

Eddy diffusivity, eddy noise and subgrid-scale modelling

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A subgrid model is presented for a passive scalar advected by a randomly prescribed frozen velocity field. In addition to an eddy diffusivity it has a term which describes the injection of noise from the subgrid scales, and a term which implicitly describes the coupling between the large eddies and the eddies just below the limit of resolution of the finite-difference grid. The construction of the model is based upon an iterative procedure which models away first the dissipation-range eddies and then the eddies of a slightly larger size, etc.

1. Introduction

Most turbulence models describe the enhancement of transport processes owing to velocity fluctuations by a gradient-diffusion hypothesis (Bradshaw 1972):

$$\langle \phi' u_j \rangle = C \partial \langle \phi \rangle / \partial r_j,$$

where ϕ' and u are the fluctuating components of the property being transported and the velocity field respectively. This hypothesis has two serious deficiencies even in the simple case of almost homogeneous isotropic turbulence:

(a) The existence of a continuum of length scales, from that of the energy-containing eddies to the Kolmogorov microscale, requires the 'constant' C to be replaced by an integral operator whose Fourier transform has a peculiar cusp-like behaviour at the bottom of the inertial range (Kraichnan 1976; Leith 1971).

(b) All detailed statistics of the small scales are lost when the original equations of motion are contracted by the process of taking the mean value. Their effect in the mean is represented by an eddy diffusivity, but the fluctuations about the mean, which should be described by an 'eddy noise', are ignored.

These deficiencies are distinct from the additional complications found in the analyses of strongly inhomogeneous flows, which often require that C be determined not by local flow properties, but rather by a transport equation for C (or for a length scale which determines C) itself.

In the context of the random advection of a passive scalar ϕ , we show that the two effects (a) and (b) are related, and that the crucial features which are omitted by a gradient-diffusion model are as follows:

(A) A description of turbulence must incorporate, as a fundamental building block, the interaction of three contiguous scales of fluctuations (the use of two widely separated scales yields gradient diffusion).

(B) The use of a constrained mean-value operation, which is limited to a partial average over the fluctuations of intermediate size, produces a contracted description

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which makes explicit the injection of eddy noise from the small to the large scales of motion.

We present a model equation for the time evolution of ϕ in the special case of a frozen (time-independent) velocity field. This model is limited in that it is suitable only for calculating the mean response of the scalar field to an external disturbance. It is unsuitable for calculating the scalar correlation function $\langle\phi\phi\rangle$, because only some of the factors which contribute to the eddy noise have been considered in detail. The linearity of the equation of motion for ϕ enables these two features to be separated and this is the reason why the passive-scalar system was chosen.

The Fourier representation of our model may be found in equation (4.8). k_0 is a cut in Fourier space located at the boundary between the energy-containing range and the inertial range of the prescribed advecting velocity field u . It is used to decompose the set of all wavenumbers $\{k\}$ into the following regions:

The supergrid region, with k such that $k \leq k_0$.

The subgrid region, with k such that $k > k_0$.

The near-grid region, with k such that $k_0 < k \leq 2k_0$.

The energy spectrum of u is specified in the inertial range by the parameter m according to $E(k) \sim 1/k^m$. Our model refers explicitly to the supergrid passive-scalar field and to the supergrid and near-grid velocity fields. The near-grid velocity field is considered to be random. A weakly wavenumber dependent eddy diffusivity $\mu(k)$ appears which implicitly depends on m . It was assumed that the subgrid velocity field is both homogeneous and isotropic. No assumptions have been made concerning the supergrid velocity field.

There are two features of our model which distinguish it from the usual subgrid models. The first is the explicit retention of coupling between the supergrid scalar modes and the near-grid velocity modes. This is one of the factors which contribute to eddy noise. We have called this coupling 'eddy advection'. The second feature is the $uu\phi$ term in (4.8), which we have called 'eddy-mediated advection'. It may be regarded as a non-local contribution to the scalar flux in real (as opposed to Fourier) space. Eddy-mediated advection represents the possibility of an exchange of scalar eddies between the supergrid and subgrid scales. Alternatively, it describes the apparent loss of local conservation of scalar density. This effect is an inherent property of measurements made on the passive-scalar system with instruments which have a spatial resolution limited to eddies with size greater than $1/k_0$.

Though this model has no direct application to the study of real turbulence because of its assumptions about the subgrid velocity field and because it is a model for a linear system, we believe that it is useful as an illustration of some of the features which a turbulence model should contain.

The mathematical method we shall use is known as the renormalization-group, though no prior familiarity with it is assumed on the part of the reader. In the past few years it has proved to be a powerful tool for understanding critical phenomena (Wilson 1975). There are significant differences between these phenomena and that of turbulence and one does not expect to find, in the application of the renormalization-group to subgrid modelling, the spectacular success exhibited in calculating the properties of critical phenomena. Our model will remain a tentative one until it has been closely compared with experiment.

2. Eddy-diffusivity models

Consider a passive scalar field $\phi(\mathbf{r}, t)$ advected by a turbulent fluid with a solenoidal velocity field $\mathbf{u}(\mathbf{r}, t)$, a prescribed random function. Then

$$\partial\phi(\mathbf{r}, t)/\partial t - \mu\nabla^2\phi(\mathbf{r}, t) = -u_j(\mathbf{r}, t)\partial\phi(\mathbf{r}, t)/\partial r_j. \quad (2.1)$$

The summation convention will be used for repeated latin subscripts j assuming the values 1, 2 and 3 in (2.1). μ is the molecular diffusivity. The Fourier transform of (2.1) is

$$\frac{\partial\phi}{\partial t}(\mathbf{k}, t) + \mu k^2\phi(\mathbf{k}, t) = -ik_j \int_{\mathbf{p}+\mathbf{q}=\mathbf{k}} d^3p u_j(\mathbf{q}, t)\phi(\mathbf{p}, t). \quad (2.2)$$

If \mathbf{u} represents strong turbulence, then its energy spectrum $E(k)$ has a long inertial range where $E(k) \sim 1/k^m$. The precise value of m is not relevant for our purposes, though the classical Kolmogorov (1941) value of $\frac{5}{3}$ is used when presenting numerical results. Let the wavenumber k_0 mark the bottom of this range, k_d the top, and let V_0 be the r.m.s. value of \mathbf{u} :

$$\frac{1}{2}V_0^2 = \frac{1}{2}\langle u_j u_j \rangle = \int_0^\infty E(k) dk \approx \int_0^{k_0} E(k) dk.$$

Typically μ is small compared with V_0/k_0 .

