

Models based on a statistical-thermodynamics analogy for the computation of varying diffusivity tensors and integration of the diffusion equation

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Abstract

The possibility is discussed of estimating space and time varying eddy diffusivities tensors based on numerically computed velocity fields of a waterbody. Valid results, are obtained with an approach derived from statistical thermodynamics analogies, which make to correspond the mean free path to the dimension of tidal vortexes.

Through the computation of the Lagrangian time scale, the possibility is also shown, to integrate the shear stress with a Fickian equation. Shear stress is evaluated through a modified von Kàrmàn formulation.

Additional approaches are also prospected in the determination of diffusivity tensors components.

Introduction

Models of complex waterbody ecosystems with chemical and biological purposes, demand the modelling of transport phenomena such as advection and diffusion. This need is determined by the influence of dilution on the relative kinetics which are effected not just through a time reversible advection mechanism, that can not lead to a steady state, but basically through an irreversible diffusion process. Steady states are similar to equilibrium states as, all intensive variables (such as temperature, chemical concentrations, biological densities) are constant in time, but they differ from these because they vary in space. In fact continuous source and open boundary conditions assure constant gradients, in the waterbody, of these intensive variables.

Fluxes of the conjugated extensive variables (heat, chemical and biological mass) are derived from gradients from Fick and Fourier laws according to eddy

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diffusivities. This dilution and the concomitant time irreversible processes, produce entropy, which is still minimum at steady state, and it is removed from the ecosystem contemporaneously with mass and heat fluxes.

In the real environment, however, and particularly in water bodies of complex topography, vector fluxes are not collinear with the corresponding gradients, and in such instances, the diffusivities constitute a transformation matrix related to the spatial coordinates and hence a tensor. Such conditions clearly refer to turbulent diffusivities strictly linked to the filed properties and not to isotropic molecular phenomena quantities. In respect to the former, however, molecular diffusivities are several order of magnitude lower and their effect is felt only in restricted and particular space such as the thermohaloclyne. In all environmental interdisciplinary models the greater uncertainty is associated to the description of processes related to the trophic chain and it increases with the growing up of complexity: this occurs beginning with nutrients, photosynthesis, primary and secondary production until the simulation is possible with continuous distribution.

For instance, in the extended simulation of seasonal phenomena all descriptive formulations require an increasing number of parameters, to account for variation of rate processes with irradiance and temperature and so the uncertainty increases further. Because of this situation, a balance between uncertainty sources is requested, it is left arbitrary the decision to where, the greater accuracy should be required for description of a phenomenon in respect to another.

In this view, even a diffusion process may be reproduced through a less accurate constant diffusivity instead of an approach involving a tensorial analysis. This practice has been successfully applied so far in the majority of applicative model, such as the eutrophication-diffusion model of the Venice lagoon¹, Florianopolis bay (Brasil) and others.

However, all efforts presently devoted to more accurately estimate trophic processes parameters, by sensitivity analysis and calibration of each single parameter², also basing on time series of structural environmental data and their accurate statistical treatments³, induce to a more detailed analysis of transport mechanisms. This demands for introduction of time and space varying diffusivity tensors whose average should be comparable to the constant value so far adopted in transport models.

Basing on dimensional analysis, several semi-empirical formulations have been elaborated in order to estimate eddy diffusivities, but they are not capable to render the complexity of eddy diffusivities in real situations. A different approach is necessary, deriving from the application of thermodynamic-statistical analogies on velocity fields computed through numerical programs, now widely available also in 3D.

The simplest analogy⁴ leads to a molecular diffusivity which is proportional to the product of a particle mean velocity between two collisions and the mean free path: the first obtained on a short time interval, and the

second, dependent only on the density, time averaged on a longer period. The most attainable procedure to represent the turbulent motion is the statistical one, but this would demand a very large number of measurements carried out in a long series of repeated similar experiments, that are not available at all. In fact only one single experiment is usually considered, which should last for a time long enough to calculate a reliable time averaged mean property. Then it is needed to find out how close this empirical mean quantity lies to the theoretical probability mean value. This conception is completely analogous to that in ordinary statistical thermodynamics, where the theoretical "mean over all possible states of the systems" (called "ensemble mean"), may also be replaced by the directly observed time-mean. Although this averaging interval seems to be tolerable, still the ergodic hypothesis must be verified, i.e. all the possible states of the system must be actually reached in that time interval, which is shown to be acceptable. The central limit theorem in statistics generates, in these cases, gaussian distributions and this may be considered as a posterior verification, instead of a prior cause.

