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IMPROVED AVERAGING METHOD FOR TURBULENT FLOW SIMULATION. PART I: THEORETICAL DEVELOPMENT AND APPLICATION TO BURGERS' TRANSPORT EQUATION

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SUMMARY

This is the first of two articles intended to develop, apply and verify a new method for averaging the momentum and mass transport equations for turbulence. The new method is based on Gaussian filtering in both the spatial and temporal domains. Application is made to the problem of momentum and scalar transport in a one-dimensional transient Burgers' flow field. No actual calculations, with the averaged equations, are presented in this paper. However, an 'exact' solution of the one-dimensional flow situation is presented as an economical tool for verifying the performance of the different turbulence models. In the second paper calculations are performed with the averaged one-dimensional equations on coarse grids, and the results are compared to the exact or fully simulated data with a statistical verification procedure.

KEY WORDS Turbulence Modelling Large Eddy Simulation Filtering One-dimensional Scalar Transport Burgers' Flow

INTRODUCTION

Whenever a system of equations describing turbulent fluctuations is to be solved numerically, on relatively coarse grids, the equations must be 'prepared' commensurate with the grid spacings. Because any numerical grid is capable of resolving only a certain portion of a rapidly fluctuating variable, a large-scale component and the remaining portion, called the subgrid-scale (SGS) component, are defined. Although not calculable, the SGSs have an important impact on the calculated large-scale components since they are responsible for receiving, scattering and dissipating the energy contained in the large-scale motion. The term 'preparing' the equations (turbulence modelling) then means replacing the total variables by their large-scale equivalents (averaging), and modelling the SGS effects in terms of the large-scale components (closure). After turbulence modelling, the equations can be solved on relatively coarse grids, since the large-scale variables vary less rapidly than the total variables.

Very recently attention has been directed towards improved methods for averaging the basic equations in order to achieve an improved representation of both the mean flow and SGS terms. Following the work of Leonard[1] new higher order spatial averaging procedures have been used

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with considerable success in formulating and solving turbulent flow problems. The critical basis of the procedure is that spatial averaging is all that is required for proper formulation. Many flows of environmental or meteorological interest are modelled under conditions which call into question whether spatial filtering or averaging is sufficient. It is therefore the objective of this paper to formulate a higher order space-time filter and test the results by intercomparison with models using the other available averaging methods and the results of a full one-dimensional 'turbulence' simulation.

RATIONALE

There are several reasons for examining space-time filtering, not the least of which is the authors' desire to model environmental flows. Such flows are dominated by: (1) very large horizontal and compressed vertical scales, (2) dynamic activity with time variation in the mean flows and perhaps non-stationarity in the turbulence characteristics and (3) the effects of interacting non-linear waves. Therefore it is anticipated that for the following reasons spatial filtering alone might not be fully adequate for use in numerical fluid dynamics models.

First, it is noted that based upon the initial suggestions of Reynolds[2] only time filtering is employed in most equation preparation. More recently in computational fluid dynamics has been the development and use of spatial filters. As reviewed in the next section, these filters do not employ any temporal filtering and rely on the elimination of temporal information through the elimination of the spatial components. The large eddy simulation method reviewed in the following section represents the most highly evolved form of spatial filtering. A thorough review of the average definition is presented by Monin and Yaglom[3] (Chapters 2 and 3), whereby the general space-time averaging definition is suggested (equation (3.1), p. 206). As to the use of this full averaging, Monin and Yaglom further go on to say that there are analysis complexities which are better approached by probabilistic methods. The analysis complexities are not clear, but appear to include an inability to arrive at solutions to such averaged equations, a problem avoided by computer solution methods. From our review of the literature no discussion as to the adequacy of space for time averaging or space and time averaging has occurred. Therefore the space-time averaging procedure is offered in this paper as a means of exploring the question of its necessity.

A second reason for developing this new averaging is to ensure complete space-time consistency in the dynamic model equations and their results. To heavily average in space and not to do so in time, because space averaging takes care of the temporal activity, seems inconsistent, i.e. it assumes and demands a full relationship between the space and time behaviours of the resolved processes for the *de facto* spatial averaging of temporal activity to be valid. If such were the case then it should be possible always to replace the three-dimensional space average with its equivalent temporal filter and achieve the same averaging result. To exactly substitute time for space filtering appears to be only possible when dealing with linear conservative waves where a clear linear relationship between space and time exists through the wave equation. In the presence of spatially and temporally variable dispersion, diffusion or turbulence the relationship between space and time would vary considerably from point to point in time and space in the flow field and therefore non-linear behaviour would be obtained. The non-linear relationship between space and time would then require both time and space filtering to ensure that the desired averaging occurred.

Additionally space for time filtering cannot be the case at all when, for example, there are source/sink terms. Source/sink terms, such as are heavily used in pollutant transport models, or the more general case of very stiff time-varying source/sink terms, can have very cyclical or oscillatory behaviours at a fixed point or volume in space. Since for many such source/sink terms there is no space dependence at all, then a spatial filter would not provide consistent averaging of these point oscillations.

A third theoretical or conceptual motivation is exemplified by the necessity of using very small time steps coupled with very large spatial scales. This represents an extreme case of the inconsistency mentioned above, and it is this very point that resulted in the investigation of space-time filtering. There must be consistency between the space-time averaging used in the equations and the physics to be resolved in the model. That same consistency must also exist between the averaged model equations and resulting numerical grid and discretizations. As is most often the case with surface water models, the spatial filter scales, as dictated by the grid size, place a definite resolution limit on the time scale of the resolved spatial phenomena. For example, if the average resolved scale spatial grid length is l, then a typical time scale of that resolution can be found if an appropriate velocity, say U, can be found. Under these conditions the typical time grid scale is $\tau = l/U$. The following problem now occurs if spatial filtering is left to perform temporal filtering as well. Because of stability restrictions, the time step δ_t actually allowed in the model is usually much less than τ, the time period of the activity permitted by the spatial grid. Therefore, the time marching scheme is resolving and the spatial grid is propagating activity with a very high frequency time characteristic and a very low spatial wave number resolution. Because the Navier–Stokes equations produce turbulence and because of the very small time step a portion of the turbulence frequency spectrum between $2\pi/\tau$ and $2\pi/\delta_t$ is being created which has not been filtered by the spatial grid. Hence a failure of the spatial filter to properly filter in time. The first step towards resolving this problem was, we felt, to learn how to time and space filter in order to remove this unwarranted frequency spectrum resolution and prohibit aliasing of these high frequency data into the long wavelengths.

Finally, and without much elaboration, it is noted that Pielke,[4] in his text on meteorological mesoscale models recommends space-time averaging as the basis for model equation preparation—but no analysis or discussion occurs in the work.

The rest of this paper and the second paper therefore present the higher order space-time filter and its evaluation. For the sake of initial or exploratory validation of the concept it is applied to the one-dimensional momentum and passive scalar transport problem. The authors fully realize that the one-dimensional problem may not possess the physics of the full 3D problem, but, as so many others have done before, we use the simplified application to allow a cost-effective first test of the procedure.