The philosophy behind many turbulence models, the subgrid models being a particular type (Deardorff 1970, 1971, 1972, 1973; Fox & Lilly 1972; Leonard 1974; Leslie 1975; Lilly 1966, 1967; Schumann 1975; Smagorinsky 1963), is that in calculations which are concerned with smoothly varying quantities only, the effect of the many, quickly evolving small scales of motion may be represented by enhanced transport coefficients in the original equation of motion. For the system described by (2.2), subgrid models would replace ϕ by its truncations at k_0

$$\phi(\mathbf{r}, t) = \int d^3k \phi(\mathbf{k}, t) e^{i\mathbf{k}\cdot\mathbf{r}} \rightarrow \int_{k \leq k_0} d^3k \phi(\mathbf{k}, t) e^{i\mathbf{k}\cdot\mathbf{r}}, \quad (2.3)$$

\mathbf{u} by an analogous truncation and μ by an eddy diffusivity $\mu_E \gg \mu$, which must be of order V_0/k_0 by dimensional analysis. The effect of these replacements is to reduce drastically the number of dynamic degrees of freedom. This reduction must somehow be made if the calculation is to fit on present-day computers. Note that, as an alternative to truncating in Fourier space, it is common to work with a finite-difference representation of (2.1) on a grid initially fine enough to resolve all the significant scales of motion. The fine grid is then replaced by a much coarser grid, the equation of motion being simultaneously adjusted to compensate for the loss of spatial resolution. This adjustment also amounts to replacing μ by μ_E .

Though the detailed prescription for calculating μ_E depends on the particular model, the following reasoning is common. The fundamental property of strong turbulence is the transfer of energy from large eddies to small. For the passive scalar, the conserved quantity which plays an analogous role to energy is the mean-square scalar fluctuation, called the scalar variance. It too is transferred to small eddies. The eddies of intermediate size, with wavenumber $k_0 < k < k_d$, serve as intermediaries in the transfer process. If the truncation indicated in (2.3) is made, the mechanism by which the now no longer referred to modes removed scalar variance from the large-scale modes must be compensated for. Since the diffusive term $\mu\nabla^2\phi$ removes scalar

variance, it might be possible to realize this compensation by suitably enhancing the numerical value of μ . To estimate this enhancement, a dimensionally correct combination of large-scale parameters is chosen. Clearly k_0^{-1} is a relevant length scale and $\langle |\partial u / \partial r| \rangle$ (with the spatial derivative evaluated on a coarse grid with mesh spacing $1/k_0$) a relevant time scale, so that

$$\mu_E \sim \frac{1}{k_0^2} \left\langle \left| \frac{\partial u}{\partial r} \right| \right\rangle.$$

The above procedure captures some of the essential physics, but it has a fundamental inconsistency, which results from following the detailed evolution of individual realizations of the supergrid modes while at the same time compensating for the effect of the unresolvable subgrid modes only in the statistical mean. While it is true that the fine-scale modes, say those with $k > 2k_0$, evolve so quickly that their effect on individual realizations may be replaced by an equivalent mean effect, there is a strong coupling between the supergrid modes and the near-grid modes which cannot be thus represented.

In place of the eddy-diffusivity models, a model is constructed which realizes the special properties of the near-grid scales. This is accomplished through the use of a constrained mean-value operation which, in a sense to be precisely defined, performs only a partial average over the near-grid modes, and thus allows them to interact implicitly with the supergrid modes, in a realization-dependent fashion.

3. Systematic elimination of high wavenumber modes

Divide the set of equations represented by (2.2) into two subsets. The first contains those equations whose left-hand side refers to a $\phi(\mathbf{k}, t)$ such that $k \leq k_0$. The second contains all the others. In principle one can eliminate explicit reference to the latter set by solving them for the high k modes in terms of the low k modes, and then substituting the results into the first set wherever any reference is made to a high k mode (Ma & Mazenko 1975). The resulting system can be further simplified by performing some kind of average over the high k velocity modes, whose statistics are presumed to be given. In practice, only an approximation to this algorithm can be accomplished.

To illustrate the kind of approximation used without being encumbered by the unwieldy algebra of many coupled equations, the following simple model will first be examined in detail:

$$dX(t)/dt + \alpha X(t) = -i(a_x + a_y)(X(t) + Y(t)), \quad (3.1)$$

$$dY(t)/dt + 2\alpha Y(t) = -i(a_x + a_y)(X(t) + Y(t)). \quad (3.2)$$

Here X and Y are two functions of time, α is a positive constant and a_x and a_y are specified time-independent random variables with zero mean and covariances $\langle a_x^2 \rangle$ and $\langle a_y^2 \rangle$ respectively. The identifications to be made with (2.2) are the following:

X is a scalar mode $\phi(k_x)$ with $k_x < k_0$,

a_x is a frozen-velocity mode $u(k_x)$,

Y is a scalar mode $\phi(k_y)$ with $k_y > k_0$,

a_y is a frozen velocity mode $u(k_y)$,

α is the damping associated with μk_x^2 ,

2α is the higher damping associated with μk_y^2 .

The equality of the right-hand sides of (3.1) and (3.2) is of no consequence. The algebraic structure of (2.2) which is preserved by the above model is that both high and low wavenumber passive-scalar modes may be advected by both high and low wavenumber velocity modes.

In the context of (3.1) and (3.2), a 'subgrid model' is obtained by solving (3.2) for $Y(t)$ in terms of $X(t)$ and then substituting this solution into (3.1) to obtain a single equation for $X(t)$. Though this can be done exactly, the corresponding operation for (2.2) is impossible. A full description of the approximations used to obtain a subgrid model of (2.2) is given in § 5. For the moment, let us content ourselves with only a brief sketch of the parallel development for (3.1) and (3.2).