The use of statistical-thermodynamical analogies in this aim, is so completely justified even though the velocity fields applied to theoretical formulations, are computed from numerical programs and not from experimental data.

If the water body to model is governed by periodical forcing functions as the tide, the tidal velocities exhibit a negligible mean value if averages during a proper time interval, and therefore in the transport phenomenon, turbulent diffusion plays the most important role.

In this case the analogy with the ultrasimplified theory of molecular diffusion suggests to substitute the particle velocity between two collisions with a mean velocity averaged in a time interval (1 hour), small compared to the tidal period (12 hours).

Using this velocity field to obtain the particle displacements, since residual currents are negligible, it is observed that almost all the different trajectories (starting at different tidal moments, from every point) are closed curves. Therefore they may be statistically described with a dispersion ellipse that includes 95% of all the trajectories points. In this way it is possible to determine the main direction of the flux vector in the Lagrangian reference system. Each ellipse is in fact characterized by the length of the major and minor axis, by the angle between the major axis and the ordinate axis of the Cartesian reference system (N-S direction) and by the eccentricity. The distribution of these four parameter in the modelled area (the central part of the Venice lagoon) is reported in Figure 1a,b,c,d. As one can see, in the majority of the points, the eccentricity is markedly different from 0 and this substantiates the need of a tensor reproducing the concentration patterns in all the different zones of the modelled area. Carrying on with the analogy, the eddy diffusivities along the canonical axes of each ellipse are determined by the products between the two ellipse semiaxes (analogous to the mean free path) and the projections of the

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hourly averaged velocities on them. The Lagrangian diffusivity tensor so computed, is represented by a diagonal matrix, having, in the principal diagonal, the two components of this vector and, outside it, zero values. To obtain the Eulerian tensor, the Lagrangian one is rotated to the orientation of the fixed Cartesian axes by applying a linear transformation and its inverse, which lead to a non diagonal but still symmetrical space and time varying diffusivity tensor with the following properties:

$K_{xx} > 0$, $K_{yy} > 0$, $K_{xy} = K_{yx}$ and $K_{xx} \cdot K_{yy} - K_{xy}^2 > 0$, as requested by the second law of thermodynamics.

Results are summarised in Figure 2a,b,c that show respectively the daily averaged diagonal components, K_{xx} and K_{yy} and the cross term, K_{xy} of the tensor. For a comparison, in Figure 2d it is shown the bathymetry of the central part of the lagoon characterized by a complex network of shallow areas and deep channels joined to the Adriatic sea through three inlets (maximum depth: 20 m).

The numerical integration of the diffusion equation in presence of a continuous point source, has been performed with a finite difference explicit method for each horizontal layer and with an implicit Laasonen scheme along each vertical column using space variable diffusivities to simulate the stratification⁵. The explicit method adopted to solve the horizontal diffusion second order partial differential equation with space and time varying diffusivity tensors, must assure the respect of the conservativity, the convergence, consistency, and stability of the solutions. To guarantee the conservativity, the most important property for chemical and biological applications, the scheme adopted is forward in time and centred in space except for the term of the scalar product of the diffused property gradient with the divergence of a vector with components K_{xx} and K_{yy} , that is forward in space. The stability condition, on the other hand, requires a quite long running time but still acceptable. Initial instabilities, though, are inevitably caused by the cross term (especially in the few grid points where K_{xy} is greater than a tenth of any of the diagonal components), but later smoothed out as the numerical integration proceeds. The results are presented in Figure 3, where the spatial distribution of a persistent pollutant is shown after 40 days of simulation. From the comparison with Figure 2d it is observed that all the deepest channels are realistically rendered also using only diffusivity tensors without any advective direct contribution.

