106t</td>
<td>26x</td>
<td>Const. K</td>
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<td>STF</td>
<td>106t</td>
<td>26x</td>
<td>Smag. K</td>
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</table>
Table 7.5  Third Group of Coarse-Grid Runs. Effect of Reynolds Number.

<table>
<thead>
<tr>
<th>Run #</th>
<th>$R_e$</th>
<th>$\Delta t$</th>
<th>$\Delta x$</th>
<th>Closure Method</th>
<th>Const. $K$</th>
<th>$w$</th>
<th>$N$</th>
<th>$M$</th>
<th>Figures</th>
</tr>
</thead>
<tbody>
<tr>
<td>A6</td>
<td>500</td>
<td>STF</td>
<td>$10\Delta t$</td>
<td>Smagorinsky</td>
<td>$14\Delta x$</td>
<td>806</td>
<td>470</td>
<td></td>
<td>8.53 through 8.62</td>
</tr>
<tr>
<td>C1</td>
<td>600</td>
<td>STF</td>
<td>$2\Delta x$</td>
<td>Smagorinsky</td>
<td>$14\Delta x$</td>
<td>806</td>
<td>470</td>
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<td>8.53 through 8.62</td>
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<td>C2</td>
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<td>C3</td>
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### Table 7.6 Fourth Group of Coarse-Grid Runs. Effect of Grid Spacings.

<table>
<thead>
<tr>
<th>Run #</th>
<th>N</th>
<th>M</th>
<th>Averaging Method</th>
<th>$\Delta_t$</th>
<th>$\Delta_x$</th>
<th>Closure Method</th>
<th>Const.</th>
<th>W</th>
<th>$R_e$</th>
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<td>470</td>
<td>STF</td>
<td>106x</td>
<td>26x</td>
<td>Smag.</td>
<td>--</td>
<td></td>
<td>500</td>
<td>8.63 through 8.67</td>
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<td>STF</td>
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</table>
Chapter VIII
RESULTS

8.1 DENSE GRID RESULTS

The following is a description of the "exact" results of solving (6.1), (6.2) and (6.3) on the dense grid. These results are plotted along with their exact-averaged equivalents in Figures 8.1 through 8.9.

Figure 8.1 shows the spatial distributions of velocity and their wave number spectra at different time steps. The purpose of this figure is to present a complete picture of the Burgers velocity field at high Reynolds numbers (R =500). Initially (Figure 7.2), the velocity distribution has almost one Fourier component at which the wave number spectrum reaches a very accentuated peak. At later time steps, the negative slopes become steeper and steeper which adds new Fourier components at smaller wave lengths or higher wave numbers. The steep negative slopes are shock fronts in which the velocity changes drastically in a short distance. When the shocks are fully developed (i.e. the negative slopes are at their steepest state), the spectrum shows an dependency in the inertial subrange.

The velocity magnitudes are diminishing because of the viscous dissipation and the lack of any external supply of
energy in Equation (6.1). However, the spatial mean of the velocity distribution remains constant at its initial value. The whole train of shocks is sweeping across the flow domain with a speed equal to the constant spatial mean. Therefore, a fixed point in space experiences the shocks passing through as shown in Figure 8.4. The frequency spectrum of velocity at this fixed location also shows an $f^{-2}$ dependency in the inertial subrange.

The relation between the exact velocity field (curves $E_2$) and its exact-averaged counterpart (curves $EA_2$) is evident in Figure 8.1. The exact-averaged field always shows smaller spectral values at high wave numbers because it is obtained by averaging or smoothing the exact field. Although difficult to observe, the shock fronts in the exact-averaged field have milder slopes than their exact equivalents.

Figure 8.2 shows the behavior of the concentration field as convected by the velocity field of Figure 8.1. Initially, the concentration is uniform across the flow domain and the wave number spectrum is zero. At later time steps the concentration gradually accumulates in low velocity regions and diminishes in regions of high velocity. This creates steep concentration slopes which are interpreted as new Fourier components at high wave numbers. The fully developed wave number spectrum shows an $\omega^2$ dependency in its inertial subrange. The number of peaks in the spatial distributions of concentration is equal to that in the velocity distributions.
(40 peaks). These peaks are sweeping across the flow domain with a speed equal to the steady mean of velocity. This is easily concluded by counting the peaks in the time history of concentration at a fixed location (10 peaks in Figure 8.6). Therefore, a distance of 12/40 units of length is covered in 1/10 unit of time. Thus the speed is 3.0 units of length/unit of time.

Since the exact-averaged concentration field is obtained by smoothing the exact field, curves EA2 show smaller spectral values (than curves E2) at high wave numbers in Figure 8.2. Milder concentration slopes are easily noticed in the EA2 distributions compared to the E2 distributions.

All spectral plots in Figures 8.1 and 8.2 show sharp peaks with gaps of low spectrum content between them. This means that both u and c signals can be decomposed into superpositions of cosine waves (Fourier components) of which the important ones show discrete gaps between their respective wave lengths.

Figure 8.3 through 8.6 show some spatial and temporal distributions of u and c, and the corresponding spectral plots as affected by the Reynolds number. It is noticed that as $Re$ increases, the steepness of u and c gradients in the shock fronts increases. Since the steep gradients correspond to high wave number and frequency components, the increasing $Re$ results in increasing spectral values at high wave numbers and high frequencies. The steeper gradients are due to
the fact that $v$ is inversely proportional to $R_e$. As $R_e$ in-creases, the importance of the molecular dissipation de-reases giving a chance for more energy to be sustained in the small-size motion. The spectral plots for the exact-averaged fields (marked EA1, EA2 and EA3) show the same kind of dependency on $R_e$.

In Figure 8.7, the velocity variance defined by Equation (7.2) (which is twice the total energy $\langle v^2/2 \rangle$) increases with higher Reynolds numbers. That is because steeper shock fronts mean larger deviations from the spatial mean. However, all variances diminish with time as a result of the con-tinuous decay in the velocity magnitudes.

The time histories of velocity skewness, as defined by Equation (7.9), show a logically expected behavior in Figure 8.7. Initially, when there is as much regions of positive slopes in the velocity distribution as there is regions of negative slopes, the value of $(\text{slope}_3^3)$ is zero. As the shocks develop, the negative slopes become steeper and steeper with time. This imposes a growing negative value on the skewness which reaches a peak when the shocks are fully developed. After this point in time, the skewness diminishes as a result of the viscous decay in $u(x,t)$. Of course, the increasing $R$ causes larger negative skewness since the negative slopes are directly proportional to $R_e$.

The kurtosis of velocity, in Figure 8.7, changes slowly with time until about the time the shocks are fully devel-
oped. At this point in time dissipation takes over and the kurtosis diminishes as \( u(x,t) \) decays. Again, increasing \( R_e \) causes larger kurtosis since the deviations from the mean are larger for higher \( R_e \).

Averaging the exact velocity field, according to the verification procedure in Chapter VII, has a uniform effect on all the three statistics plotted in Figures 8.7. The curves marked "EA" are always lower (in absolute values) than their corresponding "E" curves. This is due to the fact that the velocity deviations from its spatial mean are reduced in the exact-averaged field.

Figure 8.8 shows time plots of the concentration statistics. Since the concentration is initially uniform, i.e. with zero deviations from the mean, all the three statistics start at zero. As the concentration accumulates gradually in regions of low velocity, it deviates from its spatial mean causing the three statistics to grow larger with time. The statistics reach their peaks when the shocks are fully developed. Then, the decaying velocity forces the concentration field to go gradually back to its initial uniform distribution (see Figures 8.1 and 8.2). This causes the three concentration statistics in Figure 8.8 to decrease after reaching their maximum values.

As in the case of velocity statistics, and for the same reasons, increasing the Reynolds number causes a corresponding increase in the concentration statistics. Also, the ef-
fect of averaging on the concentration statistics is similar to its effect on the velocity statistics.

Figure 8.9 shows a time history of the individual terms of the energy equation (6.3). Since this is an exact solution on a very dense grid, turbulence modeling is not needed and terms 2, 3, and 5 are zero. The energy equation is balanced (L.H.S. = R.H.S.) which means that the results are accurate for the three different Reynolds numbers. As seen in Figure 8.7, the variance (or twice the total energy \( \langle v^2/2 \rangle \)) increases as \( R_e \) increases. Therefore, its temporal slope (the L.H.S of the energy equation) decreases. This explains the differences among the three plots in Figure 8.9.

8.2 **COARSE GRID RESULTS**

The coarse grid results of solving the modeled Equations (6.1), (6.2) and (6.3) are presented in Figures 8.10 through 8.67. These are divided into groups as shown in tables 7.3 through 7.6. The results of each group are described separately in the following subsections.

8.2.1 **Effect of Averaging Method**

Figures 8.10 and 8.11 show wave number spectra (at time 0.5) and frequency spectra (at distance 10) for the calculated \( \bar{u} \) and \( \bar{v} \). The curves marked A1 show clearly that the coarse grid is not capable of solving the original equations. The curves A2 are the results of Reynolds averaging (see Table
7.3) which improves the calculated \( \bar{u} \) and \( \bar{c} \) fields by removing some of the high frequency and high wave number fluctuations seen in A1. Curves A3 are obtained by Leonard's spatial filtering method. Further improvement over the A1 and A2 curves is evident. Finally, curves A4, A5 and A6 show that the STF method of averaging (with increasing \( \Delta_t \)) is more successful in removing the high wave number and high frequency components in the calculated \( \bar{u} \) and \( \bar{c} \).

Figures 8.12 and 8.13 show envelopes of all the spectral plots in Figures 8.10 and 8.11 compared to the corresponding exact-averaged envelopes (see Figure 8.3 for illustration of envelopes). The gradual improvement from A1 to A6 is clear. Only the STF method produces spectral distributions comparable to the corresponding exact-averaged results. A two-fold explanation can be written as follows: 1) From the physical point of view, filtering in both time and space is important since the turbulent variables possess both high frequency and high wave number components. These components are unresolvable by the coarse grid, but are removable by filtering. 2) Mathematically, the existence of the filter terms in Equation (6.1) causes the thin shock fronts to spread over longer distances and periods. This enables coarser grids to perform more stable calculations.

Time histories of the \( \bar{u} \) and \( \bar{c} \) statistics are plotted in Figures 8.14 and 8.15 and compared to their exact-averaged equivalents. Run A1 (no turbulence modelling) gives com-
pletely erroneous statistics. Runs A2 through A6 give quite similar statistics that are comparable to their exact-averaged counterparts.

The eddy viscosity, as defined in Equation 6.4, is calculated at each spatial node. The maximum value is chosen and plotted in Figure 8.16 against time. The STF curves (A4 and A6) show smoother behavior than the Reynolds (A2) and the Leonard's (A3) curves. Also the STF curves are lower than the previous ones. This is due to more efficient smoothing, or smaller $|\partial \bar{u}/\partial x|$ values, in case of STF method.

Figure 8.17 also shows the rewards of improving the averaging method. The figure presents the balance of the energy equation (6.3) for runs A1 through A6. The gap between the L.H.S. and the R.H.S. curves in the A1 plot shows the gross inaccuracy of the calculations. This gap is reduced gradually towards the A6 plot where the L.H.S. and the R.H.S. are almost identical.

The individual terms of the energy equation show their expected behavior in Figure 8.17. The L.H.S. curves are the temporal gradients of the total energy curves plotted in Figure 8.14. The nonlinear terms (terms #1) are always zero since they do not contribute to the balance of energy as explained in Chapter IV. The filter terms (2 and 3) start at zero and grow with time as the shocks develop requiring more filtering. Then, the size of the filter terms decreases as the velocity field decays. The filter terms are proportional
to their respective filter widths. The molecular and turbulent dissipation terms (4 and 5) are governed by $R_e$ and the grid spacings. Since these are constant for all runs in Figure 8.17, terms 4 and 5 show little change from one plot to another.

All terms in the R.H.S. of the energy equation present dissipation since there is no external source of energy in the flow field. It is noticed in Figure 8.17 that: 1) The nonlinear term is energy conservative, i.e. the large scale motions (constituting the nonlinear term) do not dissipate energy. 2) Most dissipation is caused by the molecular and turbulent viscosity terms, i.e. the SGS motion, and 3) The filter terms contribute very little to the dissipation which implies that they act as a media for transferring energy to the SGS motion where it is dissipated. Thus, the energy cascade phenomenon is preserved in the numerical simulation.

Finally, Figure 8.18 and 8.19 are presented to show how the results of run A6 follow closely their exact-averaged equivalents at all time steps.

8.2.2 Effect of Closure Method

Figures 8.20 through 8.27 show the results of constant eddy viscosity closure compared to Smagorinsky's closure when both are combined with Reynolds averaging. In Figure 8.20, curves B1 to B5 correspond to different values of the constant eddy viscosity (see Table 7.4). All curves are within
an acceptable range around the exact-averaged (EA2) curve. Run B2 (K=0.001) is chosen for subsequent comparisons as a representative constant K closure run.

Figures 8.21 through 8.24 show that the Smagorinsky's closure (curves A2) improves both the wave number and the frequency spectra of velocity over the constant K closure (curves B2). The A2 curves have less undesirable high wave number and high frequency components, and are closer to the exact-averaged results than the B2 curves. As shown in Figures 8.25 and 8.26, the Smagorinsky's closure also improves the velocity statistics and the energy balance over the constant K closure. Note however that, in Figures 8.21 to 8.26, the A2 results are still unsatisfactory since the Reynolds averaging method is in effect. Figure 8.27 shows that, as long as the Reynolds averaging method is used, the constant K closure is not capable of producing correct velocity spectra even with careful tuning of the value of K.

The results of constant K closure (B6 curves) and Smagorinsky's closure (curves A3), both combined with Leonard's spatial filtering, are given in Figures 8.28 through 8.34. All A3 spectral curves contain less undesirable noise, and are closer to the exact-averaged results than the B6 curves (Figures 8.28 to 8.31). The Smagorinsky's closure also improves the statistics of both velocity and concentration fields as shown in Figures 8.32 and 8.33. Figure 8.34 shows that the turbulent dissipation term (term 5) in run B6 is
smaller than its equivalent in run A3. That is because in B6 the eddy viscosity is fixed at a value smaller than its variable counterpart in run A3 shown in Figure 8.16. The less efficient turbulent dissipation in run B6 explains the existence of more noise in the spectral plots shown in Figures 8.28 through 8.31. It also explains the erratic behavior of the molecular dissipation term (term 4) in run B6 which becomes alone responsible for dissipating most of the energy flowing to the small-scale components of motion. Generally, the predictions are more accurate in run A3 than in run B6 since the gap between the L.H.S. and the R.H.S. curves is much smaller.

Figures 8.35 to 8.41 compare the results of constant K closure (run B7) to the results of Smagorinsky's closure (run A4) when both are combined with STF averaging at $\Delta_k=4\delta_k$. The group of figures 8.42 to 8.48 present the same kind of comparison but with $\Delta_k=8\delta_k$. The Smagorinsky's closure, combined with any averaging method, continues to show the same improvements discussed above over the constant K closure. It is also noticed that all results improve (become closer to their exact-averaged equivalents) as the averaging method changes from Reynolds to Leonard's to the newly suggested STF scheme.

In Figures 8.49 through 8.52, the closure method is constant K for curves B9, and Smagorinsky's K (with different values for the averaging length w) for curves B10 through
B13. The averaging method is STF with $\Delta x = 10 \delta_i$ for all runs. Again, the Smagorinsky's closure improves the velocity statistics and spectra as shown in Figures 8.49 and 8.50. Note that the effect of $w$ on these statistics and spectra is negligible.

The effect of $w$ on the eddy viscosity is apparent in Figure 8.51. When $w=0$ (curve B10), the eddy viscosity behaves erratically. As $K$ is averaged over longer distances, the curve becomes smoother and lower in magnitude. At $w=14 \delta_x$ (run A6), the eddy viscosity curve is the smoothest obtainable. Further increase of $w$ does not add any smoothness to the $K$ curve, nor does it appreciably change the values of $K$. That is why the value $w=14 \delta_x$ was chosen for all the previous STF runs.