THE GENERAL AVERAGING DEFINITION

The mathematical definition of the large-scale component, $\bar{A}(\mathbf{x}, t)$, varies from one method of averaging to another; however, all methods imply smoothing. In other words, $\bar{A}(\mathbf{x}, t)$ must be obtained from $A(\mathbf{x}, t)$ by removing the high wave number and high frequency components. High wave numbers and high frequencies are those larger than the corresponding Nyquist values of the grid. From Reference 3 a general definition of $\bar{A}(\mathbf{x}, t)$ covering all possible methods of averaging can be written as

$$\bar{A}(\mathbf{x}, t) = \int_{-\infty}^{\infty} G(\mathbf{x} - \mathbf{x}', t - t')A(\mathbf{x}', t')\mathrm{d}\mathbf{x}'\mathrm{d}t'. \tag{1}$$

This is a convolution integral in which $G(\mathbf{x}, t)$ is a weight, averaging or filter function defined as

$$G(\mathbf{x}, t) = G_t(t)\prod_{l=1}^{n} G_l(x_l), \tag{2}$$

where $G_l(x_l)$ is the component of $G(\mathbf{x}, t)$ in the x_l direction, $G_t(t)$ is the temporal component, $\mathbf{x}$ is the spatial position vector, t is time and n is the total number of spatial directions. The function $G(\mathbf{x}, t)$ must satisfy the condition

$$\int_{-\infty}^{\infty} G(\mathbf{x}-\mathbf{x}', t-t')\mathrm{d}\mathbf{x}'\mathrm{d}t = 1, \tag{3}$$

so that the large-scale component of a constant becomes the same constant.

If $\bar{A}(\mathbf{x}, t)$ is really the large-scale component (the component that can be resolved by a given coarse grid), its Fourier transform should vanish at wavelengths and wave periods equal to or smaller than twice the corresponding grid spacings. This can be easily examined by applying the convolution theorem, which states that if (1) is true then

$$F\{\bar{A}(\mathbf{x}, t)\} = F\{G(\mathbf{x}, t)\}F\{A(\mathbf{x}, t)\}, \tag{4}$$

where F denotes the Fourier transform. Equation (4) shows that the Fourier transform of $\bar{A}(\mathbf{x}, t)$ is directly proportional to the Fourier transform of the filter function. Therefore, a filter function whose Fourier transform is zero for wavelengths and periods equal to or smaller than twice the corresponding grid spacings is needed.

Using (2), equation (4) can be rewritten as

$$F\{\bar{A}(\mathbf{x}, t)\} = \underbrace{F\{G_t(t)\}\prod_{l=1}^{n} F\{G_l(x_l)\}}_{F\{G(\mathbf{x}, t)\}}F\{A(\mathbf{x}, t)\}, \tag{5}$$

which is represented by

$$\Omega_{\bar{A}}(\omega_1, \ldots, \omega_n, f) = \underbrace{\Omega_t(f)\prod_{l=1}^{n} \Omega_l(\omega_l)}_{F\{G(\mathbf{x}, t)\}}\Omega_A(\omega_1, \ldots, \omega_n, f), \tag{6}$$

where Ω is a general function, f is frequency and ω_l is wave number in the x_l direction ($l = 1, \ldots, n$). A successful averaging operation should therefore possess the following properties:

$$\Omega_t(f) = F\{G_t(t)\} = 0 \quad (\text{for } f \geqslant 1/2\delta_t), \tag{7a}$$

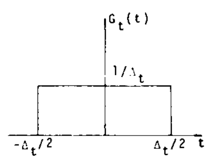
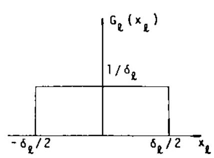
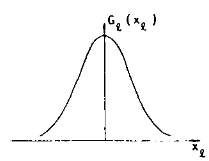
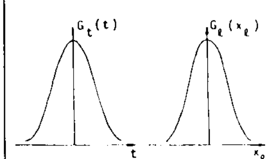
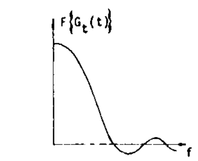
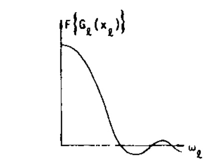
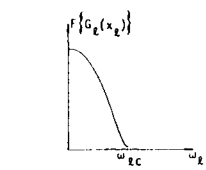
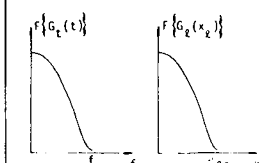
$$\Omega_1(\omega_1) = F\{G_l(x_l)\} = 0 \quad (\text{for } \omega_l \geqslant 1/2\delta_l), \tag{7b}$$

where δ_t is the temporal grid spacing and δ_l is the spatial grid spacing in the x_l direction.

There have been three filter functions used in preparing numerical models. The first three columns of Table I summarize the details of the various filters. In each column the filter function is defined and the Fourier transform behaviour specified and plotted. The first and most widely used form is Reynolds[2] averaging, a uniform temporal filter with incomplete high frequency removal. Rodi[5] and Brodkey[6] give the modelling and physics aspects of this filter. It is noted that condition (7a) is only partially satisfied and (7b) is not satisfied. Column 2 of Table I contains the more currently used uniform spatial averaging filter. Recognizing the necessity of removing the eddies smaller in size than the spatial grid, the original use of this filter was in complex meteorological models by Smagorinsky,[7] Deardorff[8-11] and Lilly.[12] Bedford and Rai[13] used this procedure in a shallow lake circulation and transport model. Again it is noted that high wave number information is not totally removed by this filter.

The first use of non-uniform weight functions was by Leonard[1] who used a Gaussian spatial filter (column 3 of Table I) and thereby initiated the large eddy simulation method. Extensive use of