Assuming that the subgrid modes evolve more quickly (a Markovian approximation) than the supergrid modes, and that the amplitude of the subgrid modes is smaller than those of the supergrid modes, it is plausible to use

$$Y(t) = -i(a_x + a_y) X(t)/2\alpha \quad (3.3)$$

as an approximate solution to (3.2). Substitute (3.3) into (3.1) to obtain

$$dX(t)/dt + \alpha X(t) = -i(a_x + a_y) X(t) - (a_x + a_y)^2 X(t)/2\alpha. \quad (3.4)$$

Since a_y corresponds to a subgrid velocity mode, which is regarded as random, it is tempting to replace (3.4) by the equation which results from the substitutions

$$\begin{aligned} a_y X(t) &\rightarrow \langle a_y \rangle X(t) = 0, \\ a_y a_x X(t) &\rightarrow \langle a_y \rangle a_x X(t) = 0, \quad a_y^2 X(t) \rightarrow \langle a_y^2 \rangle X(t). \end{aligned}$$

However, in a sense to be defined in § 5, only the last two of the above are consistent with the properties in the mean of the original system (3.1) and (3.2). With these substitutions we obtain

$$dX(t)/dt + (\alpha + \delta\alpha) X(t) = -i(a_x + a_y) X(t) - a_x^2 X(t)/2\alpha, \quad (3.5)$$

where $\delta\alpha = \langle a_y^2 \rangle/2\alpha$, as a 'subgrid model' for (3.1) and (3.2).

The interpretation of the various terms in (3.5) is:

- (i) $\delta\alpha$ is the enhancement of the molecular diffusivity by the subgrid velocity modes,
- (ii) $ia_x X$ is the advection of the supergrid scalar field by the supergrid velocity field,
- (iii) $ia_y X$ is the random advection of the supergrid scalar field by the subgrid velocity field,
- (iv) $(a_x^2/2\alpha) X$ represents the boosting of a supergrid scalar eddy into the subgrid regime by a supergrid velocity eddy (which gives the first a_x factor) and its return to the supergrid regime by its interaction with a second supergrid velocity eddy (which gives the second a_x factor).

The transformation of (3.4) into (3.5) might be described as a partial average over the subgrid velocity-field statistics. The use of a partial subgrid average, as opposed to the use of an indiscriminate total average, is one way in which this model differs from the usual ones. As a consequence the term described in (iii) appears, which would otherwise be absent. The appearance of the unusual term in (iv) may be explained by saying that an average was performed over the subgrid scales with a probability distribution function conditioned with respect to the values assumed by the supergrid scalar field. Physically this corresponds to the fact that the supergrid

scalar eddies do not constitute an isolated system. There is a constant exchange of scalar eddies across the mathematical construction in Fourier space at $k = k_0$ (or in the language of real space, an exchange from eddies resolved by the coarse finite-difference grid to the unresolved eddies lying between the grid points), which causes the subgrid scalar field to respond and react back on the supergrid scalar field.

To justify the above interpretation we must return to the original set of equations (2.2) and perform the same manipulations as led to (3.5). Since $\langle |u(k)|^2 \rangle$ falls off exponentially for $k > k_d$, there will be a negligible contribution to $\delta\mu$ from this wavenumber range. Thus, for the purpose of constructing a subgrid mode, the system represented by (2.2) may be truncated at k_d . However, even at k_d , it is clear that the approximation which led to (3.3) would be untenable if μ were small enough. For the analogue of (3.3) to be valid, when Y corresponds to a subgrid scalar mode with wavenumber k we must have

$$V_k/\mu k < 1,$$

where V_k^2 is the energy of the velocity modes in the neighbourhood of k . This ratio, which may be thought of as a wavenumber-dependent Reynolds number, assumes its largest value for $k = k_0$,

$$V_0/\mu k_0. \quad (3.6)$$

For most problems of practical interest, this Reynolds number is much larger than one.

If we could solve for the subgrid modes in terms of the supergrid modes in such a way that the eddy diffusivity appeared in (3.6) instead of the molecular diffusivity, then the estimate in (3.6) would be lowered significantly. This can be partially realized by regarding the ultimate subgrid model as the product of two subsidiary calculations. The first calculation models away the modes between k_d and $\frac{1}{2}k_d$. The effective Reynolds number for this preliminary calculation is much smaller than that in (3.6) because in place of V_0 we use

$$W = \left(\int_{\frac{1}{2}k_d}^{\infty} E(p) dp \right)^{\frac{1}{2}} \ll V_0$$

and in place of k_0 we use $\frac{1}{2}k_d$. The system (2.2) is replaced by one with an upper cut-off of $\frac{1}{2}k_d$ and with a diffusivity enhanced by the amount

$$\delta\mu \sim W/(\frac{1}{2}k_d).$$

Next, the second calculation models away the modes between $\frac{1}{2}k_d$ and k_0 . The effective Reynolds number for this calculation is smaller than that in (3.6) because μ is replaced by $\mu + \delta\mu$.

The above process, whereby the subgrid model is produced in two stages, can be further subdivided by eliminating all of the subgrid modes in several stages. If we regard the original system as a ball in Fourier space of radius k_d , then by removing the subgrid modes one shell at a time, beginning at k_d and working in to k_0 , the effective diffusivity will be built up bit by bit. When all the shells between k_0 and k_d have been removed, the effective diffusivity attains its full value μ_E , of order V_0/k_0 . In this way, the Reynolds number for the removal of a particular shell is always of order unity, and the final subgrid model has been constructed through the use of a series of uniformly valid approximations.

It remains to be determined into how many shells Fourier space should be divided in order that the most accurate subgrid model is produced. Clearly two shells are

better than one, and three better than two, but after we have passed to the limit of many shells, it is not a simple matter to decide upon the optimum number. Fortunately, the resulting model is not very sensitive to this decision. Later we shall discuss some criteria for making this choice. For the moment, simply assume that there are N shells with inner and outer radii $k_d^{(n)}$ and $k_d^{(n-1)}$ respectively ($n = 1, 2, \dots, N$), where

$$k_d^{(n)} = f^n k_d$$

and f is a parameter between zero and one. The value $n = 1$ corresponds to the outer shell, bounded by $f k_d$ and k_d , and the value $n = N$ to the innermost shell, bounded by

$$k_0 = f^N k_d \tag{3.7}$$

and k_0/f . A fractional decrease in radius is the natural choice for an energy spectrum which obeys a power law.