Figure 8.52 shows the effect of $w$ on the energy balance. Since smaller $w$ produces larger $K$ (Figure 8.51), the turbulent viscosity term (term 5) is large in B10 and small in B13. Otherwise, the effect of $w$ on the energy equation is negligible.

8.2.3 Effect of Reynolds Number
In Figures 8.53 through 8.62, the Reynolds number changes from 500 (run A6) to 800 (run C3). The effects on the wave number and frequency spectra of both $\bar{u}$ and $\bar{c}$ are shown in Figures 8.53 to 8.58. As explained in section 8.1, increasing the Reynolds number causes steeper slopes in the spatial
and temporal distributions of velocity and concentration. This makes it more difficult for the averaging procedure to spread out the shocks over longer distances and periods. Consequently, the coarse grid becomes less capable of handling the calculation. This explains the high frequency and high wave number noise (Figures 8.53 to 8.58) which is proportional to the Reynolds number.

The effect of changing \( R_e \) on the velocity and concentration statistics is shown in Figures 8.59 and 8.60. As the Reynolds number increases, the slopes of \( \bar{u} \) and \( \bar{c} \), and consequently the deviations from the mean, increase. This causes a general increase in the statistics of \( \bar{u} \) and \( \bar{c} \).

The impact of increasing \( R_e \) on the eddy viscosity is very clear in Figure 8.61. The eddy viscosity depends on \( |\partial \bar{u} / \partial x| \) which increases as \( R_e \) increases. Therefore, the eddy viscosity curves are higher for larger Reynolds numbers. The erratic behavior of the C2 and C3 curves is a result of the high wave number noise in \( u \) which is interpreted as large values of \( |\partial \bar{u} / \partial x| \).

Figure 8.62 shows the energy balance as affected by the Reynolds number. As the Reynolds number increases, the magnitude of the molecular viscosity term (term 4) decreases because \( \nu \) is inversely proportional to \( R_e \). This hinders the dissipation process and allows energy to build up at the small scales of motion. Consequently, the accuracy of the calculation diminishes as implied by the increasing gap between the L.H.S. and the R.H.S. curves.
8.2.4 Effect of Grid Spacings

Figures 8.63 through 8.67 show the effect of increasing grid spacings on the calculated $\tilde{u}$ and $\tilde{c}$ fields. When all other parameters are fixed, the increasing grid spacings cause instabilities in the $\tilde{u}$ and $\tilde{c}$ fields and accumulation of energy at the high wave numbers and frequencies (Figures 8.63 to 8.66). Numerically, the wider spacings mean larger errors in the finite difference approximations of the derivatives. This causes errors and instabilities in the calculated variables. Physically, the spatial and temporal scales of the shocks in $\tilde{u}$ and $\tilde{c}$ are too small compared to the scales of the coarser grids. In other words, the $\tilde{u}$ and $\tilde{c}$ fields include components at frequencies and wave numbers higher than the Nyquist values of the wide grids. Thus, $\tilde{u}$ and $\tilde{c}$ cannot be fully resolved by the wide grid spacings.

The energy balance plots, in Figure 8.67, show that the magnitude of the turbulent dissipation term (term 5) increases as the grid spacings increase. This is expected since the eddy viscosity $K$ in the Smagorinsky's model is directly proportional to the square of the spatial grid spacing. However, this increasing dissipation is apparently not enough to counter the build up of spectrum at high frequencies and wave numbers caused by the numerical errors. The overall accuracy of the calculation is affected by the increasing spacings as implied by the increasing gap between the L.H.S. and the R.H.S. terms.
Figure B.1: Time Evolution of Exact and Exact-Averaged Velocity Profiles.
Figure 8.1: (Continued)
Figure 8.1: (Continued)
Figure 8.2: Time Evolution of Exact and Exact-Averaged Concentration Fields.
Figure 8.3: Wave Number Spectra of Velocity at Time 0.4. Dense Grid Runs.
Figure 8.4: Frequency Spectra of Velocity at Distance 2.0. Dense Grid Runs.
Figure 8.5: Wave Number Spectra of Concentration at Time 0.4. Dense Grid Runs.
Figure 8.6: Frequency Spectra of Concentration at Distance 2.0. Dense Grid Results.
Figure 8.7: Time Histories of Exact and Exact-Averaged Velocity Statistics.
Figure 8.8: Time Histories of Exact and Exact-Averaged Concentration Statistics.
Figure 8.9: Energy Balance in the Exact Velocity Field.
Figure 8.10: Wave Number Spectra of Velocity and Concentration. Different Averaging Methods with Smagorinsky's Closure.
Figure 8.10: (Continued).
Figure 8.11: Frequency Spectra of Velocity and Concentration at Distance 10. Different Averaging Methods; Smagorinsky's Closure.
Figure 8.11: (Continued).
Figure 8.11: (continued).

[Graphs showing log spectrum, velocity, and concentration plots for different conditions.]
Figure 8.12: Comparison of Velocity Spectra. Different Averaging Methods with Smagorinsky's Closure.

Figure 8.13: Comparison of Concentration Spectra. Different Averaging Methods with Smagorinsky's Closure.
Figure 8.14: Time Histories of Velocity Statistics. Different Averaging Methods with Smagorinsky's Closure.
Figure 8.15: Time Histories of Concentration Statistics. Different Averaging Methods with Smagorinsky's Closure.
Figure 8.16: Time Histories of Maximum Eddy Viscosity. Different Averaging Methods with Smagorinsky's Closure.
Figure 8.17: Energy Balance in the Large-Scale Velocity. Different Averaging Methods with Smagorinsky's Closure.
Figure 8.18: Calculated Velocity Field by STF and Smagorinsky’s Closure Compared to its Exact-Averaged Equivalent.
Figure 8.18: (Continued)
Figure 8.18: (Continued)
Figure 8.19: Calculated Concentration Field by STF and Smagorinsky’s Closure Compared to its Exact-Averaged Equivalent.
Figure 8.19: (Continued).

[Graphs showing concentration and log spectrum data with various scales and labels.]

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Figure 8.20: Time Histories of Velocity Variance. Tuning the Constant Eddy Viscosity.
Figure 8.21: Wave Number Spectra of Velocity at time 0.2. Different Closures with Reynolds Averaging.
Figure 8.22: Wave Number Spectra of Velocity at Time 0.4. Different Closures with Reynolds Averaging.
Figure 8.23: Frequency Spectra of Velocity at Distance 2.0. Different Closures with Reynolds Averaging.
Figure 8.24: Frequency Spectra of Velocity at Distance 5.4. Different Closures with Reynolds Averaging.
Figure 8.25: Time Histories of Velocity Statistics. Different Closures with Reynolds Averaging.
Figure 8.26: Energy Balance in the Large-Scale Velocity. Different Closures with Reynolds Averaging.
Figure 8.27: Wave Number and Frequency Spectra of Velocity. Constant K Closure with Reynold's Averaging.
Figure 8.28: Wave Number Spectra of Velocity at Time 0.5. Different Closures with Leonard's Spatial Filtering.
Figure 8.29: Frequency Spectra of Velocity at Distance 10. Different Closures with Leonard's Spatial Filtering.
Figure 8.30: Wave Number Spectra of Concentration at Time 0.5. Different Closures with Leonard's Spatial Filtering.
Figure 8.31: Frequency Spectra of Concentration at Distance 10. Different Closures with Leonard's Spatial Filtering.
Figure 8.32: Time Histories of Velocity Statistics. Different Closures with Leonard's Spatial Filtering.
Figure 8.33: Time Histories of Concentration Statistics. Different Closures with Leonard's Spatial Filtering.
Figure 8.34: Energy Balance in the Large-Scale Velocity. Different Closures with Leonard's Spatial Filtering.
Figure 8.35: Wave Number Spectra of Velocity at Time 0.75. Different Closures with STF, $\Delta t = 4 \delta_t$. 
Figure 8.36: Frequency Spectra of Velocity at Distance 2.0.
Different Closures with STF, $\Delta_t = 4 \delta_t$. 
Figure 8.37: Wave Number Spectra of Concentration at Time 0.75. Different Closures with STF, $\Delta_t = 4 \delta_t$. 

- B7
- A4
- EA2
- EA2
Figure 8.38: Frequency Spectra of Concentration at Distance 2. Different Closures with STF, $\Delta t = 4 \delta t$. 
Figure 8.39: Time Histories of Velocity Statistics. Different Closures with STF, $\Delta_t = 4\delta_t$. 
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Figure 8.41: Energy Balance in the Large-Scale Velocity. Different Closures with STF, \( \Delta t = 4 \Delta t \).
Figure 8.42: Wave Number Spectra of Velocity at Time 0.3. Different Closures with STF, $\Delta_t = 8 \delta_t$. 
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Different Closures with STF, $\Delta_t = 8\delta_t$. 
Figure 8.44: Wave Number Spectra of Concentration at Time 0.3. Different Closures with STF, $\Delta_t = 8 \delta_t$. 
Figure 8.45: Frequency Spectra of Concentration at Distance 5.4. Different Closures with STF, $\Delta_t = 8 \delta_t$. 
Figure 8.46: Time Histories of Velocity Statistics. Different Closures with STF, $\Delta_t = 8 \delta_t$. 
Figure 8.47: Time Histories of Concentration Statistics. Different Closures with STF, $\Delta_l = 8 \delta_l$. 
Figure 8.48: Energy Balance in the Large-Scale Velocity. Different Closures with STF, $\Delta t = 8\delta t$. 
Figure 8.49: Time Histories of Velocity Statistics. Different Closures with STF, $\Delta_t = 10 \delta_t$. 
Figure 8.50: Wave Number and Frequency Spectra of Velocity. Different Closures with STF, $\Delta_t = 10 \delta_t$. 
Figure 8.51: Time Histories of Maximum Eddy Viscosity. Different Closures with STF, $\Delta t = 10 \delta t$. 
Figure 8.52: Energy Balance in the Large-Scale Velocity. Different Closures with STF, $\Delta_t = 10\delta_t$. 
Figure 8.53: Wave Number Spectra of Velocity at Time 0.5. Different $R_e$ with STF Averaging and Smagorinsky's Closure.
Figure 8.54: Frequency Spectra of Velocity at Distance 10. Different $R_e$ with STF Averaging and Smagorinsky's Closure.
Figure 8.55: Wave Number Spectra of Concentration at Time 0.5. Different $R_e$ with STF Averaging and Smagorinsky's Closure.
Figure 8.56: Frequency Spectra of Concentration at Distance 10. Different $R_e$ with STF Averaging and Smagorinsky's Closure.
Figure 8.57: Comparison of Velocity Spectra. Different $Re$ with STF Averaging and Smagorinsky's Closure.

Figure 8.58: Comparison of Concentration Spectra. Different $Re$ with STF Averaging and Smagorinsky's Closure.
Figure 8.59: Time Histories of Velocity Statistics. Different $R_e$ with STF Averaging and Smagorinsky's Closure.
Figure 8.60: Time Histories of Concentration Statistics. Different $R_a$ with STF Averaging and Smagorinsky's Closure.
Figure 8.61: Time History of Maximum Eddy Viscosity. Different Re with STF Averaging and Smagorinsky's Closure.
Figure 8.62: Energy Balance in the Large-Scale Velocity. Different $R_e$ with STF Averaging and Smagorinsky's Closure.
Figure 8.63: Wave Number Spectra of Velocity at Time 1.0. Different Grid Spacings with STF Averaging and Smagorinsky's Closure.
Figure 8.64: Frequency Spectra of Velocity at Distance 10. Different Grid Spacings with STF Averaging and Smagorinsky's Closure.
Figure 8.65: Wave Number Spectra of Concentration at Time 1.0. Different Grid Spacings with STF Averaging and Smagorinsky's Closure.
Figure 8.66: Frequency Spectra of Concentration at Distance 10. Different Grid Spacings with STF Averaging and Smagorinsky's Closure.
Figure 8.67: Energy Balance in the Large-Scale Velocity. Different Grid Spacings with STF Averaging and Smagorinsky's Closure.
9.1 OVERVIEW

The overall objective of this research is to improve the averaging and verification aspects of turbulence modeling. The Reynolds temporal averaging (Reynolds, 1883); the uniform spatial averaging (e.g. Lilly, 1967); and the spatial Gaussian averaging (e.g. Leonard, 1974) are reviewed in Chapter II. These methods of averaging are critically analyzed in Chapter III and the new STF method is suggested to correct their mathematical and physical shortcomings. The one-dimensional, transient equations presented in Chapter IV are used for application and experiments.

In order to verify and compare the results of the existing and the new STF methods of averaging, a statistical verification package is suggested in Chapter VII and applied to the results in Chapter VIII. The verification procedure is based on statistical and spectral comparisons between the model results and the averaged "exact" results obtained by solving the original equations on very dense grids. The results and comparisons are described in detail in Chapter VIII.
In the following sections, the results are placed into context with the present state of knowledge on turbulence modeling with Burgers flow. Similarities and improvements over the existing theory are pointed out. Finally, a list of conclusions is given at the end of this chapter.

9.2 DISCUSSION OF DENSE GRID RESULTS
The important difference between the dense grid results described in Chapter VIII and similar results in the literature is in presenting the temporal (not only the spatial) characteristics of the results. In the works of Jeng (1969); Jeng and Meecham (1971); Hosokawa and Yamamoto (1975) and Love (1980), exact solutions of the "forced" Burgers equation are considered. An extra term, in the form of a random function of x and t, is added to the equation. This term acts as an external source of energy which counters the dissipation and results in a steady state. The statistical and spectral properties of the velocity field are studied in the steady state.

In the present research, the original form of the Burgers equation is solved for the case of a randomly distributed initial velocity. Statistics and wave number spectra of velocity at different time levels are calculated to study closely the time evolution of these properties. Also, frequency spectra of velocity are calculated at different spatial locations. Both spatial and temporal statistics are
used as a basis against which the results of the modeled equations are compared. This spatial-temporal comparison is important since the new STF method of averaging, which filters in both space and time is being tested.

The exact results are described in detail in Chapter VIII. The main features can be summarized as follows:

1. As observed in all previous research, the random initial distribution of velocity gradually arranges itself into a series of shock fronts connected by regions of mild slope. See for example Figure 9.1 (Love, 1980).

2. When the shocks are fully developed, the corresponding wave number spectrum is proportional to $\omega^{-2}$ in the inertial subrange. This confirms the spectral plots given in Jeng (1969); Love(1980) and Hosokawa and Yamamoto (1975) (See Figure 9.2.). In the present research, the initial wave number spectrum is zero in the inertial subrange. As the shocks developed gradually, it was possible to observe the gradual development of the inertial subrange with the expected $\omega^{-2}$ dependency.

3. The frequency spectra of velocity, at different spatial locations, also show an $f^{-\frac{1}{2}}$ dependency in the inertial subrange. No similar results are available in the literature since all previous spectral analysis is applied to spatial distributions of velocity.

4. The variance, skewness and kurtosis of the spatial distributions of velocity are plotted against time. No similar presentation of these statistics is available in the literature. The behavior of these statistics is explained in Chapter VIII. These statistics are instrumental in verifying the results of the modeled equations according to the verification procedure.

The energy equation (6.3) is derived as in Meecham and Seigel (1964) and Love (1980). This equation gives a measure of the contribution of each term in the burgers equation to the process of energy distribution and dissipation. For the
Figure 9.1: Typical Velocity Profile, Love (1980).

Figure 9.2: Wave Number Spectrum, Jeng (1969).
dense grid results, the temporal behavior of each term in the energy equation is plotted and discussed in detail in Chapter VIII. The main features are:

1. As explicitly demonstrated by Meecham and Seigel (1964) and Love (1980), the nonlinear inertial term is energy conservative. The nonlinear energy dissipation term is always zero in all the energy balance plots in Figure 8.9.

2. The dissipation of energy is caused solely by the molecular viscosity term which represents the small scales of motion. This is in agreement with the results of Love (1980) shown in Figure 9.3.