Table I. Averaging operator definitions

	Reynolds Temporal Averaging 1882 to Present	Uniform Spatial Averaging 1950 to Present	Leonard's Spatial Filtering 1974 to Present	STF suggested by the Authors
Definition of the Large-scale component	$\bar{A}(\underline{x},t)=\int_{-\infty}^{\infty} G_t(t-t')A(\underline{x},t')dt'$	$\bar{A}(\underline{x},t)=\int_{-\infty}^{\infty} G(\underline{x}-\underline{x}')A(\underline{x}',t)d\underline{x}'$	$\bar{A}(\underline{x},t)=\int_{-\infty}^{\infty} G(\underline{x}-\underline{x}')A(\underline{x}',t)d\underline{x}'$	$\bar{A}(\underline{x},t)=\int_{-\infty}^{\infty} G(\underline{x}-\underline{x}',t-t')A(\underline{x}',t')d\underline{x}'dt'$
Definition of the filter function	$G_t(t)=\frac{1}{\Delta_t}$ for $\frac{-\Delta_t}{2}\le t\le\frac{\Delta_t}{2}$ = 0 Otherwise 	$G(\underline{x})=\prod_{\ell=1}^{n} G_\ell(x_\ell)$ where $G_\ell(x_\ell)=\frac{1}{\delta_\ell}$ for $\frac{\delta_\ell}{2}\le x_\ell\le\frac{\delta_\ell}{2}$ = 0 Otherwise 	$G(\underline{x})=\prod_{\ell=1}^{n} G_\ell(x_\ell)$ where $G_\ell(x_\ell)=\sqrt{\frac{\gamma}{\pi}}\frac{1}{\Delta_\ell}e^{-\gamma x_\ell^2/\Delta_\ell^2}$ 	$G(\underline{x},t)=G_t(t)\prod_{\ell=1}^{n} G_\ell(x_\ell)$ where $G_t(t)=\sqrt{\frac{\gamma}{\pi}}\frac{1}{\Delta_t}e^{-\gamma t^2/\Delta_t^2}$ $G_\ell(x_\ell)=\sqrt{\frac{\gamma}{\pi}}\frac{1}{\Delta_\ell}e^{-\gamma x_\ell^2/\Delta_\ell^2}$ 
Fourier transform of the Large-scale component	$F\{\bar{A}(\underline{x},t)\}=F\{G_t(t)\}.F\{A(\underline{x},t)\}$ where $F\{G_t(t)\}=\frac{\sin(f\,\Delta_t/2)}{(f\,\Delta_t/2)}$ 	$F\{\bar{A}(\underline{x},t)\}=F\{G(\underline{x})\}.F\{A(\underline{x},t)\}$ where $F\{G(\underline{x})\}=\prod_{\ell=1}^{n} F\{G_\ell(x_\ell)\}$ $=\prod_{\ell=1}^{n}\frac{\sin(\omega_\ell\delta_\ell/2)}{(\omega_\ell\delta_\ell/2)}$ 	$F\{\bar{A}(\underline{x},t)\}=F\{G(\underline{x})\}.F\{A(\underline{x},t)\}$ where $F\{G(\underline{x})\}=\prod_{\ell=1}^{n} F\{G_\ell(x_\ell)\}$ $=\prod_{\ell=1}^{n} e^{-\omega_\ell^2\Delta_\ell^2/4\gamma}$ 	$F\{\bar{A}(\underline{x},t)\}=F\{G(\underline{x},t)\}.F\{A(\underline{x},t)\}$ where $F\{G(\underline{x},t)\}=F\{G_t(t)\}.\prod_{\ell=1}^{n} F\{G_\ell(x_\ell)\}$ $=e^{-f^2\Delta_t^2/4\gamma}.\prod_{\ell=1}^{n} e^{-\omega_\ell^2\Delta_\ell^2/4\gamma}$ 

Δ_t = temporal averaging scale
Δ_l = spatial averaging scale in the x_l direction
γ = dimensionless constant with optimum value of 6
f = frequency
ω_l = wave number in the x_l direction

this filter is presented in References 14–18. For a review of the LES method especially with regard to flows of industrial or commercial application the reader is referred to the review paper by Rogallo and Moin.[19] Babajimopoulos and Bedford,[20] Bedford and Babajimopoulos[21] and Bedford[22] have used this method in lake and coastal transport calculations. In this spatial filter the high wave number components are successfully eliminated from $\bar{A}(\mathbf{x}, t)$. The cut-off wave number, ω_{lc}, is obviously a function of the filter width Δ_l and the non-dimensional constant γ. It is therefore the primary function of Δ_l and γ to bring ω_{lc} as close as possible to $1/2\delta_l$ (cycle per unit of length) in order to satisfy the requirement (7b). The constant γ is usually set equal to 6, and Δ_l is usually an integer multiple of δ_l. Note that no averaging is done in the temporal domain. In other words, the requirement (7a) is not satisfied, which means that $F\{\bar{A}(\mathbf{x}, t)\}$ has non-zero values at all frequencies.

THE NEW STF METHOD OF AVERAGING

An important physical attribute of turbulence is the fact that turbulent quantities fluctuate rapidly in both space and time. Thus, simultaneous filtering in time and space is appropriate. The general operation (1) is suggested as the basic definition of the large-scale. The filter function defined in (2) has n Gaussian spatial components as will be defined in (9), and a similarly defined temporal component. In this new space time filter (STF), equations (1), (2), (4), (5), (6), (7a) and (7b) become, respectively

$$\bar{A}(\mathbf{x}, t) = \int_{-\infty}^{\infty} G(\mathbf{x}-\mathbf{x}', t-t')A(\mathbf{x}', t')\mathrm{d}\mathbf{x}'\mathrm{d}t', \tag{8}$$

$$\begin{aligned} G(\mathbf{x}, t) &= G_t(t)\prod_{l=1}^{n} G_l(x_l) \\ &= \sqrt{(\gamma/\pi)}(1/\Delta_t)\exp(-\gamma t^2/\Delta_t^2)\prod_{l=1}^{n}\sqrt{(\gamma/\pi)}(1/\Delta_l)\exp(-\gamma x_l^2/\Delta_l^2), \end{aligned} \tag{9}$$

$$F\{\bar{A}(\mathbf{x}, t)\} = F\{G(\mathbf{x}, t)\}F\{A(\mathbf{x}, t)\}, \tag{10}$$

$$F\{\bar{A}(\mathbf{x}, t)\} = F\{G_t(t)\}\left(\prod_{l=1}^{n} F\{G_l(x_l)\}\right)F\{A(\mathbf{x}, t)\}, \tag{11}$$

$$\Omega_{\bar{A}}(\omega_1, \ldots, \omega_n, f) = \Omega_t(f)\left(\prod_{l=1}^{n}\Omega_l(\omega_l)\right)\Omega_A(\omega_1, \ldots, \omega_n, f), \tag{12}$$

$$\Omega_t(f) = F\{G_t(t)\} = \exp(-f^2\Delta_t^2/4\gamma) \simeq 0 \quad (\text{for } f \geqslant f_c), \tag{13}$$

$$\Omega_l(\omega_l) = F\{G_l(x_l)\} = \exp(-\omega_l^2\Delta_l^2/4\gamma) \simeq 0 \quad (\text{for } \omega_l \geqslant \omega_{lc}). \tag{14}$$

Equations (8)–(14) and the Figures in Table I show that $\bar{A}(\mathbf{x}, t)$ is free of any components having wave numbers and frequencies greater than or equal to $\omega_{lc}(l = 1, \ldots, n)$ and f_c. The cut-off values ω_{lc} and f_c can be brought to $1/2\delta_l$ and $1/2\delta_t$ so as to satisfy both the requirements (7a) and (7b).