After the first shell has been removed, the remaining equations of motion have a new form which resembles (3.5). If $\mu^{(1)}(k)$ is the (now wavenumber-dependent) effective diffusivity, then upon the removal of the second shell $\mu^{(1)}$ will be augmented to yield an effective diffusivity $\mu^{(2)}$, but $\mu^{(1)}$ will still appear explicitly in the $uu\phi$ term, just as in (3.5) there is still reference to α in the $a_x a_x X$ term. More generally, after n shells have been removed, the effective diffusivity is denoted by $\mu^{(n)}(k)$, and there is a memory of $\mu^{(n-1)}$, $\mu^{(n-2)}$, \dots . It can be shown inductively that (2.2) is transformed into the following system of equations if n is sufficiently large that $f^n < \frac{1}{2}$:

$$\begin{aligned} \frac{\partial \phi}{\partial t}(\mathbf{k}, t) + \mu^{(n)}(k) k^2 \phi(\mathbf{k}, t) = & -i k_j \int d^3 p u_j(\mathbf{k} - \mathbf{p}, t) \phi(\mathbf{p}, t) \\ & - k_j \sum_{h=1}^{h_{\max}} \int d^3 p \int d^3 s \frac{s_m u_j(\mathbf{k} - \mathbf{p}, t) u_m(\mathbf{p} - \mathbf{s}, t) \phi(\mathbf{s}, t)}{\mu^{(n-h)}(p) p^2}. \end{aligned} \tag{3.8}$$

The wave-vector arguments in (3.8) are constrained by $k \leq k_d^{(n)}$, and

$$|k - p| \leq 2k_d^{(n)}, \quad p \leq k_d^{(n)} \quad \text{in the first integral}$$

and

$$s \leq k_d^{(n)}, \quad |\mathbf{k} - \mathbf{p}| \leq k_d^{(n)}, \quad |\mathbf{p} - \mathbf{s}| \leq k_d^{(n)}, \quad f^{-h+1} k_d^{(n)} < p \leq f^{-h} k_d^{(n)} \quad \text{in the second integral.}$$

h_{\max} is simply an expression of the wavenumber constraint on term number h of the above summation

$$k_d^{(n-h+1)} < p = |\mathbf{p} - \mathbf{s} + \mathbf{s}| \leq |\mathbf{p} - \mathbf{s}| + s \leq 2k_d^{(n)},$$

which implies that

$$h_{\max} = (1 + \log_2(1/f))/\log_2(1/f). \tag{3.9}$$

Note that the integral of $u(q) \phi(p)$ represents advection by velocity modes which are both supergrid and subgrid with respect to the cut at $k_d^{(n)}$. When the $(n + 1)$ th shell is modelled away, $\delta\mu^{(n)}$ receives contributions from the $u\phi$ and from the $uu\phi$ terms:

$$\mu^{(n+1)}(k) = \mu^{(n)}(k) + \delta\mu^{(n)}(k), \tag{3.10}$$

$$\delta\mu^{(n)}(k) = \frac{k_m k_j}{k^2} \int d^3 p \frac{U_{mj}(\mathbf{k} - \mathbf{p})}{\mu^{(n)}(p) p^2} + \frac{k_m k_j}{k^2} \sum_{h=1}^{h_{\max}} \int d^3 p \frac{U_{mj}(\mathbf{k} - \mathbf{p})}{\mu^{(n-h)}(p) p^2}, \tag{3.11}$$

with $f k_d^{(n)} < p \leq k_d^{(n)}$, $f k_d^{(n)} < |\mathbf{k} - \mathbf{p}| \leq 2k_d^{(n)}$ in the first integral

and $f^{-h+1} k_d^{(n)} < p \leq f^{-h} k_d^{(n)}$, $f k_d^{(n)} < |\mathbf{k} - \mathbf{p}| \leq k_d^{(n)}$ in the second integral,

where $U_{mj}(\mathbf{q})$ is related to the equal-time velocity covariance, i.e.

$$\langle u_m(\mathbf{p}, t) u_j(\mathbf{q}, t) \rangle = \delta^3(\mathbf{p} + \mathbf{q}) U_{mj}(\mathbf{q}).$$

We have implicitly assumed that the subgrid velocity field is isotropic by using the single function $\mu^{(n)}(k)$ to represent the eddy diffusivity instead of using a tensor. It would not be difficult to rewrite the above equations in the anisotropic case.

The recursion relations (3.10) and (3.11), initialized by the definition $\mu^{(0)}(k) = \mu$, the molecular diffusivity, are central to the analysis which follows.

4. Self-similarity properties of the recursion relations

With a covariance $U(q)$ which goes as a power of q , we expect $\mu^{(n+1)}$ to be simply related to $\mu^{(n)}$ for large n . Technically this implies that, with a suitable choice of dependent variable, (3.10) and (3.11) can be converted into an autonomous system which refers to the index n only implicitly. In (3.11) one of the references to n is a trivial one related to the limits of integration and to the domain of definition for $\mu^{(n)}(k)$, which is $k \leq k_d^{(n)}$. The other dependence on n is through the variation of U ,

$$U(q) \sim E(q)/q^2 \sim 1/q^{m+2},$$

and from the downward shift of the limits of integration for q with increasing n . To eliminate the dependence of the domains of definition on n , we should consider the functions of k to be defined within the unit sphere $k \leq 1$,

$$\mu^{(n)}(k_d^{(n)}k),$$

and to eliminate the rising trend of U we should find a suitable diffusivity scale and use it to rescale the above functions.

Assume that U can be written in the form

$$U_{ij}(\mathbf{q}) = (C/\lambda^{m+2}) \mathcal{U}_{ij}(\mathbf{q}/\lambda),$$

where λ is any inverse length scale, \mathcal{U} is a dimensionless function, and C is a dimensional constant with the dimensions $[C] = 1/T^2 L^{m-3}$. It may be verified by direct substitution that in terms of the dimensionless functions

$$\beta^{(n)}(k) = [k_d^{(n)}]^{1/2(m+1)} C^{-1/2} \mu^{(n)}(k_d^{(n)}k), \tag{4.1}$$

defined for $k \leq 1$, (3.10) and (3.11) are equivalent to

$$\beta^{(n+1)}(k) = [\beta^{(n)}(fk) + \delta\beta^{(n)}(fk)] f^{1/2(m+1)}, \tag{4.2}$$

$$\delta\beta^{(n)}(k) = \frac{k_i k_j}{k^2} \int d^3p \frac{\mathcal{U}_{ij}(\mathbf{k}-\mathbf{p})}{\beta^{(n)}(p) p^2} + \frac{k_i k_j}{k^2} \sum_{h=1}^{h_{\max}} f^{-1/2\lambda(m+1)} \int d^3p \frac{\mathcal{U}_{ij}(\mathbf{k}-\mathbf{p})}{\beta^{(n-h)}(f^h p) p^2}, \tag{4.3}$$

with the wave-vector constraints obtained from those of (3.11) by making the replacement $k_d^{(n)} \rightarrow 1$.