Analysing, now, the ergodicity of the process, it must be observed that the points of the trajectories within the ellipses, do not have a 2D Gaussian distribution, but a toroidal one. This is unavoidable as the resolution of minor vortices, originating from the turbulent energy cascade of bigger eddies, is not possible to be simulated with the presently available advective models, and so it is not possible to smooth out the toroidal distribution set of curves. Nevertheless, the solution adopted theoretically guarantees the statistical-thermodynamic ergodicity, since the whole reachable phase space is really

reached for both the position and momentum subspace, and only the frequencies of reachability are different. For this purpose it is possible to resort to theoretical treatments, capable of taking into account the proximity of big vortexes along the main direction of the flux vector and the smaller ones present in the surroundings. However, they must strongly interact to realistically render the distributions: to this aim shear stress fluxes orthogonal to the main ones, are added, and they start to overwhelm the molecular diffusion only in an intermediate time, after which the process goes back to a Fickian law but with eddy diffusivities. During this time period, the area covered by the vortex (or of the variance σ^2)⁶ is proportional not to the time but to the cube of it. The relative determining parameter is the Lagrangian integral time scale T_L , which is computed from the ratio between the autocovariance and the variance⁷ and in the present case, it results lower than a tidal period⁸, while the stationary state requires a longer time intervals to be reached. It is so legitimized to add the shear stress component to the tensor one in a normal integration with the Fick equation for diffusion and not with a faster telegraph equation.

The classical method to obtain the shear stress for systems with an irregular geometry, is due to von Kàrmàn theory⁹: the first and second velocity derivatives are calculated in every grid point in respect to its orthogonal direction, and for dimensional reasons, the rate between the cube of the first derivative and the square of the second one is performed and multiplied by the square of the well known von Kàrmàn "universal" constant, $k=0.36\div0.4$. Another way of evaluating this contribute of the flux is due to Aris¹⁰ and Saffman¹¹, who based their analysis on the direct calculation of the zero, first and second moments of the distribution function along the main direction through their dependence on the diffusivity in the orthogonal direction, but the solution holds in non-stationary conditions of flow, and with a semi-empirical parametrization.

A further method was proposed by Carter and Okubo¹² who based their analysis on the integration of the advective diffusion equation, modifying the velocity vector components in the main direction. Both relationships seemed to be tested experimentally by Elder¹³ and Okubo and Karweit¹⁴ respectively.

The computation of the shear stress component of the eddy diffusivity, was first carried out with the Von Kàrmàn analysis, but the distribution of the results appears to be spatially almost random, Figure 4a, according to $R_1 = (\partial v / \partial n)^3 / (\partial^2 v / \partial n^2)^2$ and the frequencies distribution shows a very high variability. It is very difficult to reduce with the removal of distonormal ($R_1 \pm 3\sigma_{R1}$) values which are distributed in a range between -1.4×10^{14} and 1.6×10^{14} . Studying separately the numerator from the denominator the situation improves, but only slightly. Cutting all the values that detach from the mean more than, after few iterations, 40% of the points are excluded and about 29% are in a tight range around the mean value.



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Aware of the real difficulties encountered in the application of the method based on second derivatives to numerical computations, von Kármán dimensional logic was applied not to velocities but to the Lagrangian main components of the tensor, as made by Aris, but with a completely different theoretical approach. In this case the dimensional analysis is much easier and does not utilize neither second derivatives nor high powers. In fact it leads to this new ratio: $R_2 = (\partial K / \partial n)^2 / (\partial v / \partial n)$. In this ratio two cases have been distinguished for the denominator: in the first one the velocity is considered along its own direction, and in the second projected along the main tensor direction. While the first approach gives good results as the original, but still quite scattered, the second case shows reliable results, Figure 4b and its frequency distribution is less scattered but with a behaviour still similar to R_1 , as it is multiplied by a corrective factor obtained by the statistical comparison of R_2 and R_1 .

Adding the two shear stress components to the already computed Lagrangian eddy diffusivity tensors, and transforming in a new Eulerian matrix, the integration of the diffusion equation could be arranged with the scheme described above. Some initial instabilities appear and now they require a long computing time to disappear. To overtake this problem, super computers with high parallelism and suitable optimization will be used.

In conclusion the method here proposed is suitable to evaluate the effect of a diffusive transport with space and time eddy diffusivity tensors including also shear stress, and the results of the integration is completely conservative and also applicable to chemical and biological modelling.