The filter function (9) clearly satisfies the condition (3). Using the averaging operation (8), with the filter (9), the STF scheme for dealing with the averaging of a non-linear term, i.e. $\overline{\bar{A}\bar{B}}$, is as follows:

$$\overline{\bar{A}\bar{B}}(\mathbf{x}, t) = \int_{-\infty}^{\infty} G(\mathbf{x}-\mathbf{x}', t-t')\bar{A}\bar{B}(\mathbf{x}', t')\mathrm{d}\mathbf{x}'\mathrm{d}t'. \tag{15}$$

Expressing $\bar{A}\bar{B}(\mathbf{x}', t')$ in terms of $\bar{A}\bar{B}(\mathbf{x}, t)$ through a Taylor series expansion and neglecting higher order terms gives, after some algebra

$$\begin{aligned} \overline{\bar{A}\bar{B}} = \bar{A}\bar{B}&\int_{-\infty}^{\infty} G(\mathbf{x}-\mathbf{x}', t-t')\mathrm{d}\mathbf{x}'\mathrm{d}t' \\ &+ (\partial\bar{A}\bar{B}/\partial t)\int_{-\infty}^{+\infty} (t'-t)G(\mathbf{x}-\mathbf{x}', t-t')\mathrm{d}\mathbf{x}'\mathrm{d}t' \\ &+ \sum_{l=1}^{n}(\partial\bar{A}\bar{B}/\partial x_l)\int_{-\infty}^{\infty}(x_l'-x_l)G(\mathbf{x}-\mathbf{x}', t-t')\mathrm{d}\mathbf{x}'\mathrm{d}t' \\ &+ 0{\cdot}5(\partial^2\bar{A}\bar{B}/\partial t^2)\int_{-\infty}^{\infty}(t'-t)^2 G(\mathbf{x}-\mathbf{x}', t-t')\mathrm{d}\mathbf{x}'\mathrm{d}t' \end{aligned}$$

$$+0{\cdot}5\sum_{l=1}^{n}(\partial^2\bar{A}\bar{B}/\partial x_l^2)\int_{-\infty}^{\infty}(x_l'-x_l)^2G(\mathbf{x}-\mathbf{x}',t-t')\mathrm{d}\mathbf{x}'\mathrm{d}t'. \quad (16)$$

The components of $G(\mathbf{x}, t)$ are defined in equation (9). Note that each of these components is a Gaussian probability distribution with a zero mean; a variance equal to $\Delta_l^2/2\gamma$ or $\Delta_t^2/2\gamma$ and a unit area under the curve. Therefore, the above equation reduces to

$$\overline{\bar{A}\bar{B}} = \bar{A}\bar{B} + (\Delta_t^2/4\gamma)\partial^2\bar{A}\bar{B}/\partial t^2 + \sum_{l=1}^{n}(\Delta_l^2/4\gamma)\partial^2\bar{A}\bar{B}/\partial x_l^2. \quad (17)$$

Thus, a typical non-linear quantity is averaged as follows:

$$\begin{aligned}\overline{AB} &= \overline{(\bar{A}+A')(\bar{B}+B')}\\ &= \overline{\bar{A}\bar{B}} + \overline{\bar{A}B'} + \overline{A'\bar{B}} + \overline{A'B'}\\ &= \bar{A}\bar{B} + (\Delta_t^2/4\gamma)\partial^2\bar{A}\bar{B}/\partial t^2 + \sum_{l=1}^{n}(\Delta_l^2/4\gamma)\partial^2\bar{A}\bar{B}/\partial x_l^2\\ &\quad + \underbrace{(\overline{\bar{A}B'} + \overline{A'\bar{B}} + \overline{A'B'})}_{\text{closure}}.\end{aligned} \quad (18)$$

Notice the existence of the new temporal filter term in addition to the n spatial terms due to Leonard.[1] The cross terms $\overline{\bar{A}B'}$ and $\overline{A'\bar{B}'}$ are either neglected, according to the Reynolds rules, or modelled as by Clark *et al.*[16] Clark suggests a model for $\overline{\bar{A}B'}$ and $\overline{A'\bar{B}}$ which when combined with Leonard's filter terms reduces them to first order partial derivatives. The extension of this method to the STF procedure is below.

STF SIMPLIFICATION BY CLARK'S REDUCTIONS

The Clark *et al.*[16] reduction scheme can be easily extended to cover the newly suggested STF method. By induction from (17), the result of applying (8) to B is

$$\bar{B} = B + (\Delta_t^2/4\gamma)\partial^2B/\partial t^2 + \sum_{l=1}^{n}(\Delta_l^2/4\gamma)\partial^2B/\partial x_l^2. \quad (19)$$

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

$$B' = -(\Delta_t^2/4\gamma)\partial^2B/\partial t^2 - \sum_{l=1}^{n}(\Delta_l^2/4\gamma)\partial^2B/\partial x_l^2. \quad (20)$$

Multiplying by $\bar{A}$, expanding B into $\bar{B}+B'$, and then averaging the above equation yields

$$\overline{\bar{A}B'} = -(\Delta_t^2/4\gamma)(\overline{\bar{A}\partial^2\bar{B}/\partial t^2} + \overline{\bar{A}\partial^2B'/\partial t^2}) - \sum_{l=1}^{n}(\Delta_l^2/4\gamma)(\overline{\bar{A}\partial^2\bar{B}/\partial x_l^2} + \overline{\bar{A}\partial^2B'/\partial x_l^2}). \quad (21)$$

According to Clark *et al.*[16], B' is small by an order of magnitude than $\bar{B}$, and since B' fluctuates rapidly within the averaging scales and has a mean value of approximately zero, the second and last terms at the right can be neglected. The lowest order approximations of $\overline{\bar{A}\partial^2\bar{B}/\partial t^2}$ and $\overline{\bar{A}\partial^2\bar{B}/\partial x_l^2}$ are just $\bar{A}\partial^2\bar{B}/\partial t^2$ and $\bar{A}\partial^2\bar{B}/\partial x_l^2$. Thus equation (21) reduces to

$$\overline{\bar{A}B'} = -(\Delta_t^2/4\gamma)\bar{A}(\partial^2\bar{B}/\partial t^2) - \sum_{l=1}^{n}(\Delta_l^2/4\gamma)\bar{A}(\partial^2\bar{B}/\partial x_l^2). \quad (22)$$

Similarly

$$\overline{A'\bar{B}} = -(\Delta_t^2/4\gamma)\bar{B}(\partial^2\bar{A}/\partial t^2) - \sum_{l=1}^{n}(\Delta_l^2/4\gamma)\bar{B}(\partial^2\bar{A}/\partial x_l^2). \tag{23}$$

Using (18), (22) and (23) a typical non-linear quantity is averaged as follows:

$$\begin{aligned}\overline{AB} &= \overline{(\bar{A}+A')(\bar{B}+B')} = \overline{\bar{A}\bar{B}} + \overline{\bar{A}B'} + \overline{A'\bar{B}} + \overline{A'B'}\\ &= \bar{A}\bar{B} + (\Delta_t^2/4\gamma)\partial^2\bar{A}\bar{B}/\partial t^2 + \sum_{l=1}^{n}(\Delta_l^2/4\gamma)\partial^2\bar{A}\bar{B}/\partial x_l^2\\ &\quad - (\Delta_t^2/4\gamma)\bar{A}(\partial^2\bar{B}/\partial t)^2 - \sum_{l=1}^{n}(\Delta_l^2/4\gamma)\bar{A}(\partial^2\bar{B}/\partial x_l^2)\\ &\quad - (\Delta_t^2/4\gamma)\bar{B}(\partial^2\bar{A}/\partial t^2) - \sum_{l=1}^{n}(\Delta_l^2/4\gamma)\bar{B}(\partial^2\bar{A}/\partial x_l^2) + \overline{A'B'}\\ &= \bar{A}\bar{B} + (\Delta_t^2/2\gamma)(\partial\bar{A}/\partial t)(\partial\bar{B}/\partial t) + \sum_{l=1}^{n}(\Delta_l^2/2\gamma)(\partial\bar{A}/\partial x_l)(\partial\bar{B}/\partial x_l) + \overline{A'B'}.\end{aligned} \tag{24}$$

All filter terms, including the new temporal component, are reduced to first order partial derivatives. The quantity $\overline{A'B'}$ is to be modelled in terms of the large scales by a closure scheme.