To see simply the structure of (4.2) and (4.3) we use the hindsight afforded us by a direct numerical analysis, which indicates that the functions $\beta^{(n)}$ are smooth functions of k . If these functions are replaced by constants, the form of the above equations resembles that of

$$\beta^{(n+1)} = \left[\beta^{(n)} + \frac{(1-f)}{\beta^{(n)}} \right] f^{1/2(m+1)}. \tag{4.4}$$

The factor $1-f$ represents the vanishing of $\delta\beta^{(n)}(k)$ as f approaches 1 because of the limits of integration in (4.3). With the introduction of the difference operator Δ , defined by

$$\Delta\beta^{(n)} = \beta^{(n+1)} - \beta^{(n)},$$

(4.4) becomes

$$\Delta\beta^{(n)} = -[1-f^{\frac{1}{2}(m+1)}]\beta^{(n)} + (1-f)f^{\frac{1}{2}(m+1)}\beta^{(n)}.$$

Since

$$1-f^{\frac{1}{2}(m+1)} > 0,$$

$\beta^{(n)}$ quickly relaxes to a constant β as n increases, with

$$\beta^2 = \frac{(1-f)f^{\frac{1}{2}(m+1)}}{1-f^{\frac{1}{2}(m+1)}}.$$

Note that β is independent of the initial value $\beta^{(0)}$. Similarly the numerical solution of (4.2) and (4.3) has the property that

$$\lim_{n \rightarrow \infty} \beta^{(n)}(k) \equiv \beta(k)$$

exists, and though it depends implicitly on f , it is independent of μ , the molecular diffusivity. $\beta(k)$ is called a fixed point of the recursion relations.

The existence of a fixed point implies for the effective diffusivity, in the limit of large n , the behaviour

$$\mu^{(n)}(k) = [C/(k_d^{(n)})^{m+1}]^{\frac{1}{2}} \beta(k/k_d^{(n)}). \quad (4.5)$$

Thus, as each shell in Fourier space is removed, the functional form of $\mu^{(n)}$ remains invariant and its amplitude increases by the factor $1/f^{\frac{1}{2}(m+1)}$. When all the shells have been removed ($n = N$),

$$k_d^{(N)} = f^N k_d = k_0,$$

$$\mu^{(N)}(k) = (C/k_0^{m+1})^{\frac{1}{2}} \beta(k/k_0) \equiv \mu(k), \quad (4.6)$$

where $\mu(k)$ is the eddy diffusivity. The final subgrid model is

$$\begin{aligned} \frac{\partial \phi}{\partial t}(\mathbf{k}, t) + \mu(k) k^2 \phi(\mathbf{k}, t) = & -ik_j \int d^3 p u_j(\mathbf{k} - \mathbf{p}, t) \phi(\mathbf{p}, t) \\ & - k_j \sum_{n=1}^{h_{\max}} f^{-\frac{1}{2}n(m+1)} \int d^3 p \int d^3 s \frac{s_n u_j(\mathbf{k} - \mathbf{p}, t) u_n(\mathbf{p} - \mathbf{s}, t) \phi(\mathbf{s}, t)}{\mu(f^n p) p^2}, \end{aligned} \quad (4.7)$$

with the wave-vector constraints obtained from those of (3.8) by making the replacement $k_d^{(n)} \rightarrow k_0$.

For the spectral choice

$$U_{ij}(\mathbf{p}) = C \left(\delta_{ij} - \frac{p_i p_j}{p^2} \right) \frac{1}{4\pi p^{\frac{1}{3}}},$$

i.e. $m = \frac{5}{3}$, the function $\beta(k = 0, f)$ is displayed in table 1. In table 2 we have tabulated the function $\beta(k, f)/\beta(k = 0, f)$, for $0 \leq k \leq 1$ and $f = 0.3$ and 0.9 . Note that the thickness of the near-grid wavenumber shell $k_0 < k \leq 2k_0$ is independent of f . This is a consequence of the rules encountered in the manipulation of Fourier integrals (which give constraints of the form $\mathbf{p} + \mathbf{q} = \mathbf{k}$) and the constraint in our subgrid model, which allows explicit reference to passive-scalar modes $\phi(\mathbf{k})$ with $k \leq k_0$ only.

The limiting subgrid model obtained for $f \rightarrow 1$ is of particular interest because, for reasons to be discussed in § 5, it is believed that the models obtained for f near one are

<i>f</i>	0.3	0.5	0.7	0.8	0.9
$\beta(k=0, f)$	1.4	0.99	0.86	0.82	0.78

TABLE 1. Eddy-diffusivity fixed point as a function of the shell ratio parameter *f*.

<i>k</i>	0	0.2	0.4	0.6	0.8	1.0
$\beta(k, f=0.9)/\beta(k=0, f=0.9)$	1.0	0.96	0.93	0.91	0.89	0.88
$\beta(k, f=0.3)/\beta(k=0, f=0.3)$	1.0	0.90	0.84	0.79	0.75	0.73

TABLE 2. Eddy-diffusivity fixed point as a function of the wavenumber *k* normalized by the value at the subgrid cut-off *k*₀.

the most accurate. In addition, the analytic form of (4.7) simplifies in this limit. Consider the term in (4.7) which involves a summation over the index *h*. If *f* is close to one,

$$(p/k_0)f^h \approx 1, \quad \mu(f^h p) \approx \mu(k_0), \quad f^{-\frac{1}{2}h(m+1)} \approx (p/k_0)^{\frac{1}{2}(m+1)}.$$