The one-dimensional scalar transport equation (6.2) is heavily used in the literature for open-channel or pipe flow situations. In the present research the equation is solved for the first time in conjunction with the Burgers velocity field. The behavior of the concentration field, when convected by the Burgers velocity field, is discussed in detail in Chapter VIII. The main observation is that the concentration accumulates in regions of low velocity and diminishes in regions of high velocity. Also, its spectral distributions (in both wave number and frequency domains) show the same -$2$ slopes in the inertial subrange as do the velocity spectra. The variance, skewness and kurtosis of the concentration field are calculated and plotted against time in Figure 8.8. A detailed discussion of their behavior is given in Chapter VIII.

The exact velocity and concentration fields are averaged to extract their large-scale components. Since the modeled equations predict the large-scale components of the varia-
Figure 9.3: Total Energy and Viscous Dissipation, Love (1980).
bles, it is important to compare the modeled results to the exact-averaged and not directly to the exact results. The same principle is applied in Clark et al. (1977) and Love (1980). The statistics and spectral distributions of the exact-averaged fields are plotted and compared to their exact equivalents in Chapter VIII.

9.3 DISCUSSION OF COARSE GRID RESULTS
The only coarse grid Burgers flow simulation available in the literature is due to Love (1976); Love and Leslie (1977) and Love (1980). In these works, the Burgers equation is averaged by the Leonard's spatial filtering approach. The closure is constant $K$ or Smagorinsky's $K$ with and without the Clark's reduction. The pertinent results are summarized in Figure 9.4 in which the Leonard's method shows a noticeable improvement over the Reynolds method. Figure 9.5 shows how the value $\Delta_x = 2 \delta_x$ is chosen for the spatial filter width.

In the present research, the superiority of the Leonard's method of averaging over the traditional Reynolds method is confirmed. In addition to wave number spectral comparisons (as shown in Figure 9.4), the frequency spectra and the time histories of velocity statistics are used to verify and compare the performance of the different models. However, the intensity of turbulence, as represented by the Reynolds number and the number of shocks in the flow domain, is so high that the performance of the Leonard's method is still unsa-
Figure 9.4: Wave Number Spectrum at Steady State, Love (1976).

Figure 9.5: Tuning the Spatial Filter Width, Love (1980).
satisfactory. The new STF averaging method proved capable of handling this highly turbulent flow and produced satisfactory results in terms of the spectral and statistical properties compared to the exact-averaged equivalents. Based on the detailed discussion and comparisons given in Chapter VIII, the following points are observed:

1. When all other parameters are constant, the averaging methods show increasingly refined performance in the following order:
   a) No modeling.
   b) Reynolds averaging.
   c) Leonard's averaging.
   d) STF averaging.

2. With any given method of averaging, and when all other parameters are constant, the closure methods improve the results in the following order:
   a) No modeling.
   b) Constant K closure.
   c) Local Smagorinsky's K.
   d) Smagorinsky's K averaged over a certain length in the flow domain.

3. The performance of any turbulence model is directly affected by the Reynolds number and the grid spacings. The results presented in Chapter VIII are subject to the following limitations:
   a) The Reynolds number is less than 500.
   b) Since the weakly stable Adam-Bashforth method is used for time marching, it was found that the x-t grid spacings cannot be larger than about 5 times the corresponding spacings required for the exact solution.
   c) For numerical stability, it was also found that the Courant number \( \frac{\Delta t \, V_0}{\Delta x} \) must be kept under 0.5.
The coarse grid results of the energy equation (6.3) confirm the conclusions of Love (1980) in that the nonlinear term is conservative, and the filter terms do not dissipate much energy. They transfer energy between the large-scale motion and the small-scale motion where dissipation occurs. In the present research, a temporal filter term exists in addition to the spatial filter term. The average size of these terms, as observed in the energy balance plots, depends on the filter widths and is always small compared to the dissipation terms. However, the role of these filter terms in improving the results and preserving the energy cascade process is very noticeable.

The one-dimensional transport equation (6.2) has been solved in the literature mainly to simulate contaminant transport in open-channels. Coarse grid calculations have been conducted with the traditional Reynolds averaging method as in Holley et al. (1970) and many others. Satisfactory results are obtainable if the level of turbulence is not too high.

In the present research, coarse grid calculations are performed to simulate scalar transport in a highly turbulent Burgers flow domain. The results, presented in Chapter VIII, further confirm the role of the averaging and closure methods in improving the predictions. Again, the STF method performed better than the Leonard's and the Reynolds methods. The statistics and spectral distributions of the predicted $c$
fields are closer to their exact-averaged counterparts when the STF method is used. Also, the Smagorinsky's closure gives better results than the constant K model. The same Reynolds number and grid spacing limitations listed above apply also to the solution of the transport equation.

9.4 CONCLUSIONS

Based on the results presented in Chapter VIII, and the above discussion, the major conclusions are the following:

(1) It is important to consider the physical attributes of turbulence when deriving a mathematical method for averaging. The turbulent SGS activities in both time and space necessitate both temporal and spatial averaging of the governing equations.

(2) The suggested STF method of averaging, which employs Gaussian filters in both time and space, performs better than the existing methods in simulating the one-dimensional flow considered in this research. The improvement is verified by means of statistical and spectral comparisons with the exact-averaged results.

(3) The STF averaging procedure results in the appearance of additional spatial and temporal filter terms in the governing equations. The new terms spread out the steep slopes of the turbulent variables over longer distances and periods. This makes it easier for coarse grids to handle the calculation. The filter terms also act as a media for trans-
ferring the energy from the large-scale motion to the SGS motion where dissipation takes place. Thus the energy cascade phenomenon is preserved in the simulation.

(4) The STF method of averaging gave satisfactory results when combined with the simple Zero-Equation Models of closure. This implies that improving the averaging procedure attaches less importance to the difficult and ambiguous closure problem.

(5) The performance of any turbulent modeling scheme is a function of the intensity of turbulence which is represented by the Reynolds number. The STF averaging, with Smagorinsky's Zero-Equation closure, successfully simulated a Burgers flow at $R_e = 500$. Further increase of $R_e$ puts a severe strain on the model and necessitates smaller grid spacings.

(6) Using the STF averaging, combined with Smagorinsky's closure, satisfactory results were obtained with a grid about five times wider than that required to solve the unaveraged equations. This means that for a similar three-dimensional problem the required computer memory space can be reduced by a factor of $5^4$.

The above conclusions apply to the one-dimensional, transient Burgers type flow. The similarities between this flow and the three-dimensional Navier-Stokes flow are presented in Chapter IV. These similarities imply that the above conclusions may hold for the Navier-Stokes turbulence. Future research is recommended to test this point.
BIBLIOGRAPHY


Appendix A

MOMENTUM CALCULATION PROGRAM
// TIME=(15,20),REGION=700K
/* SETUP UNIT=TAPE9,ID=(ABCD,J274,WRITE)
  JOBPARM LINES=20000,TAPE10=20000,V=D
  EXEC PLOTV,TIME.GO=15
  GO.SOURCE DD *

REAL NEW,LO,KED,KMAX,KK,KCONST,MEAN,MEAN1,MEANP
INTEGER WL,WP1,CLOSUR,ENCAL,EXACT,TAPE
DIMENSION U(4040,4),KK(1501,3)
DIMENSION KED(1501),KMAX(2020)
DIMENSION X(4040),Y(4040)
DIMENSION NOD(5),YT(5,2505)
DIMENSION R(610),E(610),ES(612),W(612)
DIMENSION TOTEN(2505),DEDT(2505)
DIMENSION EN2(2505),EN3(2505),EN4(2505),EN5(2505)
DIMENSION EN6(2505),EN234(2505),RHS(2505)
DIMENSION EN34(2505),SDEDT(2505),MEAN(4),MEANP(2505)
**********************************************************************************
C READ DATA
C RE=REYNOLDS NUMBER
C GAM=FILTER CONSTANT
C N=NUMBER OF NODAL POINTS
C M=NUMBER OF TIME STEPS
C DX=SPATIAL GRID SPACING
C DT=TEMPORAL GRID SPACING
C LFX=_RATIO OF SPATIAL FILTER WIDTH TO GRID SPACING
C LFT =RATIO OF TEMPORAL FILTER WIDTH TO TIME STEP SIZE
C WL=NUMBER OF SPATIAL INTERVALS OVER WHICH THE EDDY VISCOSITY
C IS AVERAGED
C C=RESIDUAL FIELD COEFFICIENT
C MEAN1=MEAN VALUE OF U(X,0)
C TOTL=TOTAL LENGTH OF FLOW DOMAIN
C IF CLOSUR=0,THE EDDY VISCOSITY =0
C IF CLOSUR=1,THE EDDY VISCOSITY IS CONSTANT EQUALS TO KCONST
C IF CLOSUR=2,THE SMAGORINSKY MODEL IS USED
C WP1=NUMBER OF NODES OVER WHICH THE EDDY VISCOSITY IS AVERAGED
C DELX=SPATIAL FILTER WIDTH
C DDEL=TEMPORAL FILTER WIDTH
C LO=WAVE LENGTH OF LARGEST FOURIER COMPONENT IN U(X,0)
DATA RE,GAM,N,M,DX,DT/700.0,6.0,4027,2014,0.00298063,0.00049677/
DATA LFX,LFT/0.0,2.15/
DATA WL,CL/15,4.0/
DATA MEAN/3.00/
DATA TOTL/12.0/
DATA CLOSUR,KCONST/2,0.001/
DATA WP1=WL+1
DELX=LFX*DX
DDEL=LFT*DT
LO=0.29955047
NM1=N-1
FN=FLOAT(N)
**********************************************************************************
C CONTROL VARIABLES
C NSPEC=NUMBER OF POINTS IN WAVE NUMBER SPECTRUM
SLMAX=MAXIMUM VALUE IN LOG WAVE NUMBER SPECTRAL PLOTS
SLMIN=MINIMUM VALUE IN LOG WAVE NUMBER SPECTRAL PLOTS
WLEFT=STARTING VALUE ON THE WAVE NUMBER AXIS IN SPECTRAL PLOTS
WRIGHT=ENDING VALUE ON THE WAVE NUMBER AXIS IN SPECTRAL PLOTS
J1,J2,...,J10=TIME STEPS NUMBERS AT WHICH WAVE NUMBER SPECTRA ARE CALCULATED, ALSO STATISTICS ARE CALCULATED
COF=COEFFICIENT USED FOR PLOTTING VELOCITY DISTRIBUTIONS, RANGE OF VERTICAL AXIS=3*COF, MEAN AT THE MIDDLE
XLEN,YLEN,YLEN1=LENGTHS OF AXES IN INCHES
SLOPE=SLOPE OF INCLINED LINE IN SPECTRAL PLOTS
ASL,ASYL,AX2=TO PLACE THE INCLINED LINE
TOTEN(M+1)=STARTING VALUE IN TOTAL ENERGY PLOT
TOTEN(M+2)=INTERVAL VALUE PER INCH IN TOTAL ENERGY PLOT
NNOD=NUMBER OF NODES AT WHICH VELOCITY TRACES ARE STORED
NOD=ARRAY CONTAINING THE NODE NUMBERS AT WHICH TIME TRACES ARE STORED AND ANALYZED, SPECTRA AND STATISTICS ARE CALCULATED
M1=TIME TRACES STORED AT DIFFERENT NODES START FROM TIME STEP
NUMBER M1 AND CONTINUE TO THE LAST TIME STEP
NSPECT=NUMBER OF POINTS IN FREQUENCY SPECTRUM
SLMINT=MINIMUM VALUE ON VERTICAL AXIS OF FREQUENCY SPECTRA PLOTS
SLMAXT=MAXIMUM VALUE ON VERTICAL AXIS OF FREQUENCY SPECTRA PLOTS
WTLEFT=STARTING VALUE ON THE FREQUENCY AXIS IN SPECTRAL PLOTS
WTRIGHT=ENDING VALUE ON THE FREQUENCY AXIS IN SPECTRAL PLOTS
DEDT(M+1)=STARTING VALUE IN TIME RATE OF TOTAL ENERGY PLOT
DEDT(M+2)=INTERVAL VALUE PER INCH IN TIME RATE OF TOTAL ENERGY PLOT
IF ENCAL=1 ALL TERMS OF ENERGY EQUATION WILL BE CALCULATED
IF ENCAL=0 ONLY TOTAL ENERGY AND ITS TIME RATE WILL BE CALCULATED
IF EXACT=1 THE ORIGINAL (NON-FILTERED EQUATION) IS SOLVED
IF EXACT=0 THE FILTERED OR MODELED EQUATION IS SOLVED
IF TAPE=1 THE VELOCITY FIELD IS STORED ON TAPE
IF TAPE=0 THE VELOCITY FIELD IS NOT STORED
IF INITST=1 THE STATISTICS OF U(X,0) ARE CALCULATED
IF INITST=0 THE STATISTICS OF U(X,0) ARE NOT CALCULATED
IF TAPE=1 THE VELOCITY FIELD IS STORED ON TAPE
IF TAPE=0 THE VELOCITY FIELD IS NOT STORED
IF EXACT=1 THE ORIGINAL (NON-FILTERED EQUATION) IS SOLVED
IF EXACT=0 THE FILTERED OR MODELED EQUATION IS SOLVED

DATA PI,NSPEC,SLMAX,SLMIN/3.14159,604,-2.3,-7.0/
DATA WLEFT/-0.86/
DATA WRIGHT/2.22/
DATA J1,J2,J3,J4,J5,J6,J7,J8,J9,J10/102,202,303,404,504,605,806,10
$08,1511,2014/
DATA COF/0.3333333333/
DATA LMASK1,LMASK2,XLEN,YLEN,YLEN1/ZFFFF,ZOFF,5.0,2.0,5.0/
DATA SLOPE,XS1,YS1,AX2/-2.0,3.0,4.8,4.5/
DATA TOTEN(M+1)=0.0
DATA TOTEN(M+2)=0.0022
DATA NNOD,NOD/5,1,672,1812,3356,4027/
DATA M1,NSPECT,SLMINT,SLMAXT/1,403,-7.0,-3.0/
DATA WT,WTR/0.1,3.0/
DATA DEDT(M+1)=-0.04
DATA DEDT(M+2)=0.01
DATA MEANP(M+1)=2.992
DATA MEANP(M+2)=0.002
DATA KMAX(M+1)=0.0008
KMAX(M+2)=0.0008
ENCAL=1
EXACT=1
TAPE=1
INITST=1
NSMTH=40

C ******************************************************************
C SET INITIAL VELOCITY DISTRIBUTION
READ (3,960) (U(I,3),I=1,N)
SUM=0.00
DO 10 I=1,N
10 SUM=SUM+U(I,3)
MEAN(3)=SUM/FN
DO 20 I=1,N
20 U(I,3)=U(I,3)-MEAN(3)+MEAN1
DO 30 I=1,N
30 U(I,2)=U(I,3)
U(I,1)=U(I,3)
30 CONTINUE
IF(TAPE.EQ.1) WRITE (8) (U(I,3),I=1,N)
MEAN(1)=MEAN1
MEAN(3)=MEAN1
MEAN(2)=MEAN1
MEAN(1)=MEAN1