ONE-DIMENSIONAL APPLICATION

For testing purposes the three-dimensional Navier–Stokes and scalar transport equations are extremely inefficient and expensive. Therefore many researchers resort to one-dimensional momentum and scalar transport equations to investigate certain problems in turbulence modelling. Burgers[23,24] 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 non-linear 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 closure models. Typical of these studies are References 25–35. The one-dimensional momentum and scalar transport equations are described as follows.

From the above papers the form of the unaveraged momentum equation is

$$\partial u/\partial t + a(u\partial u/\partial x) = \nu(\partial^2 u/\partial x^2). \tag{25}$$

When $a = 1{\cdot}0$ then the non-linear term is written as $(1/2)\partial(u^2)/\partial x$. In this equation u is the velocity and ν is the kinematic viscosity.

For the contaminant transport equation a somewhat non-standard form is selected, i.e. for scalar c,

$$\partial c/\partial t + \beta(u\partial c/\partial x) = \alpha(\partial^2 c/\partial x^2) + s, \tag{26}$$

where $\beta = 1{\cdot}0$ and the source/sink term s is specified as $c\partial u/\partial x$. In so doing turbulent flux can be maintained continually throughout the calculation by the source/sink term while also permitting an effective test of the filter.

If the values of u and c are given for all x at $t = 0$, the above equations can be solved for the behaviour of u and c as functions of x and t for $t > 0$. At first glance, the equations are seen to retain the inertial (advective) and dissipative (diffusive) natures of the corresponding three-dimensional equations. Further, Burgers' equation describes the formation and decay of weak shock waves in compressible fluids. Thus, equations (25) and (26) are important in their own right, as well as being

Table II. The average Burgers' equation

Unaveraged (A1)	$\frac{\partial u}{\partial t}+\frac{1}{2}\frac{\partial}{\partial x}[uu] = \nu\frac{\partial^2 u}{\partial x^2}$
Reynolds averaging (A2)	$\frac{\partial \bar{u}}{\partial t}+\frac{1}{2}\frac{\partial}{\partial x}[\bar{u}\bar{u}] = \nu\frac{\partial^2 \bar{u}}{\partial x^2}-\frac{1}{2}\frac{\partial}{\partial x}\left\{\overline{u'u'}\right\}$
Uniform spatial averaging	$\frac{\partial \bar{u}}{\partial t}+\frac{1}{2}\frac{\partial}{\partial x}[\bar{u}\bar{u}] = \nu\frac{\partial^2 \bar{u}}{\partial x^2}-\frac{1}{2}\frac{\partial}{\partial x}\left\{(\overline{\bar{u}\bar{u}}-\bar{u}\bar{u})+2\overline{\bar{u}u'}+\overline{u'u'}\right\}$
Leonard's averaging	$\frac{\partial \bar{u}}{\partial t}+\frac{1}{2}\frac{\partial}{\partial x}\left[\bar{u}\bar{u}+\frac{\Delta_x^2}{4\gamma}\frac{\partial^2 \bar{u}\bar{u}}{\partial x^2}\right] = \nu\frac{\partial^2 \bar{u}}{\partial x^2}-\frac{1}{2}\frac{\partial}{\partial x}\left\{2\overline{\bar{u}u'}+\overline{u'u'}\right\}$
Leonard's averaging and Clark's reduction (A3)	$\frac{\partial \bar{u}}{\partial t}+\frac{1}{2}\frac{\partial}{\partial x}\left[\bar{u}\bar{u}+\frac{\Delta_x^2}{2\gamma}\frac{\partial \bar{u}^2}{\partial x}\right] = \nu\frac{\partial^2 \bar{u}}{\partial x^2}-\frac{1}{2}\frac{\partial}{\partial x}\left\{\overline{u'u'}\right\}$
STF	$\frac{\partial \bar{u}}{\partial t}+\frac{1}{2}\frac{\partial}{\partial x}\left[\bar{u}\bar{u}+\frac{\Delta_t^2}{4\gamma}\frac{\partial^2 \bar{u}\bar{u}}{\partial t^2}+\frac{\Delta_x^2}{4\gamma}\frac{\partial^2 \bar{u}\bar{u}}{\partial x^2}\right] = \nu\frac{\partial^2 \bar{u}}{\partial x^2}-\frac{1}{2}\frac{\partial}{\partial x}\left\{2\overline{\bar{u}u'}+\overline{u'u'}\right\}$
STF with Clark's reduction (A4-A6)	$\frac{\partial \bar{u}}{\partial t}+\frac{1}{2}\frac{\partial}{\partial x}\left[\bar{u}\bar{u}+\frac{\Delta_t^2}{2\gamma}\frac{\partial \bar{u}^2}{\partial t}+\frac{\Delta_x^2}{2\gamma}\frac{\partial \bar{u}^2}{\partial x}\right] = \frac{\partial^2 \bar{u}}{\partial x^2}-\frac{1}{2}\frac{\partial}{\partial x}\left\{\overline{u'u'}\right\}$