These approximations transform (4.7) into

$$\frac{\partial \phi(\mathbf{k}, t)}{\partial t} + \mu(k) k^2 \phi(\mathbf{k}, t) = -ik_j \int d^3p u_j(\mathbf{k} - \mathbf{p}, t) \phi(\mathbf{p}, t) - \frac{k_j}{\mu(k_0) k_0^{\frac{1}{2}(m+1)}} \int d^3p \int d^3s \frac{s_n u_j(\mathbf{k} - \mathbf{p}, t) u_n(\mathbf{p} - \mathbf{s}, t) \phi(\mathbf{s}, t)}{p^{\frac{1}{2}(3-m)}}, \quad (4.8)$$

with the constraints $k \leq k_0$ and

$$|\mathbf{k} - \mathbf{p}| \leq 2k_0, \quad p \leq k_0 \quad \text{in the first integral}$$

and

$$s \leq k_0, \quad |\mathbf{k} - \mathbf{p}| \leq k_0, \quad |\mathbf{p} - \mathbf{s}| \leq k_0, \quad k_0 < p \leq 2k_0 \quad \text{in the second integral.}$$

Equations (4.2) and (4.3) also assume a simple form in the limit $f \rightarrow 1$. It can be shown that their fixed-point solution $\beta(k)$ is then determined by

$$k \frac{d\beta(k)}{dk} + \frac{(m+1)}{2} \beta(k) = \frac{1}{\beta(1)} [A(k) + B(k)], \quad (4.9)$$

where

$$A(k) = \frac{1}{2k} \int_{1 \leq q \leq 1+k} \frac{\sin^2(k, q, 1) dq}{q^{m+1}},$$

$$B(k) = \frac{1}{2k} \int_{1 \leq p \leq 1+k} \sin^2(k, 1, p) p^{\frac{1}{2}(m-1)} dp$$

and $\sin^2(k, p, q)$ is the square of the sine of the angle defined by the *k* and *q* legs of the **k**, **p**, **q** wave-vector triangle. The numerical solution of (4.9) is in good agreement with the extrapolation of the solutions to (4.2) and (4.3) for $f = 0.8$ and $f = 0.9$.

In (4.8) the significance of the value $m = 3$, as the dividing point between two different regimes of behaviour, is clearly seen. Note that even for $f \neq 1$ the exponent $\frac{1}{2}(3 - m) = 2 - \frac{1}{2}(m + 1)$ simply expresses the competition between the decrease in *p*, for $p \sim k_d^{(n)}$, and the increase in $\mu^{(n)}$ with *n* in the determination of a typical diffusion time $\tau^{(n)}$:

$$\tau^{(n)} = [\mu^{(n)}(p) p^2]^{-1} \sim [k_d^{(n)}]^{\frac{1}{2}(m-3)}. \quad (4.10)$$

For the Markovian aspect of the approximation used in (3.3) to be valid, the subgrid scalar modes must evolve more quickly than the supergrid modes, which implies that $\tau^{(n)} > \tau^{(n-1)}$, or that $m < 3$. This division at $m = 3$, in the context of subgrid-scale modelling, has been previously noted by Kraichnan (1976) for different reasons.

5. Nature of the approximations used in deriving the model

The approximations used in obtaining (3.8), (3.10) and (3.11) are of four different kinds. While they do not coincide with those used in the more standard schemes, such as Kraichnan's (1970) direct-interaction approximation, the latter can be used to generate the former (see Wilson 1975, p. 789). For simplicity their detailed description will be in the context of the transformation from (3.1) and (3.2) to (3.5). The first assumes that within the subgrid scales the scalar variance decreases with increasing wavenumber. It is then reasonable to solve (3.2) by a perturbation method by inserting a formal expansion parameter δ in front of Y on the right-hand side of the equation and solving for Y in terms of X as a power series in δ . The series is truncated, and δ is set equal to one. Second, it is assumed that the subgrid scalar modes evolve more quickly than the supergrid modes, and we therefore make the approximation that $Y(t)$ quickly decays to the steady-state solution of (3.2). This is called a Markovian approximation. For example, the formal expansion of Y to zeroth order in δ , and subsequent Markovian approximation, yields (3.3). Though this approximation is useful, it is not absolutely necessary. It is well known that eddy diffusivities are time dependent (Taylor 1959; Csanady 1973). For our subgrid model, this implies the presence of time histories, one of which is schematically represented by

$$\frac{\partial \phi(\mathbf{k}, t)}{\partial t} + k^2 \int_0^t \mu(k, t-t') \phi(\mathbf{k}, t') dt' = \dots$$

If ϕ varies slowly over the time scales of $\mu(k, t-t')$, which are of magnitude k_0/V_0 , then this can be replaced by

$$\partial \phi(\mathbf{k}, t) / \partial t + \mu(k) k^2 \phi(\mathbf{k}, t) = \dots,$$

where

$$\mu(k) = \int_0^\infty \mu(k, t) dt.$$

A detailed analysis shows that our 'Markovian' approximation merely amounts to having derived recursion relations for $\mu(k)$, and not for $\mu(k, t)$. The hypothesis of a frozen velocity field enables one to study $\mu(k)$ directly. The calculation of $\mu(k, t)$ for a frozen velocity field, and more generally for a velocity field with a time dependence characteristic of fully developed turbulence, does not appear to be difficult. The third approximation is an arbitrary one, and we have no justification for it except to say that without one like it we could not proceed. It may be regarded as an implicit constraint on the number of terms retained in the expansion in δ . We assume that a consistent model is produced by retaining only those terms in (3.1), after Y has been substituted for according to the first two approximations, which contain no more than two factors of the form a_x or a_y . For the real subgrid model it means that terms of the form $uu\phi$ are retained but that terms of the form $uuu\phi$, $uuuu\phi$, ..., have been ignored.

The fourth and last approximation is concerned with the procedure for partial averaging. Since the goal of subgrid modelling is to replace the initial set of equations by a smaller set which is equivalent to the first modulo the calculation of statistical

properties, we demand that the transformation induced by partial averaging should leave these properties invariant. The precise criterion we have chosen is based on the Taylor-series representation of the solution to (3.4). In this representation it is required that the mean value of $X(t)$, with respect to a_y , be invariant up to and including terms of order a^2 . This criterion allows us to replace (3.4) by (3.5). Note that this is consistent with the retention of terms of order a^2 in the third approximation. If the third approximation were expanded to retain terms of order a^4 , which correspond to terms of the form $uuuu\phi$ in the real subgrid model, then the invariance criterion would be extended to include terms of order a^4 .

In addition to the questions concerning the details of the above approximations there remains the choice of the parameter f , which determines in how many stages the modes between k_0 and k_d are modelled away. The value of f would not matter if a subgrid model could be constructed with sufficient accuracy. This does not mean that the form of the resulting equations would look the same, only that they would yield the same numerical results for a given calculation of the supergrid scalar field. Our model equation (4.7) depends on f implicitly through the function $\mu(k)$ and explicitly through the detailed form of the eddy-mediated advection term. Since (4.7) represents the beginning of a perturbation expansion of an exact model, it is possible that the differences between the models produced for two different choices of f are partially compensatory.