C ******************************************************************
C CALCULATE AND PLOT STATISTICS OF U(X,0)
DO 40 I=1,N
40 X(I)=(I-1)*DX
X(N+1)=0.0
X(N+2)=X(N)/XLEN
Y(N+1)=MEAN1-1.5*COF
Y(N+2)=(3.0*COF)/YLEN
IF(INITST.EQ.0) GO TO 170
J=1
DO 50 I=1,N
50 Y(I)=U(I,3)
SUM1=0.0
SUM2=0.0
SUM3=0.0
SUM4=0.0
DO 60 I=1,N
TERM=Y(I)-MEAN1
SUM1=SUM1+TERM*TERM
SUM2=SUM2+Y(I)*Y(I)
SUM3=SUM3+TERM*TERM*TERM
SUM4=SUM4+TERM*TERM*TERM*TERM
60 CONTINUE
STDV=SQR(T(SUM1/N))
VAR=STDV*STDV
RMS=SQR(T(SUM2/N))
SKEW=SUM3/(N*STDV*VAR)
AKURT=SUM4/(N*VAR*VAR)
TIME=(J-1)*DT
WRITE (6,970) J,TIME,MEAN1,STDV,VAR,RMS,SKEW,AKURT
WRITE (6,1080) (Y(I),I=1,101)
SUM1=0.0
SUM2=0.0
DUDX1=(U(2,3)-U(N-1,3))/(2.*DX)
DO 70 I=2,NM1
DUDX=(U(I+1,3)-U(I-1,3))/(2.*DX)
SUM1=SUM1+DUDX*DUDX*DUDX
SUM2=SUM2+DUDX*DUDX
70 SUM1=SUM1+2.*DUDX1*DUDX1*DUDX1
SUM2=SUM2+2.*DUDX1*DUDX1
SK=(SUM1/N)/((SUM2/N)**1.5)
WRITE (6,1200) SK
CALL PLOTS (0,0,0)
CALL AXIS (2.0,7.8,-8,XLEN,0.,X(N+1),X(N+2))
CALL AXIS (2.0,7.8,-8,HVEL0CITY,8,YLEN,90.,Y(N+1),Y(N+1))
CALL PLOT (2.0,7.8,-3)
CALL LINE (X,Y,N,1,0,0)
CALL HLINE (0.,XLEN,YLEN,LMASK1)
CALL VLINE (0.,XLEN,YLEN,LMASK1)
CALL PLOT (-2.,-7.8,-3)
DO 80 I=1,N
80 Y(I)=Y(I)-MEAN1
DO 100 IP=1,NSPEC
IQF=N-IP+1
SUM=0.0
DO 90 IQ=1,IQF
90 SUM=SUM+Y(IQ)*Y(IQ+IP-1)
100 R(IP)=SUM/(N-IP+1)
DO 120 IH=1,NSPEC
SUM=0.0
DO 110 IP=1,NSPEC
EPS=1.0
IF(IP.EQ.1.OR.IP.EQ.NSPEC) EPS=0.5
110 SUM=SUM+EPS*R(IP)*COS((IH-1)*(IP-1)*PI/(NSPEC-1))
120 E(IH)=2.*DX*SUM/PI
ES(1)=0.54*E(1)+0.46*E(2)
ES(NSPEC)=0.54*E(NSPEC)+0.46*E(NSPEC-1)
NSPEC=NSPEC-1
DO 130 I=2,NSPEC
130 ES(I)=0.23*E(I-1)+0.46*E(I)+0.23*E(I+1)
SUM=0.5*(ES(I)+ES(NSPEC))
DO 140 I=2,NSPEC
140 ES=SUM+ES
AREA=(PI*SUM)/(NSPEC*DX)
DO 150 I=1,NSPEC
150 W(I)=(I-1)/(2.*DX*NSPEC)
W(I)=(W(I)+W(2))/2.
DO 160 I=1,NSPEC
W(I)=ALOG10(W(I))
IF(ES(I).LT.(10.0**(SLMIN))) ES(I)=10.0**(SLMIN)
160 ES(I)=ALOG10(ES(I))
W(NSPEC+1)=WLEFT
W(NSPEC+2)=(WRIGHT-W(NSPEC+1))/XLEN
ES(NSPEC+1)=SLMIN
ES(NSPEC+2)=(SLMAX-SLMIN)/YLEN1
CALL AXIS (2.0,2.3,15HLLOG WAVE NUMBER,-15,XLEN,0.,W(NSPEC+1),W(NSPEC+1))
CALL AXIS (2.0,2.3,12HLLOG SPECTRUM,12,YLEN1,90.,ES(NSPEC+1),ES(NSPEC+1))
CALL PLOT (2.0,2.3,-3)
CALL LINE (W,ES,NSPEC,1,0,0)
CALL HLINE (0.,XLEN,YLEN1,LMASK1)
CALL VLINE (0.,YLEN1,XLEN,LMASK1)
CALL NUMBER (0.2,4.73,0.07,4HTIME,0.,4)
CALL NUMBER (XSYM,YSYM,0.07,TIME,0.,-1)
WRITE (6,990) (W(I),1=1,NSPEC)
WRITE (6,990) (ES(I),1=1,NSPEC)
WRITE (6,1010) AREA
CONTINUE
C
STORE VELOCITY TRACES AT SOME CHOSEN NODES
DO 180 K=1,NNOD

K = NOD(K)

YT(K,1)=U(K,3)
CONTINUE
C
CALCULATE MOLECULAR VISCOSITY
NEW=(L0*MEAN1)/RE
C
CALCULATE MAXIMUM EDDY VISCOSITY AT TIME ZERO
IF(EXACT.EQ.1) GO TO 220
DO 200 I=1,N
SUM=0.0
DO 190 II=1,WPI

II=I-WL/2+II-1
IIIM1=I+II-1
IIIM1=IIIM1-1
IF(IIIM1.LT.1) IIIM1=IIIM1+N-1
IF(IIIM1.GT.N) IIIM1=IIIM1-N+1
SUM=SUM+ABS(U(IIIM1,3)-U(IIIM1,3))
KED(I)=SUM*C*DX/(2.*WPI)
IF(CLOSUR.EQ.0) KED(I)=0.0
IF(CLOSUR.EQ.1) KED(I)=KCONST
CONTINUE
IF (TAPE.EQ.1 AND CLOSUR.EQ.2 AND EXACT.EQ.0) WRITE (8) (KED(I),I=11,N)
KMAX(I)=KED(I)
DO 210 I=2,N
210 IF(KMAX(I).LT.KED(I)) KMAX(I)=KED(I)
220 CONTINUE

C ***************CALCULATE COEFFICIENTS***********************
C
A1=-DT/(4.*DX)
A2=DT/(32.*DX)
A3=-(3.*DELT*DELT*DELT)/(64.*GAMMA*DX*DX*DX)
A4=-(DELT*DELT)/(32.*GAMMA*DX*DX)
A5=(3.*DT*NEW)/(2.*DX*DX)
A6=(3.*DT)/(16.*DX*DX)
AB=-A2/3.
AD=-A4/3.
AE=-A5/3.
AF=-A6/3.

C ***************START TIME LOOP*******************************
C
DO 600 J=2,M

C ***************Sweep over space*******************************
C
IF(ENCAL.EQ.0) GO TO 230
SUME2=0.0
SUME3=0.0
SUME4=0.0
SUME5=0.0
SUME6=0.0
230 CONTINUE
DO 340 I=1,N

C ***************Boundary condition*************************
C
IP1=I+1
IP2=I+2
IM1=I-1
IM2=I-2
IF(IP1.GT.N) IP1=IP1-N+1
IF(IP2.GT.N) IP2=IP2-N+1
IF(IM1.LT.1) IM1=IM1+N-1
IF(IM2.LT.1) IM2=IM2+N-1

C
TERM1=AI*(U(IP1,3)*U(IP1,3)-U(IM1,3)*U(IM1,3)+2.*U(I,3)*(U(IP1,3)-U(IM1,3)))
TERM2=A2*(U(IP2,3)*U(IP2,3)-U(IM2,3)*U(IM2,3)+2.*U(I,3)*(U(IP2,3)-U(IM2,3)))
TERM1E=AI*(ABS(U(IP1,3)-MEAN(3))**2-1ABS(U(IM1,3)-MEAN(3))**2*22.*(U(I,3)-MEAN(3))*(U(IP1,3)-U(IM1,3)))
\[
\begin{align*}
\text{TERM2E} &= A2 \cdot (\text{ABS}(U(IP2,3) - \text{MEAN}(3))^2 - \\
& \quad 1 \cdot \text{ABS}(U(IM2,3) - \text{MEAN}(3))^2) \\
& \quad - 22 \cdot *(U(I,3) - \text{MEAN}(3)) \cdot (U(IP2,3) - U(IM2,3)) \\
\text{IF} \text{EXACT.EQ.1} \text{GO TO 240}
\end{align*}
\]

\[
\begin{align*}
\text{TERM3} &= A3 \cdot ((U(IP2,3) - U(I,3)) \cdot (U(IP2,3) - U(I,3)) - (U(I,3) - U(IM2,3)) \cdot (U(1,3) - U(IM2,3))) \\
\text{TERM4} &= A4 \cdot \text{ABS}(U(IM2,3) - U(IM2,2)) \cdot (U(IM1,3) - U(IM1,2)) \cdot (U(IP1,3) - U(IP1,2)) \cdot (U(IP2,3) - U(IP2,2)) \\
& \quad - 2 \cdot (U(IP1,3) - U(IP1,2)) \cdot (U(IP1,3) - U(IP1,2)) \\
\text{TERM4E} &= A4 \cdot \text{ABS}(U(IM2,3) - U(IM2,2) + \text{DIFM})^2 - \\
& \quad 2 \cdot \text{ABS}(U(IM1,3) - U(IM1,2) + \text{DIFM})^2 - \\
& \quad 3 \cdot \text{ABS}(U(IP1,3) - U(IP1,2) + \text{DIFM})^2
\end{align*}
\]

\[
\begin{align*}
240 & \text{CONTINUE} \\
\text{TERM5} &= A5 \cdot (U(IP1,3) - 2 \cdot U(I,3) + U(IM1,3)) \\
\text{IF} \text{EXACT.EQ.1} \text{GO TO 260}
\end{align*}
\]

\[
\begin{align*}
\text{SUM1} &= 0.0 \\
\text{SUM2} &= 0.0 \\
\text{DO} 250 \text{II=1,WP1} \\
\text{IIPL}=\text{II-1} \\
\text{IIPL}=\text{II} + 2 \\
\text{IIPL}=\text{II-2} \\
\text{IF} \text{IIPL.LT.1} \text{IIPL}=\text{IIPL+N-1} \\
\text{IF} \text{IIPL.LT.1} \text{IIPL}=\text{IIPL+N-1} \\
\text{IF} \text{IIPL.LT.1} \text{IIPL}=\text{IIPL+N-1} \\
\text{SUM1} &= \text{SUM1} + \text{ABS}(U(IP2,3) - U(I,3)) \\
\text{SUM2} &= \text{SUM2} + \text{ABS}(U(IM1,3) - U(IM2,3)) \\
250 & \text{CONTINUE} \\
\text{TERM61} &= \text{SUM1}/\text{WP1} \\
\text{TERM62} &= \text{SUM2}/\text{WP1} \\
\text{KK}(IP1,3) &= \text{TERM61} \cdot (C \cdot \text{DX}/2.) \\
\text{IF} \text{CLOSUR.EQ.0} \text{KK}(IP1,3) &= 0.0 \\
\text{IF} \text{CLOSUR.EQ.1} \text{KK}(IP1,3) &= \text{KCONST} \\
\text{KK}(IM1,3) &= \text{TERM62} \cdot (C \cdot \text{DX}/2.) \\
\text{IF} \text{CLOSUR.EQ.0} \text{KK}(IM1,3) &= 0.0 \\
\text{IF} \text{CLOSUR.EQ.1} \text{KK}(IM1,3) &= \text{KCONST} \\
\text{TERM6} &= A6 \cdot (U(IP2,3) - 2 \cdot U(I,3) + U(IM2,3)) \\
\text{IF} \text{EXACT.EQ.1} \text{GO TO 270}
\end{align*}
\]

\[
\begin{align*}
\text{TERM6} &= A6 \cdot (U(IP1,3) - U(IM1,3) - U(IM1,3) - U(IM2,3)) \\
260 & \text{CONTINUE} \\
\text{TERM7} &= AA \cdot (U(IP1,3) - U(IM1,3) - U(IM1,3) - U(IM2,3)) \\
\text{TERM8} &= AB \cdot (U(IP2,3) - U(IM2,3) - U(IM2,3) - U(IM2,3)) \\
\text{IF} \text{EXACT.EQ.1} \text{GO TO 270}
\end{align*}
\]