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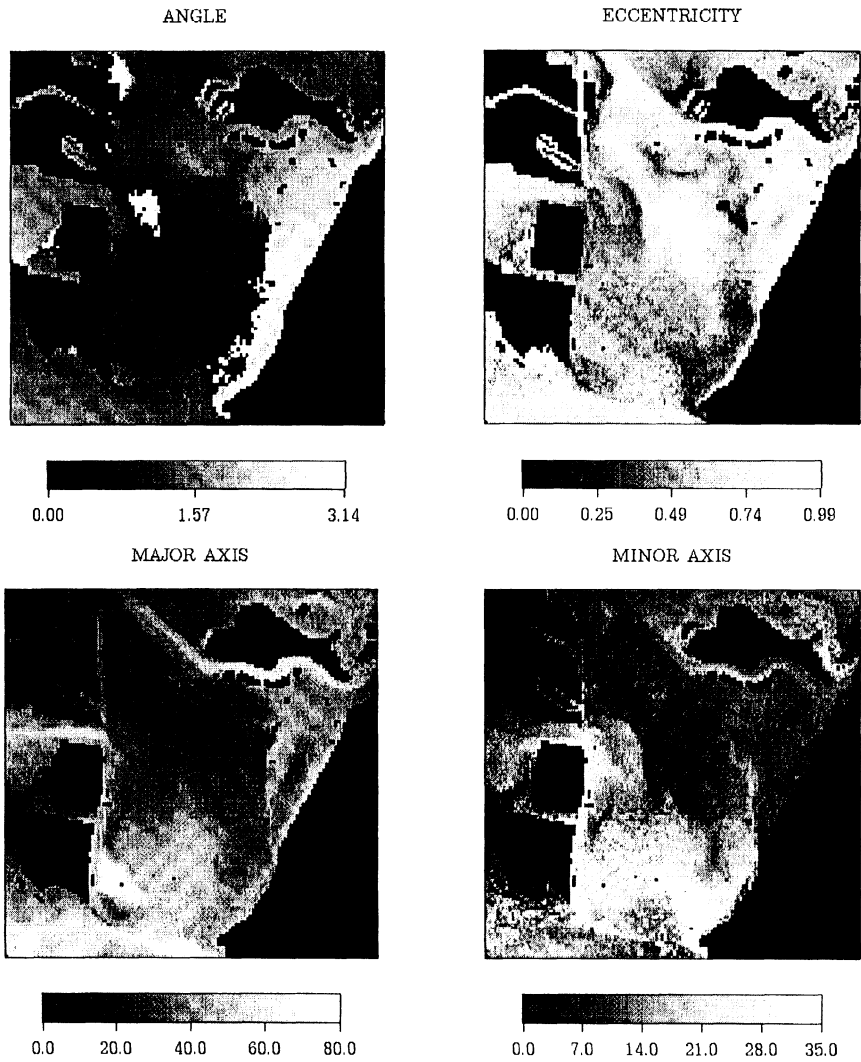


Figure 1: Parameters of the dispersion ellipse. a) major axis; b) minor axis; c) angle; d) eccentricity.