Table III. Averaged one-dimensional scalar transport equation

Unaveraged (A1)	$\frac{\partial c}{\partial c}+\frac{\partial}{\partial x}[uc] = \alpha\frac{\partial^2 c}{\partial x^2}$
Reynolds averaging (A2)	$\frac{\partial \bar{c}}{\partial t}+\frac{\partial}{\partial x}[\bar{u}\bar{c}] = \alpha\frac{\partial^2 \bar{c}}{\partial x^2}-\frac{\partial}{\partial x}\left\{\overline{u'c'}\right\}$
Uniform spatial Averaging	$\frac{\partial \bar{c}}{\partial t}+\frac{\partial}{\partial x}[\bar{u}\bar{c}] = \alpha\frac{\partial^2 \bar{c}}{\partial x^2}-\frac{\partial}{\partial x}\left\{(\overline{\bar{u}\bar{c}}-\bar{u}\bar{c})+\overline{\bar{u}c'}+\overline{u'\bar{c}}+\overline{u'c'}\right\}$
Leonard's averaging	$\frac{\partial \bar{c}}{\partial t}+\frac{\partial}{\partial x}\left[\bar{u}\bar{c}+\frac{\Delta_x^2}{4\gamma}\frac{\partial^2 \bar{u}\bar{c}}{\partial x^2}\right] = \alpha\frac{\partial^2 \bar{c}}{\partial x^2}-\frac{\partial}{\partial x}\left\{\overline{\bar{u}c'}+\overline{u'\bar{c}}+\overline{u'c'}\right\}$
Leonard's averaging with Clark's reduction (A3)	$\frac{\partial \bar{c}}{\partial t}+\frac{\partial}{\partial x}\left[\bar{u}\bar{c}+\frac{\Delta_x^2}{2\gamma}\frac{\partial \bar{u}}{\partial x}\frac{\partial \bar{c}}{\partial x}\right] = \alpha\frac{\partial^2 \bar{c}}{\partial x^2}-\frac{\partial}{\partial x}\left\{\overline{u'c'}\right\}$
STF	$\frac{\partial \bar{c}}{\partial t}+\frac{\partial}{\partial x}\left[\bar{u}\bar{c}+\frac{\Delta_t^2}{4\gamma}\frac{\partial^2 \bar{u}\bar{c}}{\partial t^2}+\frac{\Delta_x^2}{4\gamma}\frac{\partial^2 \bar{u}\bar{c}}{\partial x^2}\right] = \alpha\frac{\partial^2 \bar{c}}{\partial x^2}-\frac{\partial}{\partial x}\left\{\overline{\bar{u}c'}+\overline{u'\bar{c}}+\overline{u'u'}\right\}$
STF with Clark's reduction (A4–A6)	$\frac{\partial \bar{c}}{\partial t}+\frac{\partial}{\partial x}\left[\bar{u}\bar{c}+\frac{\Delta_t^2}{2\gamma}\frac{\partial \bar{u}}{\partial t}\frac{\partial \bar{c}}{\partial t}+\frac{\Delta_x^2}{2\gamma}\frac{\partial \bar{u}}{\partial x}\frac{\partial \bar{c}}{\partial x}\right] = \alpha\frac{\partial^2 \bar{c}}{\partial x^2}-\frac{\partial}{\partial x}\left\{\overline{u'c'}\right\}$

one-dimensional tools for testing approximations designed for Navier–Stokes turbulence models.

To solve equations (25) and (26) on coarse grids, the total variables u and c must be replaced by their large-scale components $\bar{u}$ and $\bar{c}$. This is achieved by letting $u = \bar{u} + u'$ and $c = \bar{c} + c'$ in the non-linear terms and then averaging to yield

$$\partial\bar{u}/\partial t + (1/2)\partial[\overline{\bar{u}\bar{u}} + 2\overline{\bar{u}u'} + \overline{u'u'}]/\partial x = \nu\partial^2\bar{u}/\partial x^2, \qquad (27)$$

$$\partial\bar{c}/\partial t + \partial[\overline{\bar{u}\bar{c}} + \overline{\bar{u}c'} + \overline{u'\bar{c}} + \overline{u'c'}]/\partial x = \alpha\partial^2\bar{c}/\partial x^2. \qquad (28)$$

Using the various averaging methods, the final forms of the averaged equations are given in Tables II and III. The terms between braces are to be modelled in terms of the large-scale variables through a suitable closure procedure.

After closure, the averaged equations in Tables II and III can be solved on coarser grids. The chosen values for ν and α determine the level of turbulence. For the resulting $\bar{u}$ and $\bar{c}$ fields, time histories of the spatial mean, variance, skewness and kurtosis can be calculated and plotted. Also, wave number spectra at fixed instants in time, and frequency spectra at fixed locations are easily obtainable for both $\bar{u}$ and $\bar{c}$ distributions. These statistical properties can be compared to the corresponding properties of an 'exact' u and c field which can be obtained by solving the original equations on a very dense grid.

AN EXACT SOLUTION FOR A DYNAMIC BURGERS' FLOW FIELD

Equations (25) and (26) are one-dimensional. Thus, a full simulation of all the scales of motion, on very dense grids, is economically feasible. The resulting 'exact' features provide a basis against which the results of solving the averaged equations, on coarse grids, can be verified. A sample exact solution is presented in Figures 1–5. The initial $u(x, 0)$ is a train of sine waves, and the initial $c(x, 0)$ is uniform over the spatial domain. The boundary conditions are periodic, and the viscosity, ν, is very small (high Reynolds number). The diffusivity, α, is equal to ν (unit Schmidt number). The spatial domain is divided into 4000 intervals and the total time of simulation is divided into 2000 time steps. The finite difference scheme employs the fourth order accurate discretization used by Kwak *et al.*[14] for the non-linear terms. The viscosity and diffusivity terms are discretized by the usual centred second order schemes. For time marching, the explicit Adams–Bashforth procedure is implemented.

The most important behavioural aspect of the solution $u(x, t)$ is that, owing to the non-linear terms, the absolute value of $(\partial u/\partial x)$ grows larger with time in regions where it 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, $u(x, t)$, gradually decays with time as a result of the dissipative term. Figure 1 demonstrates this behaviour. It is also known that Burgers' equation is capable of propagating the shocks through the spatial flow domain with a speed equal to the spatial mean of $u(x, t)$ which remains constant with time. Thus point B in Figure 1 feels the shocks passing through it from left to right. Therefore, a time history of velocity at point B (Figure 3) shows the shocks developing in time, as well as the gradual decay due to viscous dissipation.

Figure 2 shows the concentration field as advected by the velocity of Figure 1. A time history of concentration at point **B** is also given in Figure 3. The most important aspect of the solution, $c(x, t)$, is that the pollutant accumulates in regions of low velocity and diminishes in regions of high velocity. This results in the existence of regions and periods in which the slopes $\partial c/\partial x$ and $\partial c/\partial t$ are very steep. Figure 4 shows wave number and frequency spectra for both velocity and concentration. Note the very apparent feature of -2 slope in the inertial subrange of all the full log

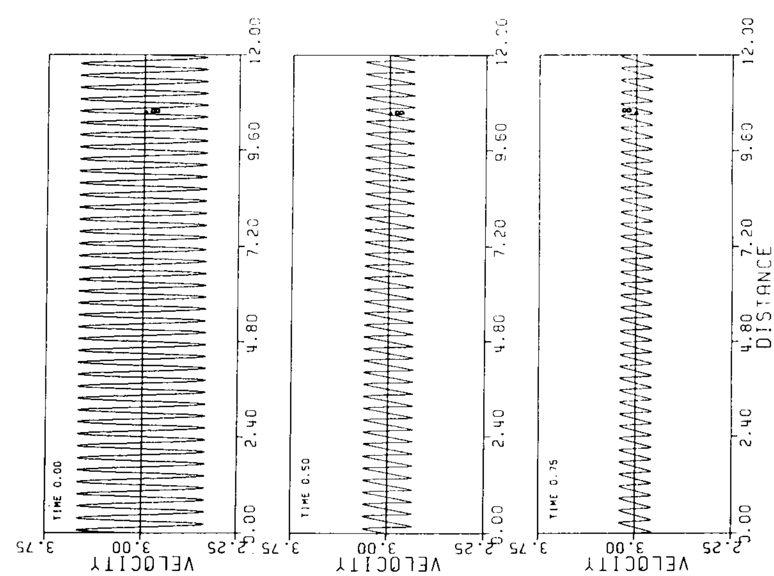


Figure 1. An exact solution of equation (25)