\[
\begin{align*}
\text{TERM8a} &= AC \cdot (U(IP2,3) - U(IM2,3) - U(IM2,3) - U(IM2,3)) \cdot (U(IP2,3) - U(IM2,3)) \\
\text{TERM8b} &= AD \cdot (U(IP2,3) - U(IM2,3) - U(IM2,3) - U(IM2,3)) \cdot (U(IP2,3) - U(IM2,3)) \\
\text{TERM8c} &= AE \cdot (U(IP1,3) - U(IM1,3) - U(IM1,3) - U(IM2,3)) \\
\text{IF} \text{EXACT.EQ.1} \text{GO TO 270}
\end{align*}
\]
SUM1=0.0
SUM2=0.0
DO 280 II=1,WP1
III=1-WL/2+II-1
IIIP2=III+2
IIIM2=III-2
IF(III.LT.1) III=III+N-1
IF(IIIP2.LT.1) IIIP2=IIIP2+N-1
IF(III.GT.N) III=III-N+1
IF(IIIP2.GT.N) IIIP2=IIIP2-N+1
SUM1=SUM1+ABS(U(IIIP2,2)-U(III,2))
SUM2=SUM2+ABS(U(III,2)-U(IIIM2,2))
280 CONTINUE
TERMF1=SUM1/WP1
TERMF2=SUM2/WP1
KK(IP1,2)=TERMF1*(C*DX/2.)
IF(CLOSURE.EQ.0) KK(IP1,2)=0.0
IF(CLOSURE.EQ.1) KK(IP1,2)=KCONST
KK(IM1,2)=TERMF2*(C*DX/2.)
IF(CLOSURE.EQ.0) KK(IM1,2)=0.0
IF(CLOSURE.EQ.1) KK(IM1,2)=KCONST
TERMF=AF*(KK(IP1,2)*(U(IP2,2)-U(I,2))-KK(IM1,2)*(U(IM2,2)-U(I,2)))
290 CONTINUE
IF(EXACT.EQ.1) GO TO 300
U(I,4)=U(I,3)+TERM1+TERM2+TERM3+TERM4+TERM5+TERM6+TERM7+TERM8+TERM9
300 U(I,4)=U(I,3)+TERM1+TERM2+TERM5+TERM6+TERM7+TERM8+TERM9
310 CONTINUE
IF(ENCAL.EQ.0) GO TO 330
SUME2=(U(I,3)-MEAN(3))*(TERM1E+TERM2E)+SUME2
IF(EXACT.EQ.1) GO TO 320
SUME3=(U(I,3)-MEAN(3))*(TERM3)+SUME3
SUME4=(U(I,3)-MEAN(3))*(TERM4E)+SUME4
320 CONTINUE
SUME5=(U(I,3)-MEAN(3))*(TERM5)+SUME5
IF(EXACT.EQ.1) GO TO 330
SUME6=(U(I,3)-MEAN(3))*(TERM6)+SUME6
330 CONTINUE
340 CONTINUE
C ******************************************************
C CALCULATE ENERGY EQUATION AT THE PREVIOUS TIME STEP
SUM=0.0
DO 350 I=1,N
SUM=SUM+ABS(U(I,3)-MEAN(3))**2
TOTEN(J-1)=0.5*SUM/FN
IF(ENCAL.EQ.0) GO TO 370
FACT=2./(3.*DT*FN)
EN2(J-1)=SUM2*FACT
IF(EXACT.EQ.1) GO TO 360
EN3(J-1)=SUM3*FACT
EN4(J-1)=SUM4*FACT
350 CONTINUE
360 CONTINUE 
EN5(J-1)=SUM*FACT 
IF(EXACT.EQ.1) GO TO 370 
EN6(J-1)=SUM*FACT 
370 CONTINUE 
C ******************************************************
C CALCULATE MAXIMUM EDDY VISCOSITY AT THIS TIME STEP 
IF(EXACT.EQ.1) GO TO 430 
DO 410 I=1,N 
SUM=0.0 
DO 400 II=1,WP1 
II1=1-WL/2+II-1 
IIIP1=II1+1 
IIIM1=II1-1 
IF(IIIP1.LT.1) IIIP1=IIIP1+N-1 
IF(IIIM1.LT.1) IIIM1=IIIM1+N-1 
IF(IIIP1.GT.N) IIIP1=IIIP1-N+1 
IF(IIIM1.GT.N) IIIM1=IIIM1-N+1 
400 SUM=SUM+ABS(U(IIIP1,4)-U(IIIM1,4)) 
KED(I)=SUM*C*D*X/(2.*WP1) 
IF(CLOSUR.EQ.0) KED(I)=0.0 
IF(CLOSUR.EQ.1) KED(I)=KCONST 
410 CONTINUE 
KMAX(J)=KED(I) 
DO 420 I=2,N 
420 IF(KMAX(J).LT.KED(I)) KMAX(J)=KED(I) 
430 CONTINUE 
C ******************************************************
C CALCULATE AND PLOT STATISTICS OF U(X,T) AT SOME CHOSEN TIME STEPS 
DO 440 I=1,N 
440 Y(I)=U(I,4) 
SUM=0.0 
DO 450 I=1,N 
450 SUM=SUM+Y(I) 
MEAN(4)=SUM/FN 
SUM1=0.0 
SUM2=0.0 
SUM3=0.0 
SUM4=0.0 
DO 460 I=1,N 
TERM=Y(I)-MEAN(4) 
SUM1=SUM1+TERM*TERM 
SUM2=SUM2+Y(I)*Y(I) 
SUM3=SUM3+TERM*TERM*TERM 
SUM4=SUM4+TERM*TERM*TERM*TERM 
460 CONTINUE 
STDV=SQRT(SUM1/N) 
VAR=STDV*STDV 
RMS=SQRT(SUM2/N) 
SKEW=SUM3/(N*STDV*VAR) 
AKURT=SUM4/(N*VAR*VAR) 
TIME=(J-1)*DT
WRITE (6,970) J, TIME, MEAN(4), STDV, VAR, RMS, SKEW, AKURT
WRITE (6,1080) (Y(I), I=1,101)
SUM1=0.0
SUM2=0.0
DUDX1=(U(2,4)-U(N-1,4))/(2.*DX)
DO 470 I=2,NM1
DUDX=(U(I+1,4)-U(I-1,4))/(2.*DX)
SUM1=SUM1+DUDX*DUDX*DUDX
470 SUM2=SUM2+DUDX*DUDX
SUM1=SUM1+2.*DUDX1*DUDX1*DUDX1
SUM2=SUM2+2.*DUDX1*DUDX1
SK=(SUM1/N)/((SUM2/N)**1.5)
WRITE (6,1200) SK
CALL PLOTS (0,0,0)
CALL AXIS (2.0,7.8,8HDISTANCE,-8,XLEN,0.,X(N+1),X(N+2))
CALL AXIS (2.0,7.8,8HVELOCITY,8,YLEN,90.,Y(N+1),Y(N+2))
CALL PLOT (2.0,7.8,-3)
CALL LINE (X,Y,N,1,0,0)
CALL HLINE (0.,XLEN,YLEN,LMASK1)
VCORD=(MEAN(4)-Y(N+1))/Y(N+2)
CALL HLINE (0.,XLEN,VCORD,LMASK1)
CALL VLINE (0.,YLEN,XLEN,LMASK1)
CALL PLOT (-2.,-7.8,-3)
DO 480 I=1,N
480 Y(I)=Y(I)-MEAN(4)
DO 500 IP=1,NSPEC
IQF=N-IP+1
SUM=0.0
DO 490 IQ=1,IQF
490 SUM=SUM+Y(IQ)*Y(IQ+IP-1)
500 R(IP)=SUM/(N-IP+1)
DO 520 IH=1,NSPEC
SUM=0.0
DO 510 IP=1,NSPEC
EPS=1.0
IF(IP.EQ.1.OR.IP.EQ.NSPEC) EPS=0.5
510 SUM=SUM+EPS*R(IP)*COS((IH-1)*(IP-1)*PI/(NSPEC-1))
520 E(IH)=2.*DX*SUM/PI
ES(I)=0.54*E(I)+0.46*E(2)
ES(NSPEC)=0.54*E(NSPEC)+0.46*E(NSPEC-1)
NNSPEC=NSPEC-1
DO 530 I=2,NNSPEC
530 ES(I)=0.23*ES(I-1)+0.54*E(I)+0.23*E(I+1)
SUM=0.5*ES(I)+ES(NSPEC)
DO 540 I=2,NNSPEC
540 SUM=SUM+ES(I)
AREA=(PI*SUM)/(NNSPEC*DX)
DO 550 I=1,NSPEC
550 W(I)=(I-1)/(2.*DX*NNSPEC)
W(I)=(W(I)+W(2))/2.
DO 560 I=1,NSPEC
W(I)=ALOG10(W(I))
IF(ES(I).LT.(10.0**(SLMIN))) ES(I)=10.0**(SLMIN)
560 ES(I)=ALOG10(ES(I))
W(NSPEC+1)=WLEFT
W(NSPEC+2)=(WRIGHT-W(NSPEC+1))/XLEN
ES(NSPEC+1)=SLMIN
ES(NSPEC+2)=(SLMAX-SLMIN)/YLEN
CALL AXIS (2.0,2.3,15LOG WAVE NUMBER,-15,XLEN,0.,W(NSPEC+1),W(NSPEC+2))
CALL AXIS (2.0,2.3,12LOG SPECTRUM,12,YLEN1,90.,ES(NSPEC+1),ES(NSPEC+2))
CALL PLOT (2.0,2.3,-3)
CALL LINE (W,ES,NSPEC,1,0,0)
CALL HLINE (0.,XLEN,YLEN1,LMASK1)
CALL VLINE (0.,YLEN1,XLEN,LMASK1)
CALL SYMBOL (0.2,4.73,0.07,4HTIME,0.,4)
CALL NUMBER (0.55,4.73,0.07,TIME,0.,+2)

YS2=YS1+SLOPE*(X-S2-XS1)*W(NSPEC+2)/ES(NSPEC+2)
CALL PLOT (XS2,YS2,+2)

XSYM=(XS2+XS1)/2.+0.1
YSYM=(YS1+YS2)/2.+0.1
CALL NUMBER (XSYM,SYM,0.14,SLOPE,0.,-1)
CALL PLOT (0.,0.,+999)
WRITE (6,1000)
WRITE (6,990) (ES(I),I=1,NSPEC)
WRITE (6,1010) AREA
CONTINUE

C*****************************************************************************
C STORE VELOCITY TRACES AT SOME CHOSEN NODES
DO 580 K=1,NMOD
KKK=NOD(K)
580 Y(K,J)=U(KKK,4)

C*****************************************************************************
C PREPARE FOR NEXT TIME STEP
IF (TAPE.EQ.1) WRITE (8) (U(I,4),I=1,N)
IF (TAPE.EQ.1.AND.CLOSUR.EQ.2.AND.EXACT.EQ.0) WRITE (8) (KED(I),I=11,N)
DO 590 I=1,N
U(I,1)=U(I,2)
U(I,2)=U(I,3)
U(I,3)=U(I,4)

590 CONTINUE
MEAN(2)=MEAN(3)
SUM3=0.0
DO 591 I=1,N
SUM3=SUM3+U(I,3)
MEAN(3)=SUM3/FN
MEANP(1)=MEAN(3)
DIFM=MEAN(2)-MEAN(3)

C*****************************************************************************
C*****************************************************************************
C END TIME LOOP
CONTINUE

C*****************************************************************************
C*****************************************************************************
C PLOT ENERGY EQUATION WITH TIME
TOTEN(M)=2.*TOTEN(M-1)-TOTEN(M-2)
DO 610 J=1,M

610 X(J)=(J-1)*DT
X(M+1)=0.0
X(M+2)=X(M)/XLEN
WRITE (6,1230)
WRITE (6,1030) (MEANP(J),J=1,M)
CALL PLOTS (0,0,0)
IF (EXACT.EQ.1) CALL SCALE (MEANP,YLEN1,M,+1)
CALL AXIS (1.5,3.5,4HTIME,-4,XLEN,0.,X(M+1),X(M+2))
CALL AXIS (1.5,3.5,4HMEAN,4,YLEN1,90.,MEANP(M+1),MEANP(M+2))
CALL PLOT (1.5,3.5,-3)
CALL LINE (X,MEANP,M,1,0,0)
CALL HLINE (0.,XLEN,YLEN1,LMASK1)
CALL VLINE (0.,YLEN1,XLEN,LMASK1)
CALL PLOT (0.,0.,+999)
MM1=M-1
DEDT(1)=(TOTEN(2)-TOTEN(1))/DT
DEDT(M)=(TOTEN(M)-TOTEN(M-1))/DT
DO 620 J=2,MM1

620 DEDT(J)=(TOTEN(J+1)-TOTEN(J-1))/(2.*DT)
WRITE (6,1020)
WRITE (6,1030) (TOTEN(J),J=1,M)
CALL PLOTS (0,0,0)
CALL AXIS (1.5,3.5,4HTIME,-4,XLEN,0.,X(M+1),X(M+2))
CALL AXIS (1.5,3.5,12HTOTAL ENERGY,12,YLEN1,90.,TOTEN(M+1),TOTEN(M+2))
CALL PLOT (1.5,3.5,-3)
CALL LINE (X,TOTEN,M,1,0,0)
CALL HLINE (0.,XLEN,YLEN1,LMASK1)
CALL VLINE (0.,YLEN1,XLEN,LMASK1)
CALL PLOT (0.,0.,+999)
WRITE (6,1040)
WRITE (6,1030) (DEDT(J),J=1,M)
SUM=0.000000
DO 630 J=1,M

630 SUM=SUM+DEDT(J)
DEDTM=SUM/FLOAT(M)
ZERO=(-DEDT(M+1))/(DEDT(M+2))
IF (NSMTH.EQ.0) GO TO 634
DO 632 J=1,M
JS1=J-NSMTH/2
JS2=J+NSMTH/2
IF (J.LE.(NSMTH/2)) JS1=1
IF (J.GE.(M-NSMTH/2)) JS2=M
SUM=0.0
DO 631 JS=JS1,JS2

631 SUM=SUM+DEDT(JS)
SDEDT(J)=SUM/(JS2-JS1+1)
CONTINUE
WRITE (6,1220)
WRITE (6,1030) (SDEDT(J),J=1,M)
SDEDT(M+1) = DEDT(M+1)
SDEDT(M+2) = DEDT(M+2)
CALL PLOTS(0.0,0.0)
CALL AXIS(1.5,3.5,4HTIME,-4,XLEN,0.,X(M+1),X(M+2))
CALL AXIS(1.5,3.5,25HTIME RATE OF TOTAL ENERGY,25,YLEN1,9)
CALL PLOT(1.5,3.5,-3)
CALL LINE(X,SDEDT,M,1.0,0.0)
CALL LINE(0.,XLEN,YLEN1,LMASK1)
CALL LINE(0.,XLEN,ZERO,LMASK2)
CALL LINE(0.,YLEN1,XLEN,LMASK1)
SUM = 0.0
DO 633 J = 1,M
633 SUM = SUM + SDEDT(J)
SDEDTM = SUM/FLOAT(M)
CALL SYMBOL(0.2,4.73,0.07,4HMEAN,0.,4)
CALL NUMBER(0.55,4.73,0.07,SDEDTM,0.,+8)
CALL PLOT(0.,0.,+999)
634 CONTINUE
IF (ENCAL.EQ.0) GO TO 780
EN2(M) = 2.*EN2(M-1) - EN2(M-2)
IF (EXACT.EQ.1) GO TO 640
EN3(M) = 2.*EN3(M-1) - EN3(M-2)
EN4(M) = 2.*EN4(M-1) - EN4(M-2)
640 CONTINUE
EN5(M) = 2.*EN5(M-1) - EN5(M-2)
IF (EXACT.EQ.1) GO TO 650
EN6(M) = 2.*EN6(M-1) - EN6(M-2)
650 CONTINUE
DO 670 J = 1,M
660 CONTINUE
IF (EXACT.EQ.1) RHS(J) = EN2(J) + EN5(J)
IF (EXACT.NE.1) RHS(J) = EN2(J) + EN3(J) + EN4(J)
670 CONTINUE
EN2(M+1) = DEDT(M+1)
EN3(M+1) = DEDT(M+1)
EN4(M+1) = DEDT(M+1)
EN5(M+1) = DEDT(M+1)
EN6(M+1) = DEDT(M+1)
EN34(M+1) = DEDT(M+1)
EN234(M+1) = DEDT(M+1)
RHS(M+1) = DEDT(M+1)
RHS(M+2) = DEDT(M+2)
RHS(M+3) = DEDT(M+3)
RHS(M+4) = DEDT(M+4)
RHS(M+5) = DEDT(M+5)
RHS(M+6) = DEDT(M+6)
WRITE (6,1120)
238

WRITE (6,990) (EN2(J),J=1,M)
SUM=0.000000
DO 680 J=1,M

680 SUM=SUM+EN2(J)
EN2M=SUM/FLOAT(M)
CALL PLOTS (0,0,0)
CALL AXIS (1.5,3.5,4HTIME,-4,XLEN,0.,X(M+1),X(M+2))
CALL AXIS (1.5,3.5,13HINERTIAL TERM,13,YLEN1,90.,EN2(M+1),EN2(M+2))
CALL PLOT (1.5,3.5,-3)
CALL LINE (X,EN2,M,1,0,0)
CALL HLINE (0.,XLEN,YLEN1,MASK1)
CALL VLINE (0.,YLEN1,XLEN,MASK1)
CALL SYMBOL (0.2,4.73,0.07,4HMEAN,0.,4)
CALL NUMBER (0.55,4.73,0.07,EN2M,0.,+8)
CALL PLOT (0.,0.,999)
IF(EXACT.EQ.1) GO TO 710
WRITE (6,1130)
WRITE (6,990) (EN3(J),J=1,M)
SUM=0.000000
DO 690 J=1,M

690 SUM=SUM+EN3(J)
EN3M=SUM/FLOAT(M)
CALL PLOTS (0,0,0)
CALL AXIS (1.5,3.5,4HTIME,-4,XLEN,0.,X(M+1),X(M+2))
CALL AXIS (1.5,3.5,17HSPACE FILTER TERM,17,YLEN1,90.,EN3(M+1),EN3(M+2))
CALL PLOT (1.5,3.5,-3)
CALL LINE (X,EN3,M,1,0,0)
CALL HLINE (0.,XLEN,YLEN1,MASK1)
CALL VLINE (0.,YLEN1,XLEN,MASK1)
CALL SYMBOL (0.2,4.73,0.07,4HMEAN,0.,4)
CALL NUMBER (0.55,4.73,0.07,EN3M,0.,+8)
CALL PLOT (0.,0.,999)
WRITE (6,1140)
WRITE (6,990) (EN4(J),J=1,M)
SUM=0.000000
DO 700 J=1,M