At present we do not have any quantitative estimates for the choice of f which would yield an optimal model. Such an estimate could be obtained by constructing the subgrid model which retains terms of the form $uuuu\phi$, and then varying f until the change produced in the original model (4.7) by these additional terms is minimized. Qualitatively it is felt that the optimal value of f is closer to one than to zero because if the successive shells in Fourier space that are being modelled away are thin, the effective diffusivity has time to adjust to the energy in the velocity modes being discarded. The use of an f which is near one in no way limits the range of interactions between the various passive-scalar and velocity-field modes in Fourier space.

6. Subgrid modelled scalar transport

The unusual $uu\phi$ term in (4.8) has a simple interpretation in physical space. If the inverse Fourier transform of (4.8) is taken, and $\mu(k)$ replaced by its value at k_0 , we obtain

$$\partial\phi(\mathbf{r}, t)/\partial t = -\nabla \cdot \mathbf{j}(\mathbf{r}, t). \quad (6.1)$$

$\phi(\mathbf{r}, t)$ is given by (2.3) and

$$\mathbf{j}(\mathbf{r}, t) = -\mu(k_0)\nabla\phi(\mathbf{r}, t) + \phi(\mathbf{r}, t)\mathbf{u}_<(\mathbf{r}, t) + \phi(\mathbf{r}, t)\mathbf{u}_>(\mathbf{r}, t) + \phi_{NL}(\mathbf{r}, t)\mathbf{u}_<(\mathbf{r}, t), \quad (6.2)$$

with

$$\begin{aligned} \mathbf{u}_<(\mathbf{r}, t) &= \int_{p \leq k_0} d^3p \mathbf{u}(\mathbf{p}, t) e^{i\mathbf{p} \cdot \mathbf{r}}, \\ \mathbf{u}_>(\mathbf{r}, t) &= \int_{k_0 < p \leq 2k_0} d^3p \mathbf{u}(\mathbf{p}, t) e^{i\mathbf{p} \cdot \mathbf{r}}, \\ \phi_{NL}(\mathbf{r}, t) &= -\int \frac{d^3r'}{(2\pi)^3} g(\mathbf{r} - \mathbf{r}') \nabla' \cdot [\phi(\mathbf{r}', t)\mathbf{u}_<(\mathbf{r}', t)]. \end{aligned}$$

where

$$g(r) = \frac{1}{\mu(k_0)k_0^{\frac{1}{2}(m+1)}} \int_{k_0 < p \leq 2k_0} d^3p \frac{e^{i\mathbf{p} \cdot \mathbf{r}}}{p^{\frac{1}{2}(3-m)}}.$$

The first two contributions to the scalar flux \mathbf{j} are expected. They correspond to gradient diffusion and supergrid velocity-field advective transport respectively. The third represents 'eddy advection' by the near-grid velocity field, and is looked upon as a random quantity. If we consider the subgrid model to be a description of the original passive-scalar system based upon observations made through a microscope whose resolution is limited to objects with spatial dimension greater than $1/k_0$, then eddy advection is the advection of clearly seen scalar eddies by invisible velocity eddies. The last contribution to \mathbf{j} is the supergrid advection of a non-local scalar density ϕ_{NL} . Looking through our microscope, it would be described by the following sequence of events:

- (i) A velocity eddy is seen advecting a scalar eddy at a spatial location \mathbf{r}' .
- (ii) The scalar eddy disappears from view.
- (iii) It reappears distributed at other space points \mathbf{r} , with a density ϕ_{NL} proportional to $g(\mathbf{r} - \mathbf{r}')$, being advected by visible velocity eddies.

Since this sequence represents the advection of a scalar eddy which has descended into the subgrid scales and then re-emerged, let us call it 'eddy-mediated advection'.

It is instructive to consider a numerical example of eddy-mediated advection in Fourier space. Let the superscale velocity field be given by

$$u_x(\mathbf{q}) = V[\delta(q_y - k_2) + \delta(q_y + k_2)]\delta(q_x)\delta(q_z), \quad u_y = u_z = 0,$$

with $k_2 < k_0$ and V a constant with the dimensions of velocity. Let there also be a time-independent source of passive scalar $S(\mathbf{q})$ on the right-hand side of (4.8):

$$S(\mathbf{q}) = [\delta(q_x - k_1) + \delta(q_x + k_1)]\delta(q_y)\delta(q_z),$$

with $k_1 < k_0$. We wish to compare the various contributions to the damping of the passive scalar ϕ . Since eddy advection represents the effect of a continuum of random velocity modes, its contribution is more or less additive and smoothly varying with the parameters k_1 and k_2 . Let us therefore ignore it in the comparison between eddy diffusivity, supergrid advection and eddy-mediated advection. Consider the following two cases.

Case I:

$$(k_1^2 + k_2^2)^{\frac{1}{2}} \leq k_0, \quad k_0 < [k_1^2 + (2k_2)^2]^{\frac{1}{2}} \leq 2k_0.$$

There are six supergrid scalar modes: $\phi(\pm k_1, 0, 0)$ and $\phi(\pm k_1, \pm k_2, 0)$. The latter four are implicitly coupled to the subgrid modes by eddy-mediated advection. Omitting the effects of eddy advection, and approximating $\mu(k)$ by $\mu(k_0)$, we obtain the following set of equations from (4.8):

$$\begin{aligned} \mu(k_0) k_1^2 \phi(k_1, 0, 0) &= -ik_1 V[\phi(k_1, k_2, 0) + \phi(k_1, -k_2, 0)] + 1, \\ \mu(k_0) (k_1^2 + k_2^2) \phi(k_1, k_2, 0) &= -ik_1 V\phi(k_1, 0, 0) - \frac{k_1^2 V^2 \phi(k_1, k_2, 0)}{\mu(k_0) k_0^{\frac{1}{2}(m+1)} (k_1^2 + 4k_2^2)^{\frac{1}{2}(3-m)}}, \end{aligned}$$

with identical equations for $\phi(k_1, \pm k_2, 0)$. The delta functions in wavenumber belonging to the scalar modes have been suppressed. Solving these equations for $\phi(k_1, 0, 0)$ it is found that

$$\phi^{-1}(k_1, 0, 0) = \mu(k_0) k_1^2 + \frac{2k_1^2 V^2}{\mu(k_0) (k_1^2 + k_2^2) + k_1^2 V^2 / \mu(k_0) k_0^{\frac{1}{2}(m+1)} (k_1^2 + 4k_2^2)^{\frac{1}{2}(3-m)}}.$$