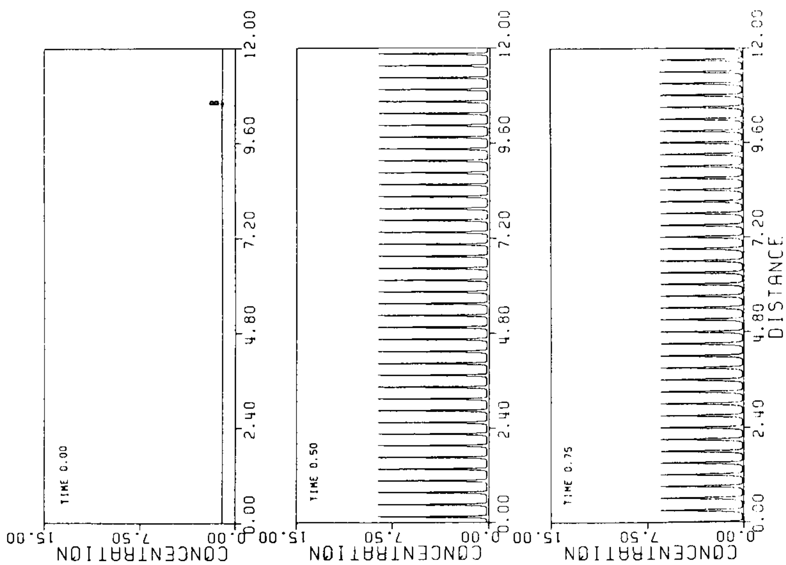


Figure 2. An exact solution of equation (26)

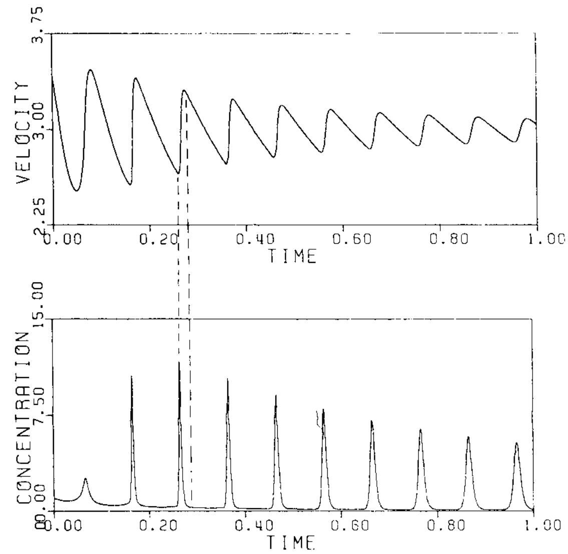


Figure 3. Time histories of u and c at point B

spectral plots. This feature is due to the existence of shocks in both the spatial and temporal distributions of u and c.

Another important aspect of the Burgers' flow is the temporal behaviour of the total energy contained in the flow field. Since the spatial mean of $u(x, t)$ remains constant with time, only the energy associated with the deviations from the mean is of interest. This total energy, per unit mass, is measured by $\langle v^2/2\rangle$ where v is the velocity u minus its spatial mean, and $\langle\,\rangle$ denotes averaging over all nodes. An 'energy equation' describing the temporal variation of $\langle v^2/2\rangle$ can be derived from (25) in the following form:[36]

$$\partial\langle v^2/2\rangle\partial t = -(1/2)\langle v\partial v^2/\partial x\rangle + \nu\langle v\partial^2 v/\partial x^2\rangle. \tag{29}$$

Time histories of each term in (29) are plotted in Figure 5. Note that the inertial term is energy conservative and that the energy decay is due solely to the viscous dissipation which reaches a peak when the shocks are fully developed.

The importance of the energy equation (29) 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 the filter and eddy viscosity terms is expected. The STF averaged equation, with Clark's reduction, is used to derive an energy equation for the temporal variation of the total energy $\langle\bar{v}^2/2\rangle$ associated with the large-scale motion. As in Reference 36, the equation reads

$$\begin{aligned}\partial\langle\bar{v}^2/2\rangle/\partial t = &-(1/2)\langle\bar{v}\partial\bar{v}^2/\partial x\rangle - (\Delta_t^2/4\gamma)\langle\bar{v}\partial(\partial\bar{v}/\partial t)^2/\partial x\rangle - (\Delta_x^2/4\gamma)\langle\bar{v}\partial(\partial\bar{v}/\partial x)^2/\partial x\rangle\\ &+ \nu\langle\bar{v}\partial^2\bar{v}/\partial x^2\rangle - (1/2)\langle\bar{v}\partial\{\overline{u'u'}\}/\partial x\rangle.\end{aligned} \tag{30}$$

An energy analysis in the fashion of Figure 5 is useful in studying the role of each of the new terms in the production, transfer and dissipation of energy.

The existence of the shocks or steep slopes in the u and c distributions is what makes equations (25) and (26) 'model equations for turbulence'. These shocks vary rapidly with space and time and, thus, a very dense grid must be used for the numerical solution, or a coarse grid turbulence modelling scheme must be implemented. The existence of the shocks in both the spatial and