700 SUM=SUM+EN4(J)
EN4M=SUM/FLOAT(M)
CALL PLOTS (0,0,0)
CALL AXIS (1.5,3.5,4HTIME,-4,XLEN,0.,X(M+1),X(M+2))
CALL AXIS (1.5,3.5,16HTIME FILTER TERM,16,YLEN1,90.,EN4(M+1),EN4(M+2))
CALL PLOT (1.5,3.5,-3)
CALL LINE (X,EN4,M,1,0,0)
CALL HLINE (0.,XLEN,YLEN1,MASK1)
CALL VLINE (0.,YLEN1,XLEN,MASK1)
CALL SYMBOL (0.2,4.73,0.07,4HMEAN,0.,4)
CALL NUMBER (0.55,4.73,0.07,EN4M,0.,+8)
CALL PLOT (0.,0.,999)
CONTINUE
WRITE (6,1150)
WRITE (6,990) (EN5(J),J=1,M)
SUM=0.00000
DO 720 J=1,M
SUM=SUM+EN5(J)
EN5M=SUM/FLOAT(M)
.calls plots (0,0,0)
call axis (1.5,3.5,4HTIME,-4,XLEN,0..X(M+1),X(M+2))
call axis (1.5,3.5,24HMOLECULAR VISCOSITY TERM,24,YLEN1,90..EN5(M 11),EN5(M+2))
call plot (1.5,3.5,-3)
call line (X,EN5,M,1,0,0)
call hline (0.,XLEN,YLEN1,LMASK1)
call hline (0.,XLEN,ZERO,LMASK2)
call vline (0.,YLEN1,XLEN,LMASK1)
call symbol (0.2,4.73,0.07,4HMEAN,0.,4)
call number (0.55,4.73,0.07,EN5M,0.,+8)
call plot (0.,0.,+999)
IF(EXACT.EQ.1) GO TO 760
WRITE (6,1160)
WRITE (6,990) (EN6(J),J=1,M)
SUM=0.00000
DO 730 J=1,M
SUM=SUM+EN6(J)
EN6M=SUM/FLOAT(M)
.calls plots (0,0,0)
call axis (1.5,3.5,4HTIME,-4,XLEN,0..X(M+1),X(M+2))
call axis (1.5,3.5,24HTURBULENT VISCOSITY TERM,24,YLEN1,90..EN6(M 11),EN6(M+2))
call plot (1.5,3.5,-3)
call line (X,EN6,M,1,0,0)
call hline (0.,XLEN,YLEN1,LMASK1)
call hline (0.,XLEN,ZERO,LMASK2)
call vline (0.,YLEN1,XLEN,LMASK1)
call symbol (0.2,4.73,0.07,4HMEAN,0.,4)
call number (0.55,4.73,0.07,EN6M,0.,+8)
call plot (0.,0.,+999)
WRITE (6,1170)
WRITE (6,990) (EN34(J),J=1,M)
SUM=0.00000
DO 740 J=1,M
SUM=SUM+EN34(J)
EN34M=SUM/FLOAT(M)
.calls plots (0,0,0)
call axis (1.5,3.5,4HTIME,-4,XLEN,0..X(M+1),X(M+2))
call axis (1.5,3.5,19HSUM OF FILTER TERMS,19,YLEN1,90..EN34(M+1),E 1N34(M+2))
call plot (1.5,3.5,-3)
call line (X,EN34,M,1,0,0)
call hline (0.,XLEN,YLEN1,LMASK1)
call hline (0.,XLEN,ZERO,LMASK2)
call vline (0.,YLEN1,XLEN,LMASK1)
call symbol (0.2,4.73,0.07,4HMEAN,0.,4)
CALL NUMBER (0.55, 4.73, 0.07, EN34M, 0., +8)
CALL PLOT (0., 0., +999)
WRITE (6, 1180)
WRITE (6, 990) (EN234(J), J = 1, M)
SUM = 0.000000
DO 750 J = 1, M
    SUM = SUM + EN234(J)
    EN234M = SUM / FLOAT(M)
    CALL PLOTS (0, 0, 0)
    CALL AXIS (1.5, 3.5, 4HTIME, -4, XLEN, 0., X(M+1), X(M+2))
    CALL AXIS (1.5, 3.5, 32HSUM OF INERTIAL AND FILTER TERMS, 32, YLEN1, 90)
    CALL PLOT (1.5, 3.5, -3)
    CALL LINE (X, EN234M, 1, 0, 0)
    CALL HLINE (0., XLEN, YLEN1, LMASK1)
    CALL HLINE (0., XLEN, ZERO, LMASK2)
    CALL VLINE (0., YLEN1, XLEN, LMASK1)
    CALL SYMBOL (0.2, 4.73, 0.07, 4HMEAN, 0., 4)
    CALL NUMBER (0.55, 4.73, 0.07, EN234M, 0., +8)
    CALL PLOT (0., 0., +999)
    750 CONTINUE
WRITE (6, 1190)
WRITE (6, 990) (RHS(J), J = 1, M)
SUM = 0.000000
DO 770 J = 1, M
    SUM = SUM + RHS(J)
    RHSM = SUM / FLOAT(M)
    CALL PLOTS (0, 0, 0)
    CALL AXIS (1.5, 3.5, 4HTIME, -4, XLEN, 0., X(M+1), X(M+2))
    CALL AXIS (1.5, 3.5, 6HR.H.S., 6, YLEN1, 90., RHS(M+1), RHS(M+2))
    CALL PLOT (1.5, 3.5, -3)
    CALL LINE (X, RHSM, 1, 0, 0)
    CALL HLINE (0., XLEN, YLEN1, LMASK1)
    CALL HLINE (0., XLEN, ZERO, LMASK2)
    CALL VLINE (0., YLEN1, XLEN, LMASK1)
    CALL SYMBOL (0.2, 4.73, 0.07, 4HMEAN, 0., 4)
    CALL NUMBER (0.55, 4.73, 0.07, RHSM, 0., +8)
    CALL PLOT (0., 0., +999)
    770 CONTINUE
C ******************************************************************************
C PLOT MAXIMUM EDDY VISCOSITY WITH TIME
IF (EXACT.EQ.1) GO TO 790
WRITE (6, 1050)
WRITE (6, 990) (KMAX(J), J = 1, M)
CALL PLOTS (0, 0, 0)
CALL AXIS (1.5, 3.5, 4HTIME, -4, XLEN, 0., X(M+1), X(M+2))
CALL AXIS (1.5, 3.5, 18MAX EDDY VISCOSITY, 18, YLEN1, 90., KMAX(M+1), KM1AX(M+2))
    CALL PLOT (1.5, 3.5, -3)
    CALL LINE (X, KMAXM, 1, 0, 0)
    CALL HLINE (0., XLEN, YLEN1, LMASK1)
    CALL VLINE (0., YLEN1, XLEN, LMASK1)
    CALL PLOT (0., 0., +999)
    790 CONTINUE
C PLOT VELOCITY TRACES AND FREQUENCY SPECTRA AT SOME CHosen NODES
Y(M+1)=MEAN1-1.5*COF
Y(M+2)=(3.0*COF)/YLEN
IF(NNOD.EQ.0) GO TO 950
DO 940 K=1,NNOD
DO 800 J=1,M
800 Y(J)=YT(K,J)
   CALL PLOTS (0,0,0)
   CALL AXIS (2.0,7.8,4,TIME,-4,XLEN,0.,X(M+1),X(M+2))
   CALL AXIS (2.0,7.8,8,VELOCITY,8,YLEN,90.,Y(M+1),Y(M+2))
   CALL PLOT (2.0,7.8,-3)
   CALL LINE (X,Y,M,1,0,0)
   CALL HLINE (0.,XLEN,YLEN,LMASK1)
   CALL VLINE (0.,YLEN,XLEN,LMASK1)
   CALL PLOT (-2.,-7.8,-3)
N=M-M1+1
NSPEC=NSPECT
DO 810 I=1,N
810 Y(I)=Y(M1+I-1)
   SUM=0.0
   DO 820 I=1,N
820 SUM=SUM+Y(I)
   AVER=SUM/N
   DO 830 I=1,N
830 TERM=Y(I)-AVER
   SUM1=SUM1+TERM*TERM
   SUM2=SUM2+Y(I)*Y(I)
   SUM3=SUM3+TERM*TERM*TERM
   SUM4=SUM4+TERM*TERM*TERM*TERM
   CONTINUE
STDV=SQR(SUM1/N)
VAR=STDV*STDV
RMS=SQR(SUM2/N)
SKEW=SUM3/(N*STDV*VAR)
AKURT=SUM4/(N*VAR*VAR)
DO 840 I=1,N
840 Y(I)=Y(I)-AVER
   DO 860 IP=1,NSPEC
   IQF=N-IP+1
   SUM=0.0
   DO 850 IQ=1,IQF
850 SUM=SUM+Y(IQ)*Y(IQ+IP-1)
860 R(IP)=SUM/(N-IP+1)
   DO 880 IH=1,NSPEC
   SUM=0.0
   DO 870 IP=1,NSPEC
   EPS=1.0
   IF(IP.EQ.1.OR.IP.EQ.NSPEC) EPS=0.5
870 SUM=SUM+EPS*R(IP)*COS((1H-1)*(IP-1)*PI/(NSPEC-1))
242

880 E(IH) = 2.*DT*SUM/PI
     ES(1) = 0.54*E(1) + 0.46*E(2)
     ES(NSPEC) = 0.54*E(NSPEC) + 0.46*E(NSPEC-1)
     NNSPEC = NSPEC - 1
     DO 890 I = 2, NNSPEC
890 ES(I) = 0.23*E(I-1) + 0.54*E(I) + 0.23*E(I+1)
     SUM = 0.5*(ES(1) + ES(NSPEC))
     DO 900 I = 2, NNSPEC
900 SUM = SUM + ES(I)
     AREA = (PI*SUM)/(NNSPEC*DT)
     DO 910 I = 1, NSPEC
910 W(I) = (I-1)/(2.*DT*NNSPEC)
     W(I) = (W(I) + W(2))/2.
     DO 920 I = 1, NSPEC
     W(I) = ALOG10(W(I))
920 IF (ES(I) .LT. (10.0**(SLMINT))) ES(I) = 10.0**(SLMINT)
     ES(I) = ALOG10(ES(I))
     W(NSPEC+1) = WTL
     W(NSPEC+2) = (WTR-WTL)/XLEN
     ES(NSPEC+1) = SLMINT
     ES(NSPEC+2) = (SLMAXT-SLMINT)/YLEN1
     CALL AXIS (2.0, 2.3, 13HLOG FREQUENCY, -13, XLEN, 0, W(NSPEC+1), W(NSPEC+2))
     CALL AXIS (2.0, 2.3, 12HLOG SPECTRUM, 12, YLEN1, 90, ES(NSPEC+1), ES(NSPEC+2))
     CALL PLOT (2.0, 2.3, 3)
     CALL LINE (W, ES, NSPEC, 1, 0, 0)
     CALL VLINE (0, XLEN, YLEN1, LMASK1)
     CALL HLINE (0, XLEN, YLEN1, LMASK1)
     DIST = (MOD(K)-1)*DX
     CALL SYMBOL (0.2, 4.73, 0.07, BDISTANCE, 0, 8)
     CALL NUMBER (0.9, 4.73, 0.07, DIST, 0, 2)
     YS2 = YS1 + SLOPE*(XS2-XS1)*W(NSPEC+2)/ES(NSPEC+2)
     CALL PLOT (XS1, YS1, 3)
     CALL PLOT (XS2, YS2, 2)
     XSYM = (XS2 + XS1)/2 + 0.1
     YSYM = (YS1 + YS2)/2 + 0.1
     CALL NUMBER (XSYM, YSYM, 0.14, SLOPE, 0, -1)
     CALL PLOT (0, 0, +999)
     WRITE (6, 1060) NOD(K)
     DIST = (MOD(K)-1)*DX
     WRITE (6, 1210) DIST
     WRITE (6, 1100) M1, M
     WRITE (6, 1110) AVER, STDV, VAR, RMS, SKEW, AKURT
     IF (K.NE.1) GO TO 930
     WRITE (6, 1070)
     WRITE (6, 990) (W(I), I = 1, NSPEC)
930 CONTINUE
     WRITE (6, 1000)
     WRITE (6, 990) (ES(I), I = 1, NSPEC)
     WRITE (6, 1010) AREA
     WRITE (6, 1090)
     WRITE (6, 990) (YT(K, J), J = 1, M)
940 CONTINUE
243

CONTINUE

STOP

C

C

960 FORMAT (F16.8)

970 FORMAT ('1',5X,'TIME STEP NUMBER',I5,/,5X,'TIME=',F8.5,/,5X,'MEAN=',

F6.4,/,5X,'STANDARD DEVIATION=',F6.4,/,5X,'VARIANCE=',F8.6,/,5X,

2'RMS=',F6.4,/,5X,'SKEWNESS=',F9.5,/,5X,'KURTOSIS=',F9.5,///,5X,'V

3ELocity DISTRIBUTATION AT THE FIRST 101 NODES',///)

980 FORMAT (///,5X,'LOG WAVE NUMBERS',///)

990 FORMAT (10F10.5)

1000 FORMAT (///,5X,'LOG SPECTRUM',///)

1010 FORMAT (///,5X,'AREA UNDER SPECTRUM=',F8.6,///)

1020 FORMAT (10F12.6)

1030 FORMAT (///,5X,'TIME HISTORY OF VELOCITY',///)

1040 FORMAT ('1',5X,'RATE OF TOTAL ENERGY',///)

1050 FORMAT ('1',5X,'MAXIMUM EDDY VISCOSITY',///)

1060 FORMAT ('1',5X,'NODE NUMBER',I5,///)

1070 FORMAT (5X,'LOG FREQUENCIES',///)

1080 FORMAT (5F20.10)

1090 FORMAT (///,5X,'TIME HISTORY OF VELOCITY',///)

1100 FORMAT (5X,'THE POINTS FROM TIME STEP NUMBER',I5,5X,'TO TIME STEP

1NUMBER',I5,5X,'ARE INVOLVED IN CALCULATING THE FOLLOWING STATI

2ICS',///)

1110 FORMAT (5X,'MEAN=',F6.4,/,5X,'STANDARD DEVIATION=',F6.4,/,5X,'VARI

1ANCE=',F8.6,/,5X,'RMS=',F6.4,/,5X,'SKEWNESS=',F9.5,/,5X,'KURTOSIS=

2',F9.5,///)

1120 FORMAT ('1',5X,'INERTIAL TERM',///)

1130 FORMAT ('1',5X,'SPACE FILTER TERM',///)

1140 FORMAT ('1',5X,'TIME FILTER TERM',///)

1150 FORMAT ('1',5X,'MOLECULAR VISCOSITY TERM',///)

1160 FORMAT ('1',5X,'EDDY VISCOSITY TERM',///)

1170 FORMAT ('1',5X,'SUM OF FILTER TERMS',///)

1180 FORMAT ('1',5X,'SUM OF INERTIAL AND FILTER TERMS',///)

1190 FORMAT ('1',5X,'R.H.S.',///)

1200 FORMAT (///,5X,'SKEWNESS AS DEFINED IN CLARK ET AL. 1977=',F9.5,///)

1210 FORMAT (5X,'DISTANCE=',F5.2,///)

1220 FORMAT ('1',5X,'SMOOTHED RATE OF TOTAL ENERGY',///)

1230 FORMAT ('1',5X,'TIME HISTORY OF MEAN',///)

END

/*

GO.FTO3FO01 DD DSN=TS0413.INVEL3,DISP=(OLD,CATLG),

UNIT=USERDA,

DCB=(LRECL=16,BKSIZE=3120,RECFM=FBS),SPACE=(TRK,(200,100),RLSE)

GO.FTO8FO01 DD UNIT=TAPE9,DISP=(NEW,KEEP),DSN=FT700,

LABEL=(3,SL),VOL=(,RETAIN,SER=ABCD),DCB=(BLKSIZE=5000)

GO.DATA DD *

*/

/*
Appendix B

TRANSPORT CALCULATION PROGRAM
// TIME=(15,20), REGION=700K
/*SETUP UNIT=TAPE9, ID=(ABCD, J274, READ)
/*SETUP UNIT=TAPE9, ID=(EHG, H143, WRITE)
/*JOBPARM LINES=20000, TAPEIO=20000
/*JOBPARM V=D
// EXEC PLOTV, TIME.GO=15
// GO.SOURCE DD 

REAL NEW, KK, KCONST, MEAN

INTEGER CLOSUR, EXACT, TAPE

DIMENSION U(4040,3), KK(1500,3), C(4040,4), DD(1500,3)
DIMENSION X(4040), Y(4040)
DIMENSION NOD(5), YT(5,2500)
DIMENSION R(610), E(610), ES(612), W(612)
DIMENSION T0TCN(2510)

READ DATA

RE=REYNOLDS NUMBER
GAMA=FILTER CONSTANT
M=NUMBER OF NODAL POINTS
M=NUMBER OF TIME STEPS
DX=SPATIAL GRID SPACING
DT=TEMPORAL GRID SPACING
LFX=RATIO OF SPATIAL FILTER WIDTH TO GRID SPACING
LFT=RATIO OF TEMPORAL FILTER WIDTH TO TIME STEP SIZE
TOTL=TOTAL LENGTH OF FLOW DOMAIN