Case II:

$$k_0 < (k_1^2 + k_2^2)^{\frac{1}{2}} \leq 2k_0.$$

The point of view we adopt is that in the first case $(k_1^2 + k_2^2)^{\frac{1}{2}}$ is marginally less than k_0 , and that the second case is obtained from the first by increasing k_1 by a small amount. There are two supergrid scalar modes, $\phi(\pm k_1, 0, 0)$, which are coupled to other modes only through eddy-mediated advection:

$$\begin{aligned} \mu(k_0) k_1^2 \phi(k_1, 0, 0) &= -k_1^2 V^2 \phi(k_1, 0, 0) / \mu(k_0) k_0^{\frac{1}{2}(m+1)} (k_1^2 + k_2^2)^{\frac{1}{2}(3-m)} + 1, \\ \phi^{-1}(k_1, 0, 0) &= \mu(k_0) k_1^2 + k_1^2 V^2 / \mu(k_0) k_0^{\frac{1}{2}(m+1)} (k_1^2 + k_2^2)^{\frac{1}{2}(3-m)}. \end{aligned}$$

Since in a typical supergrid realization $V = o(V_0)$ and k_1 and k_2 are both $o(k_0)$, the responses of ϕ in these two cases are computed to be comparable. Physically, the responses should be identical since we have supposed the two cases to be marginally different when viewed from the full set of scalar equations. Though identical responses were not found it has been demonstrated how eddy-mediated advection accounts for the loss of damping associated with the coupling of one supergrid scalar mode to another, which occurs when supergrid interactions boost an eddy into the higher wavenumbers of the subgrid scale. A subgrid model which had only an eddy-diffusivity term would be forced to have a diffusivity which rose sharply for wavenumbers approaching k_0 to compensate for the above effect.

7. Time-dependent velocity fields and the transfer of scalar variance

The determination of what constitutes a realistic choice for the turbulent velocity field \mathbf{u} is not simple. It is commonly assumed that the physically realized \mathbf{u} may be represented by a Gaussian process with the same mean and covariance. This assumption is not entirely satisfactory in the context of constructing a subgrid model.

Consider the subgrid modelling step in which the $(n+1)$ th Fourier-space shell, i.e. modes with wavenumbers k satisfying the condition

$$k_d^{(n+1)} < k \leq k_d^{(n)},$$

is removed. A partial average is performed over the velocity modes in this shell, conditioned with respect to the velocity modes whose wavenumbers are smaller than $k_d^{(n+1)}$. If \mathbf{u} is represented by a Gaussian process and if $k_d^{(n)}$ is in the inertial range, then the modes in the $(n+1)$ th shell are independent of the modes of smaller wavenumber because the inertial-range covariance is diagonal. However, the corresponding physically realized velocity-field modes are not independent. In effect, if one takes as given the velocity field due to the eddies which are larger than $1/k$, then the evolution of a randomly chosen eddy of size $1/k$ is determined (except for a phase factor) by its internal shear. As a result, its two-time covariance $\langle \mathbf{u}(\mathbf{k}, t) \mathbf{u}(-\mathbf{k}, t') \rangle$ decays to zero when $|t-t'|$ is comparable to the eddy turnover time

$$\tau(k) \sim (\epsilon^{\frac{1}{3}} k^{\frac{2}{3}})^{-1},$$

where ϵ is the energy transfer rate per unit mass. This contrasts with the unconditioned covariance, whose decay is determined by the advective dephasing time $1/kV_0$ (Kraichnan 1964).

This analysis suggests the use of a Gaussian velocity field whose two-time covariance decays according to $\tau(k)$ and whose equal-time covariance is again determined by the Kolmogorov spectrum. We believe that the subgrid model constructed from such a velocity field is suitable for calculations of $\langle\phi\rangle$ but of doubtful utility for calculations of $\langle\phi^2\rangle$; it is the inhomogeneities in the large-scale velocity and passive-scalar eddies which determine the transfer of scalar variance across k_0 , and its calculation is therefore sensitive to the modelling of these inhomogeneities. Similar difficulties stand in the way of constructing a subgrid model for turbulence itself.

Though we have little to say about the construction of a subgrid model which is suitable for the calculation of both $\langle\phi\rangle$ and $\langle\phi^2\rangle$, let us mention one qualitative feature: the presence of a random scalar source, which has been omitted from (4.8). This source represents subgrid passive-scalar fluctuations. Technically, such a term arises when the partial-averaging criterion, which was used to replace (3.4) by (3.5), is supplemented by the requirement that $\langle X^2\rangle$ be invariant.

8. Summary and closing comments

A subgrid model for the random advection of a passive scalar ϕ has been presented in the special case of a frozen velocity field. Its application is limited to the calculation of the mean value of ϕ because only one of the contributions to the fluctuations of ϕ has been included.

There are two principal differences between this model and the usual subgrid models. These arise from the recognition of the strong coupling between the large (supergrid) eddies and the (near-grid) eddies lying just below the limit of resolution of the finite-difference grid. One is the explicit injection of noise from the near-grid eddies into the supergrid eddies. The other is a new mode of scalar transport: 'eddy-mediated advection'.

The implications of our analysis are not confined to the class of models which are narrowly defined as 'subgrid'. Any model which attempts to describe scalar transport by simple advection and gradient diffusion will have difficulty in handling the above-mentioned contributions to the scalar flux.

The inspiration for this work (but none of its deficiencies) came from Jackson Herring, who pointed out the inconsistency between the usual subgrid models and the predictability studies, and from David Leslie, whose seminar and preprint (1975) provided the impetus to begin. I should also like to thank Robert Kraichnan for an informative conversation on subgrid modelling, and for a preprint (1976) of his work on eddy viscosity. Thanks also go to Uriel Frisch for helping me to organize my thoughts. This work was begun while I was with the Advanced Study Program of the National Center for Atmospheric Research, Boulder, Colorado, which is sponsored by the National Science Foundation.

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