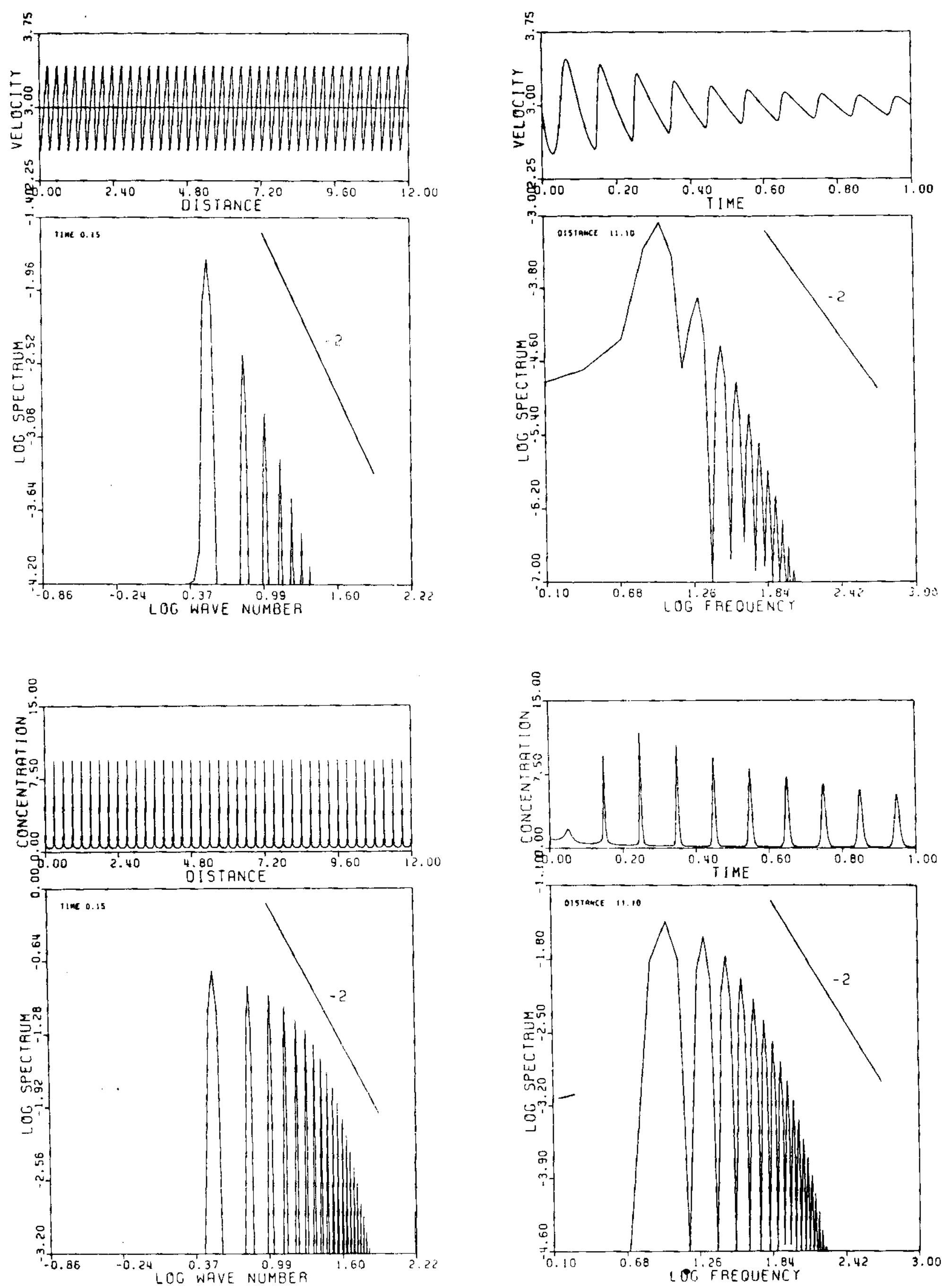


Figure 4. Wave number and frequency spectra of u and c

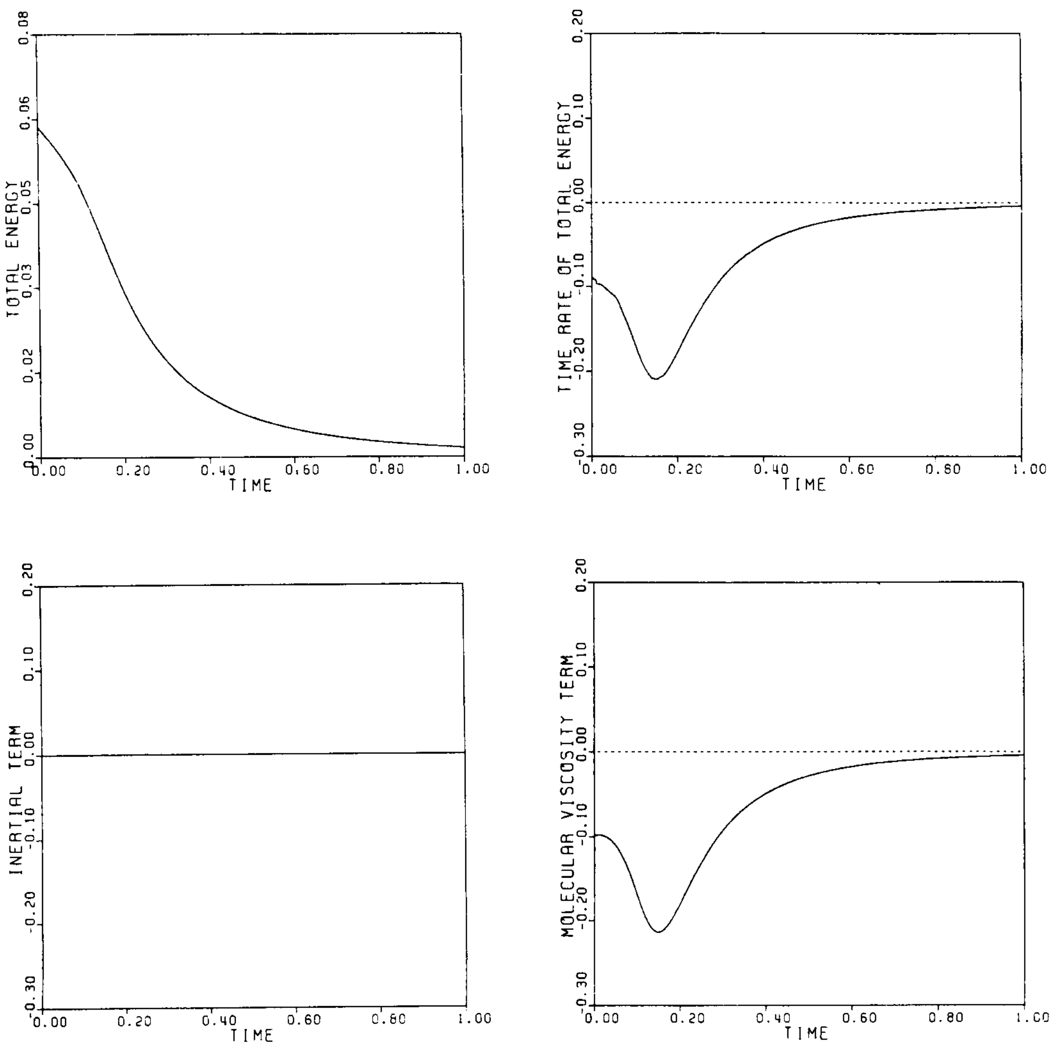


Figure 5. An exact solution of equation (29)

temporal domains is of special importance to this research since a new averaging procedure based upon both space and time filtering is suggested for such coarse grid modelling. The exact solution constitutes a valid test of the new procedure. The companion paper (Part II) presents this test.

CONCLUSIONS

In this paper a review of the spatial and temporal averaging procedures used in the formulation of numerical models is presented. Based upon deficiencies in the processing of high frequency and wave number information, a new spatial and temporal filter is presented. For this filter the rules of averaging as presented by Leonard[1] are shown to be applicable, as is Clark's reduction. To test the filter and its hypothesized improvements a dynamic Burgers' equation and transport problem is identified and solved with a mesh dense enough to constitute an exact solution. In addition to the time and space development of shocks in the solution an energetics analysis of the exact solution is presented. A sequel to this paper presents a comparison of results of the Burgers' coarse grid solution, solved with the new filter to data generated from this exact solution.

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