IF CLOSUR=0, THE EDDY VISCOSITY = 0 AND EDDY DIFFUSIVITY = 0.
IF CLOSUR=1, THE EDDY VISCOSITY IS CONSTANT AND EQUALS TO KCONST
ALSO THE EDDY DIFFUSIVITY IS CONSTANT AND EQUAL TO DCONST
IF CLOSUR=2, THE SMAGORINSKY MODEL IS USED. THE EDDY VISCOSITY IS
TAKEN FROM THE SOLUTION OF THE MOMENTUM EQUATION AND DEVIDED
BY ST TO OBTAIN THE EDDY DIFFUSIVITY.
NEW = MOLECULAR VISCOSITY
CINIT = INITIAL UNIFORM CONCENTRATION.
SM = MOLECULAR SCHMIDT NUMBER. THE MOLECULAR DIFFUSIVITY (ALPHA)
IS OBTAINED BY DIVIDING NEW BY SM.
ST = TURBULENT SCHMIDT NUMBER.
DDELX=SPATIAL FILTER WIDTH
DDELX=TEMPORAL FILTER WIDTH

DATA RE,GAMA/700.0,6.0/
DATA N,M,DX,DT/4027,2014,0.00298063,0.00049677/
DATA LFX,LFT/2.10/
DATA TOTL/12.0/
DATA CLOSUR,KCONST/2.0,0.001/
DATA NEW,CINIT,SM,ST/0.00128379,1.0,1.0,1.0/
DDELX=LFX+DX
DDELX=DT
NMI=N-1
FN=FLOAT(N)
DCONST=KCONST/ST

CONTROL VARIABLES
NSPEC=NUMBER OF POINTS IN WAVE NUMBER SPECTRUM
SLMAX=MAXIMUM VALUE IN LOG WAVE NUMBER SPECTRAL PLOTS
SLMIN=MINIMUM VALUE IN LOG WAVE NUMER SPECTRAL PLOTS
C WLEFT=STARTING VALUE ON THE WAVE NUMBER AXIS IN SPECTRAL PLOTS
C WRIGHT=ENDING VALUE ON THE WAVE NUMBER AXIS IN SPECTRAL PLOTS
C J1,J2,.....,J10=TIME STEPS NUMBERS AT WHICH WAVE NUMBER SPECTRA
C ARE CALCULATED, ALSO STATISTICS ARE CALCULATED
C XLEN,YLEN,YLEN1=LENGTHS OF AXES IN INCHES
C SLOPE=SLOPE OF INCLINED LINE IN SPECTRAL PLOTS
C XS1,YS1,XS2=TO PLACE THE INCLINED LINE
C TOTCN(M+1)=STARTING VALUE IN TOTAL MASS PLOT
C TOTCN(M+2)=INTERVAL VALUE PER INCH IN TOTAL MASS PLOT
C MNOD=NUMBER OF NODES AT WHICH VELOCITY TRACES ARE STORED
C MOD=ARRAY CONTAINING THE NODE NUMBERS AT WHICH TIME TRACES ARE
C STORED AND ANALYZED, SPECTRA AND STATISTICS ARE CALCULATED
C M1-TIME TRACES STORED AT DIFFERENT NODES START FROM TIME STEP
C NUMBER M1 AND CONTINUE TO THE LAST TIME STEP
C NSPECT=NUMBER OF POINTS IN FREQUENCY SPECTRUM
C SLMINT=MINIMUM VALUE ON VERTICAL AXIS OF FREQUENCY SPECTRA PLOTS
C SLMAXT=MAXIMUM VALUE ON VERTICAL AXIS OF FREQUENCY SPECTRA PLOTS
C WTL=STARTING VALUE ON THE FREQUENCY AXIS IN SPECTRAL PLOTS
C WTR=ENDING VALUE ON THE FREQUENCY AXIS IN SPECTRAL PLOTS
C DCDT(M+1)=STARTING VALUE IN TIME RATE OF TOTAL MASS PLOT
C DCDT(M+2)=INTERVAL VALUE PER INCH IN TIME RATE OF TOTAL MASS PLOT
C IF EXACT=1 THE ORIGINAL (NON-FILTERED EQUATION) IS SOLVED
C IF EXACT=0 THE FILTERED OR ModeLED EQUATION IS SOLVED
C IF TAPE=1 THE CONCENTRATION FIELD IS STORED ON TAPE
C IF TAPE=0 THE CONCENTRATION FIELD IS NOT STORED
C IF INITST=1 THE STATISTICS OF C(X,0) ARE CALCULATED
C IF INITST=0 THE STATISTICS OF C(X,0) ARE NOT CALCULATED
C CMINT,CMAX ARE VERTICAL AXIS LIMITS IN CONCENTRATION PLOTS.
DATA P1,NSPECT,SLMAX,SLMIN/3.14159,604,0.0,-4.5/
DATA WLEFT/-0.86/
DATA WRIGHT/2.22/
DATA J1,J2,J3,J4,J5,J6,J7,J8,J9,J10/102,202,303,404,504,605,806,10
DATA 08,1511,2014/
DATA LMASK1,LMASK2,XLEN,YLEN,YLEN1/ZFFF,Z00FF,5.0,2.0,5.0/
DATA SLOPE,XS1,YS1,XS2/-2.0,3.0,4.8,4.5/
DATA TOTCN(M+1)=0.50
DATA TOTCN(M+2)=0.2000
DATA NMOD,MOD/5.1,672,1812,3356,4027/
DATA M1,NSPECT,SLMIN,SLMAX/1,403,-4.6,-1.1/
DATA WTL,WTR/0.10,3.0/
DATA EXACT,TAPE,INITST/1,1,1/
DATA CMINT,CMAX/0.0,7.0/
C******************************************************************************
C SET INITIAL CONDITIONS
C READ (3) (U(I,3),I=1,N)
C IF(CLOSUR.EQ.2.AND.EXACT.EQ.0) READ (3) (KK(I,3),I=1,N)
C DO 10 I=1,N
C U(I,2)=U(I,3)
C U(I,1)=U(I,3)
C C(I,3)=CINIT
C C(I,2)=C(I,3)
C C(I,1)=C(I,3)
C IF (EXACT.EQ.1) GO TO 10
C DD(I,3)=KK(I,3)/ST
247

DD(I,2)=DD(I,3)
10 CONTINUE
   IF(TAPE.EQ.1) WRITE (8) (C(I,3),I=1,N)
C ******************************************************************
C CALCULATE AND PLOT STATISTICS OF C(X,0)
   DO 20 I=1,N
   X(I)=(I-1)*DX
   X(N+1)=0.0
   X(N+2)=X(N)/XLEN
   Y(N+1)=CMIN
   Y(N+2)=(CMAX-CMIN)/YLEN
   IF(INITST.EQ.0) GO TO 140
   J=1
   DO 30 I=1,N
   30 Y(I)=C(I,3)
   SUM1=0.0
   SUM2=0.0
   SUM3=0.0
   SUM4=0.0
   DO 40 I=1,N
       TERM=Y(I)-CINIT
       SUM1=SUM1+TERM*TERM
       SUM2=SUM2+Y(I)*Y(I)
       SUM3=SUM3+TERM*TERM*TERM
       SUM4=SUM4+TERM*TERM*TERM*TERM
   40 CONTINUE
   STDV=SQR(SUM1/N)
   VAR=STDV*STDV
   RMS=SQR(SUM2/N)
   SKEW=SUM3/((N*STDV*VAR)
   AKURT=SUM4/(N*VAR*VAR)
   TIME=(J-1)*DT
   WRITE (6,600) J,TIME,CINIT,STDV,VAR,RMS,SKEW,AKURT
   WRITE (6,700) (Y(I),1=1,101)
   CALL PLOTS (0,0,0)
   CALL AXIS (2.0,7.8,8HDISTANCE,-8,XLEN,0.,X(N+1),X(N+2))
   CALL AXIS (2.0,7.8,13HCONCENTRATION,13,YLEN,90.,Y(N+1),Y(N+2))
   CALL PLOT (2.0,7.8,-3)
   CALL LINE (X,Y,N,0,0)
   CALL HLINE (0.,XLEN,YLEN,LMASK1)
   CALL VLINE (0.,YLEN,XLEN,LMASK1)
   CALL PLOT (-2.,-7.8,-3)
   DO 50 I=1,N
   50 Y(I)=Y(I)-CINIT
   DO 70 IP=1,NSPEC
   IQF=N-IP+1
   SUM=0.0
   DO 60 IQ=1,IQF
       SUM=SUM+Y(IQ)*Y(IQ+IP-1)
   60 R(IP)=SUM/(N-IQF)
   DO 90 IH=1,NSPEC
   SUM=0.0
   DO 80 IP=1,NSPEC
   EPS=1.0
IF(IP.EQ.1.OR.IP.EQ.NSPEC) EPS=0.5
80 SUM=SUM+EPS*R(IP)*COS((IH-1)*(IP-1)*PI/(NSPEC-1))
90 E(IH)=2.*DX/SUM/PI
   ES(I)=0.54*E(I)+0.46*E(I+1)
   ES(NSPEC)=0.54*E(NSPEC)+0.46*E(NSPEC-1)
   NNSPEC=NSPEC-1
DO 100 I=2,NNSPEC
100 ES(I)=0.23*E(I-1)+0.54*E(I)+0.23*E(I+1)
   SUM=0.5*(ES(I)+ES(NSPEC))
DO 110 I=2,NSPEC
110 SUM=SUM+ES(I)
   AREA=(PI*SUM)/(NSPEC*DX)
   SUM=0.5*(ES(1)+ES(NSPEC))
DO 120 I=1,NSPEC
120 W(I)=(I-1)/(2.*DX*NNSPEC)
   W(I)=(W(I)+W(2))/2.
   W(I)=ALOG10(W(I))
IF(ES(I).LT.(10.0**(SLMIN))) ES(I)=10.0**(SLMIN)
   ES(I)=ALOG10(ES(I))
   W(NSPEC+1)=WLEFT
   W(NSPEC+2)=(WRIGHT-W(NSPEC+1))/XLEN
   ES(NSPEC+1)=SLMIN
   ES(NSPEC+2)=(SLMAX-SLMIN)/YLEN1
   CALL AXIS (2.0,2.3,15LOG WAVE NUMBER,-15,XLEN,0.,W(NSPEC+1),W(NSPEC+2))
   CALL AXIS (2.0,2.3,12LOG SPECTRUM,12,YLEN1,90.,ES(NSPEC+1),ES(NSPEC+2))
   CALL PLOT (2.0,2.3,-3)
   CALL LINE (W,ES,NSPEC,1,0,0)
   CALL HLINE (0.,XLEN,YLEN1,LXLEN)
   CALL VLINE (0.,YLEN1,XLEN,LXLEN)
   CALL SYMBOL (0.2,4.7,0.07,4HTIME,0.,4)
   CALL NUMBER (0.55,4.73,0.07,TIME,0.,2)
   YS2=YS1+SLOPE*(XS2-XS1)*W(NSPEC+2)/ES(NSPEC+2)
   CALL PLOT (XS1,YS1,+3)
   CALL PLOT (XS2,YS2,+2)
   XSYM=(XS2+XS1)/2.+0.1
   YSYM=(YS1+YS2)/2.+0.1
   CALL NUMBER (XSYM,YSYM,0.14,SLOPE,0.,-1)
   CALL PLOT (0.,0.,+999)
   WRITE (6,610)
   WRITE (6,620) (W(I),I=1,NSPEC)
   WRITE (6,630)
   WRITE (6,640) ARE
   140 CONTINUE

C ******************************************************
C STORE CONCENTRATION TRACES AT SOME CHOSEN NODES
D0 150 K=1,NNOD
   KKK=NODE(K)
   YT(K,1)=C(KKK,3)
C ******************************************************
C CALCULATE MOLECULAR DIFFUSIVITY
   ALPHA=NEW/SM
CALCULATE COEFFICIENTS

\[ A_1 = \frac{-D_T}{2 \times D_X} \]
\[ A_2 = \frac{D_T}{16 \times D_X} \]
\[ A_3 = \frac{-3 \times D_ELX \times D_ELX \times D_T}{32 \times GAMA \times D_X \times D_X \times D_X} \]
\[ A_4 = \frac{-D_ELT \times D_ELT}{16 \times GAMA \times D_X \times D_T} \]
\[ A_5 = \frac{3 \times D_T \times ALPHA}{2 \times D_X \times D_X} \]
\[ A_6 = \frac{3 \times D_T}{8 \times D_X \times D_X} \]

AA = \frac{-A_1}{3}

AB = \frac{-A_2}{3}

AC = \frac{-A_3}{3}

AD = \frac{-A_4}{3}

AE = \frac{-A_5}{3}

AF = \frac{-A_6}{3}

START TIME LOOP

DO 410 J=2,M

SWEEP OVER SPACE

DO 220 I=1,N

BOUNDARY CONDITION

IP1=I+1
IP2=I+2
IM1=I-1
IM2=I-2

IF(IP1.GT.N) IP1=IP1-N+1
IF(IP2.GT.N) IP2=IP2-N+1
IF(IM1.LT.1) IM1=IM1+N-1
IF(IM2.LT.1) IM2=IM2+N-1

TERM1 = A1 \times (U(IP1,3) \times C(IP1,3)-U(IM1,3) \times C(IM1,3)+1 \times U(I,3) \times (C(IP1,3)-C(IM1,3)))

TERM2 = A2 \times (U(IP2,3) \times C(IP2,3)-U(IM2,3) \times C(IM2,3)+1 \times U(I,3) \times (C(IP2,3)-C(IM2,3)))

TERM3 = A3 \times ((U(IP2,3)-U(I,3)) \times (C(IP2,3)-C(I,3))-(U(I,3)-U(IM2,3)) \times (C(I,3)-C(IM2,3)))

TERM4 = A4 \times ((U(IM2,3)-U(IM2,2)) \times (C(IM2,3)-C(IM2,2)) - 8 \times (U(IM1,3)-U(I,3)) \times (C(IM1,3)-C(IM1,2)) + 8 \times (U(IP1,3)-U(IP1,2)) \times (C(IP1,3)-C(IP1,2)) - (U(IP2,3)-U(IP2,2)) \times (C(IP2,3)-C(IP2,2))

160 CONTINUE

TERM5 = A5 \times (C(IP1,3)-2 \times C(I,3)+C(IM1,3))

IF(EXACT.EQ.1) GO TO 170

IF(CLOSUR.EQ.0) DD(IP1,3)=0.0
IF(CLOSUR.EQ.1) DD(IP1,3)=DCONST
IF(CLOSUR.EQ.0) DD(IM1,3)=0.0
IF(CLOSUR.EQ.1) DD(IM1,3)=DCONST
250

**TERM 6** = \( A_6 \times (DD(IP1,3) \times (C(IP2,3) - C(I,3)) - DD(IM1,3) \times (C(I,3) - C(IM2,3))) \)

**CONTINUE**

**TERM A** = \( A_A \times (U(IP1,2) \times C(IP1,2) - U(IM1,2) \times C(IM1,2) + 1.0 \times U(I,2) \times (C(IP1,2) - C(IM1,2)) + C(I,2) \times (U(IP1,2) - U(IM1,2))) \)

**TERM B** = \( A_B \times (U(IP2,2) \times C(IP2,2) - U(IM2,2) \times C(IM2,2) + 1.0 \times U(I,2) \times (C(IP2,2) - C(IM2,2)) + C(I,2) \times (U(IP2,2) - U(IM2,2))) \)

**IF** (EXACT.EQ.1) **GO TO** 180

**TERM C** = \( A_C \times ((U(IP2,2) - U(I,2)) \times (C(IP2,2) - C(I,2)) - (U(I,2) - U(IM2,2)) \times (C(IM2,2) - C(IM1,2))) \)

**TERM D** = \( A_D \times ((U(IM2,2) - U(IM1,2)) \times (C(IM2,2) - C(IM2,1)) - 8.0 \times (U(IM1,2) - U(I,2)) \times (C(IM1,2) - C(IM1,1)) + 8.0 \times (U(IP1,2) - U(IP1,1)) \times (C(IP2,2) - C(IP1,2)) - (U(IP2,2) - U(IP1,2)) \times (C(IP2,2) - C(IP2,1))) \)

**CONTINUE**

**TERM E** = \( A_E \times (C(IP1,2) - 2.0 \times C(I,2) + C(IM1,2)) \)

**IF** (EXACT.EQ.1) **GO TO** 190

**IF** (CLOSUR.EQ.0) DD(IP1,2) = 0.0

**IF** (CLOSUR.EQ.1) DD(IP1,2) = DCONST

**IF** (EXACT.EQ.0) DD(IM1,2) = 0.0

**IF** (CLOSUR.EQ.1) DD(IM1,2) = DCONST

**TERM F** = \( A_F \times (DD(IP1,2) \times (C(IP2,2) - C(I,2)) - DD(IM1,2) \times (C(I,2) - C(IM2,2))) \)

**GO TO** 190

**CONTINUE**

**IF** (EXACT.EQ.1) **GO TO** 200

\( C(I,4) = C(I,3) + \text{TERM 1} + \text{TERM 2} + \text{TERM 3} + \text{TERM 4} + \text{TERM 5} + \text{TERM 6} + \text{TERM A} + \text{TERM B} + \text{TERM C} \)

**GO TO** 210

**CONTINUE**

**C**

**CALCULATE TOTAL MASS AT THE PREVIOUS TIME STEP**

**SUM** = 0.0

**DO** 230 I = 1, N

**SUM** = **SUM** + **C(I,3)**

**CONTINUE**

**TOTCH(J-1)** = **SUM** / FN

**C**

**CALCULATE AND PLOT STATISTICS OF C(X,T) AT SOME CHOSEN TIME STEPS**


**DO** 240 I = 1, N

**Y(I)** = **C(I,4)**

**SUM** = 0.0

**DO** 250 I = 1, N

**SUM** = **SUM** + **Y(I)**

**MEAN** = **SUM** / FN

**SUM1** = 0.0

**SUM2** = 0.0

**SUM3** = 0.0

**SUM4** = 0.0

**DO** 260 I = 1, N

**TERM** = **Y(I)** - **MEAN**

**SUM1** = **SUM1** + **TERM** \* **TERM**

**SUM2** = **SUM2** + **Y(I)** \* **Y(I)**

**SUM3** = **SUM3** + **TERM** \* **TERM** \* **TERM**
SUM4 = SUM4 + TERM*TERM*TERM*TERM

CONTINUE

STDV = SQRT(SUM1/N)
VAR = STDV*STDV
RMS = SQRT(SUM2/N)
SKEW = SUM3/(N*STDV*VAR)
AKURT = SUM4/(N*VAR*VAR)

TIME = (J-1)*DT
WRITE (6,600) J, TIME, MEAN, STDV, VAR, RMS, SKEW, AKURT
WRITE (6,700) (Y(I), I=1,101)
SUM1 = 0.0
SUM2 = 0.0
DUDX1 = (C(2,4) - C(N-1,4))/(2.*DX)
DO 270 I=2,N
DUDX = (C(I+1,4) - C(I-1,4))/(2.*DX)
SUM1 = SUM1 + DUDX*DUDX*DUDX
SUM2 = SUM2 + DUDX*DUDX
270 SUM1 = SUM1 + 2.*DUDX1*DUDX1*DUDX1
SUM2 = SUM2 + 2.*DUDX1*DUDX1
SK = (SUM1/N)/((SUM2/N)**1.5)
WRITE (6,740) SK
CALL PLOTS (0,0,0)
CALL AXIS (2.0,7.8,8HDISTANCE,8,XLEN,0.,X(N+1),X(N+2))
CALL AXIS (2.0,7.8,13HC0NCENTRATI0N,13,YLEN,90.,Y(N+1),Y(N+2))
CALL PLOT (2.0,7.8,-3)
CALL LINE (X,Y,N,1,0,0)
CALL HLINE (0.,XLEN,YLEN,LMASK1)
CALL VLINE (0.,YLEN,XLEN,LMASK1)
CALL PLOT (-2.,-7.8,-3)
DO 280 I=1,N
280 Y(I) = Y(I) - MEAN
DO 300 IP=1,NSPEC
IQF = N-IP+1
SUM = 0.0
DO 290 IQ=1,IQF
290 SUM = SUM + Y(IQ)*Y(IQ+IP-1)
DO 300 R(IP) = SUM/(N-IP+1)
DO 320 IH=1,NSPEC
SUM = 0.0
DO 310 IP=1,NSPEC
EPS = 1.0
IF(IP.EQ.1.OR.IP.EQ.NSPEC) EPS = 0.5
310 SUM = SUM + EPS*R(IP)*COS((IH-1)*(IP-1)*PI/(NSPEC-1))
320 E(IH) = 2.*DX*SUM/PI
ES(1) = 0.54*E(I)+0.46*E(2)
ES(NSPEC) = 0.54*E(NSPEC)+0.46*E(NSPEC-1)
NNSPEC = NSPEC-1
DO 330 I=2,NNSPEC
330 ES(I) = 0.23*E(I-1)+0.54*E(I)+0.23*E(I+1)
SUM = 0.5*(ES(I)+ES(NSPEC))
DO 340 I=2,NNSPEC
340 SUM = SUM + ES(I)
AREA = (PI*SUM)/(NNSPEC*DX)
DO 350 I=1,NSPEC
252

350 W(I)=(I-1)/(2.*DX*NSPEC)
W(I)=(W(I)+W(2))/2.
DO 360 I=1,NSPEC
W(I)=ALOG10(W(I))
IF(ES(I).LT.(10.0**(SLMIN))) ES(I)=10.0**(SLMIN)
360 ES(I)=ALOG10(ES(I))
W(NSPEC+1)=WLEFT
W(NSPEC+2)=(WRIGHT-W(NSPEC+1))/XLEN
ES(NSPEC+1)=SLMIN
ES(NSPEC+2)=(SLMAX-SLMIN)/YLEN
CALL AXIS (2.0,2.3,15HLOG WAVE NUMBER,-15,XLEN,0.,W(NSPEC+1),W(NSPEC+2))
CALL AXIS (2.0,2.3,12HLOG SPECTRUM,12,YLEN,90.,ES(NSPEC+1),ES(NSPEC+2))
CALL PLOT (2.0,2.3,-3)
CALL LINE (W,ES,NSPEC,1,0,0)
CALL HLINE (0.,XLEN,YLEN1,LMASK1)
CALL VLINE (0.,YLEN1,XLEN,LMASK1)
CALL SYMBOL (0.2,4.73,0.07,4HTIME,0.,4)
CALL NUMBER (0.55,4.73,0.07,TIME,0.,+2)
YS2=YS1+SLOPE*(XS2-XS1)*W(NSPEC+2)/ES(NSPEC+2)
CALL PLOT (XS1,YS1,3)
CALL PLOT (XS2,YS2,2)
XSYM=(XS2+XS1)/2.+0.1
YSYM=(YS1+YS2)/2.+0.1
CALL NUMBER (XSYM,YSYM,0.14,SLOPE,0.,-1)
CALL PLOT (0.,0.,+999)
WRITE (6,630)
WRITE (6,620) (ES(I),I=1,NSPEC)
WRITE (6,640) AREA
CONTINUE
C
***************************************************************
C
C
C

370 CONTINUE

C
***************************************************************
C
C
C

380 YT(K,J)=C(KK,K))
C
***************************************************************
C
C
C

390 CONTINUE

C
***************************************************************
C
C
C

390 CONTINUE

C
***************************************************************
C
C
C

400 CONTINUE


END TIME LOOP

CONTINUE

PLOT TOTAL MASS WITH TIME

TOTCN(M) = 2.*TOTCN(M-1) - TOTCN(M-2)

DO 420 J=1,M

X(J) = (J-1)*DT

X(M+1) = 0.0

X(M+2) = X(M)/XLEN

MM1 = M-1

WRITE (6,650)

WRITE (6,660) (TOTCN(J), J=1,M)

CALL PLOTS (0,0,0)

CALL AXIS (1.5,3.5,4*TIME,-4,XLEN,0.,X(M+1),X(M+2))

CALL AXIS (1.5,3.5,10*TOTAL MASS,10,YLEN1,90.,TOTCN(M+1),TOTCN(M+2))

CALL PLOT (1.5,3.5,-3)

CALL LINE (X,TOTCN,M,1,0,0)

CALL HLINE (0.,XLEN,YLEN1,LMASK1)

CALL VLINE (0.,YLEN1,XLEN,LMASK1)

CALL PLOT (0.,0.,+999)

PLOT CONCENTRATION TRACES AND FREQUENCY SPECTRA AT SOME CHOSEN NODES

Y(M+1) = CMIN

Y(M+2) = (CMAX-CMIN)/YLEN

IF (NNOD.EQ.0) GO TO 590

DO 580 K=1,NNOD

DO 440 J=1,M

Y(J) = YT(K,J)

CALL PLOTS (0,0,0)

CALL AXIS (2.0,7.8,4*TIME,-4,XLEN,0.,X(M+1),X(M+2))

CALL AXIS (2.0,7.8,13*CONCENTRATION,13,YLEN90.,Y(M+1),Y(M+2))

CALL PLOT (2.0,7.8,-3)

CALL LINE (X,Y,M,1,0,0)

CALL HLINE (0.,XLEN,YLEN1,LMASK1)

CALL VLINE (0.,YLEN1,XLEN,LMASK1)

CALL PLOT (-2.,-7.8,-3)

N = M-M1+1

NSPEC = NSPECT

DO 450 I=1,N

Y(I) = Y(M1+I-1)

SUM = 0.0

DO 460 I=1,N

SUM = SUM + Y(I)

MEAN = SUM/N

SUM1 = 0.0

SUM2 = 0.0

SUM3 = 0.0
SUM4=0.0
DO 470 I=1,N
TERM=Y(I)-MEAN
SUM1=SUM1+TERM*TERM
SUM2=SUM2+Y(I)*Y(I)
SUM3=SUM3+TERM*TERM*TERM
SUM4=SUM4+TERM+TERM*TERM*TERM
470 CONTINUE
STDV=SQR(SUM1/N)
VAR=STDV*STDV
RMS=SQR(SUM2/N)
SKEW=SUM3/(N*STDV*VAR)
AKURT=SUM4/(N*VAR*VAR)
DO 480 I=1,N
480 Y(I)=Y(I)-MEAN
DO 500 IP=1,NSPEC
IQF=N-IP+1
SUM=0.0
DO 490 IQ=1,IQF
490 SUM=SUM+Y(IQ)*Y(IP-1)
500 R(IP)=SUM/(N-IP+1)
DO 520 IH=1,NSPEC
SUM=0.0
DO 510 IP=1,NSPEC
EPS=1.0
IF(IP.EQ.1.OR.IP.EQ.NSPEC) EPS=0.5
510 SUM=SUM+EPS*R(IP)*COS((IH-1)*(IP-1)*PI/(NSPEC-1))
520 E(IH)=2.*DT*SUM/PI
ES(NSPEC)=0.54*E(1)+0.46*E(2)
NSPEC=NSPEC-1
DO 530 I=2,NSPEC
530 ES(I)=0.23*E(I-1)+0.54*E(I)+0.23*E(I+1)
SUM=0.5*(ES(1)+ES(NSPEC))
DO 540 I=2,NSPEC
540 SUM=SUM+ES(I)
AREA=(PI*SUM)/(NSPEC*DT)
DO 550 I=1,NSPEC
550 W(I)=(I-1)/(2.*DT*NSPEC)
DO 560 I=1,NSPEC
560 W(I)=ALOG10(W(I))
IF(ES(I).LT.(10.0**(SLMINT))) ES(I)=10.0**(SLMINT)
560 ES(I)=ALOG10(ES(I))
W(NSPEC+1)=WTL
W(NSPEC+2)=(WTR-WTL)/XLEN
ES(NSPEC+1)=SLMINT
ES(NSPEC+2)=(SLMAXT-SLMINT)/YLEN
CALL AXIS (2.0,2.3,13,LOG FREQUENCY,-13,XLEN,0.,W(NSPEC+1),W(NSPEC+2))
CALL AXIS (2.0,2.3,12,LOG SPECTRUM,12,YLEN1,90.,ES(NSPEC+1),ES(NSPEC+2))
CALL PLOT (2.0,2.3,-3)
CALL LINE (W,ES,NSPEC,1,0,0)
CALL HLINE (0.,XLEN,YLEN1,LMASK1)
CALL VLINE (0.,YLEN1,XLEN,LMASK1)
DIST=(NOD(K)-1)*DX
CALL SYMBOL (0.2,4.73,0.07,8HDISTANCE,0.,8)
CALL NUMBER (0.9,4.73,0.07,DIST,0.,+2)
YS2=YS1+SLOPE*(XS2-XS1)*W(NSPEC+2)/ES(NSPEC+2)
CALL PLOT (XS1,YS1,+3)
CALL PLOT (XS2,YS2,+2)
XSYM=(XS2+XS1)/2.+0.1
YSYM=(YS1+YS2)/2.+0.1
CALL NUMBER (XSYM,YSYM,0.14,SLOPE,0.,-1)
CALL PLOT (0.,0.,+999)
WRITE (6,680) NOD(K)
DIST=(NOD(K)-1)*DX
WRITE (6,750) DIST
WRITE (6,720) M1,M
WRITE (6,730) MEAN,STDV,VAR,RMS,SKEW,AKURT
IF(K.NE.1) GO TO 570
WRITE (6,690)
570 CONTINUE
WRITE (6,630)
WRITE (6,620) (W(I),I=1,NSPEC)
580 CONTINUE
WRITE (6,640) AREA
WRITE (6,610) (YT(K,J),J=1,M)
590 CONTINUE
STOP
C
C
C
600 FORMAT ('1',5X,'TIME STEP NUMBER',15/,5X,'TIME=',F8.5,,5X,'MEAN=',
       F6.4,,5X,'STANDARD DEVIATION=',F6.4,,5X,'VARIANCE=',F8.6,,5X,
       2'RMS=',F6.4,,5X,'SKEWNESS=',F9.5,,5X,'KURTOSIS=',F9.5,///,5X,'C
CONCENTRATION DISTRIBUTION AT THE FIRST 101 NODES',///)
610 FORMAT (///,5X,'LOG WAVE NUMBERS',///)
620 FORMAT (10F10.5)
630 FORMAT (///,5X,'LOG SPECTRUM',///)
640 FORMAT (///,5X,'AREA UNDER SPECTRUM=',F8.6,///)
650 FORMAT ('1',5X,'TOTAL MASS',///)
660 FORMAT (10F12.6)
680 FORMAT ('1',5X,'NODE NUMBER',15,/)  
690 FORMAT (5X,'LOG FREQUENCIES',///)
700 FORMAT (5F20.10)
710 FORMAT (///,5X,'TIME HISTORY OF CONCENTRATION',///)
720 FORMAT (5X,'THE POINTS FROM TIME STEP NUMBER',15,5X,'TO TIME STEP
1NUMBER',15,/,5X,'ARE INVOLVED IN CALCULATING THE FOLLOWING STATIS
2ICS',///)
730 FORMAT (5X,'MEAN=',F6.4,,5X,'STANDARD DEVIATION=',F6.4,,5X,'VARI
1ANCE=',F8.6,,5X,'RMS=',F6.4,,5X,'SKEWNESS=',F9.5,,5X,'KURTOSIS=2',F9.5,///)
740 FORMAT (///,5X,'SKEWNESS AS DEFINED IN CLARK ET AL. 1977=',F9.5,///,1/)

750  FORMAT (5X,'DISTANCE=',F5.2,///)
END
/*
//GO.FT03F001 DD UNIT=TAPE9,DISP=(OLD,KEEP),DSN=FT700,
// LABEL=(3,SL),VOL=(),RETAI N,SER=ABCD),DCB=(BLKSIZE=5000)
//GO.FT08F001 DD UNIT=TAPE9,DISP=(NEW,KEEP),DSN=FT700C,
// LABEL=(3,SL),VOL=(),RETAI N,SER=EF GH),DCB=(BLKSIZE=5000)
//GO.DATA DD *
/*
//