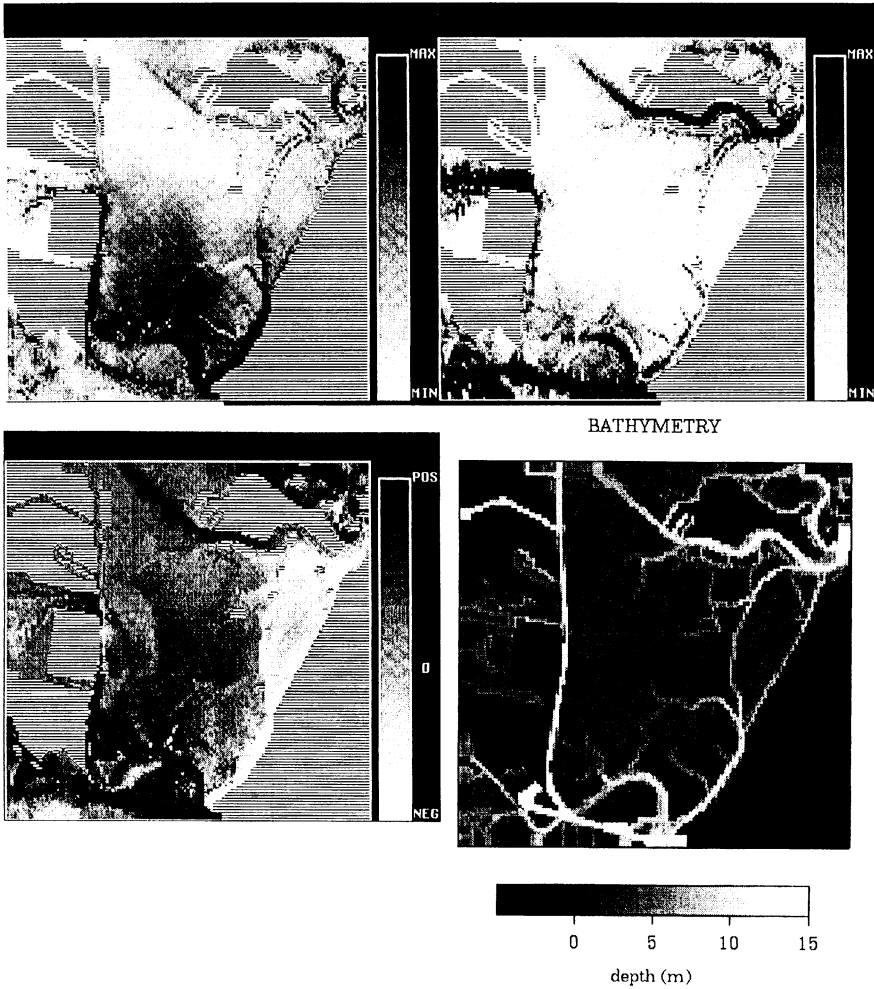


Figure 2: Tidal averaged Eulerian diffusivity tensors components. A) N-S component K_{xx} ; b) E-W component K_{yy} ; c) diagonal component K_{xy} ; d) bathymetry of the Venice Lagoon.

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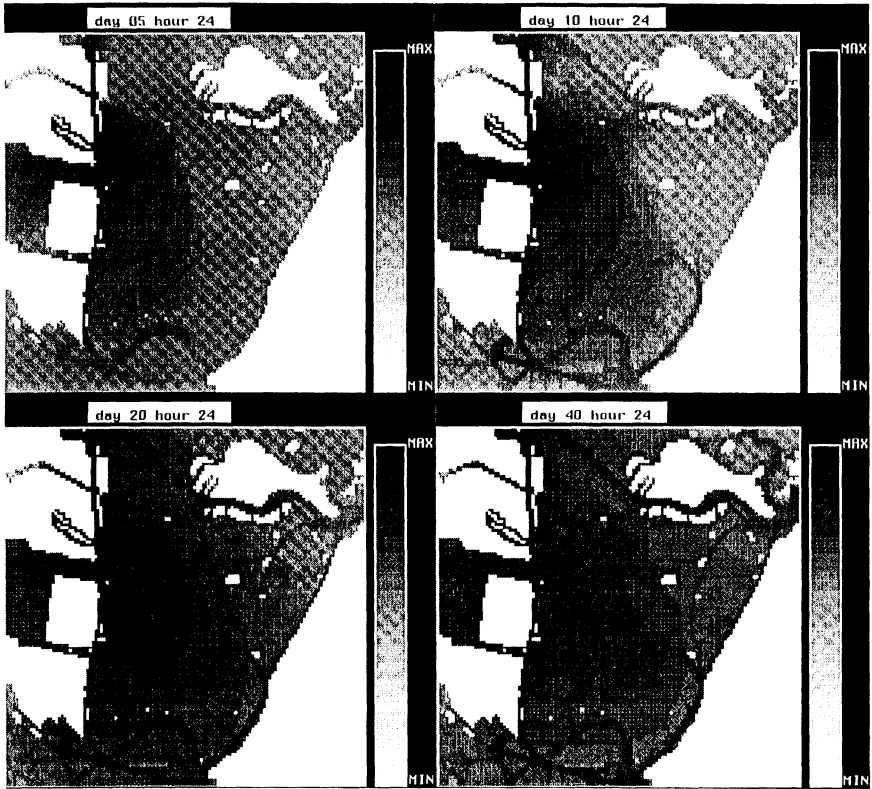


Figure 3: Integration results showing the distribution pattern of a passive tracer continuously released from a source point after: a) 5 days; b) 10 days; c) 20 days; d) 40 days.

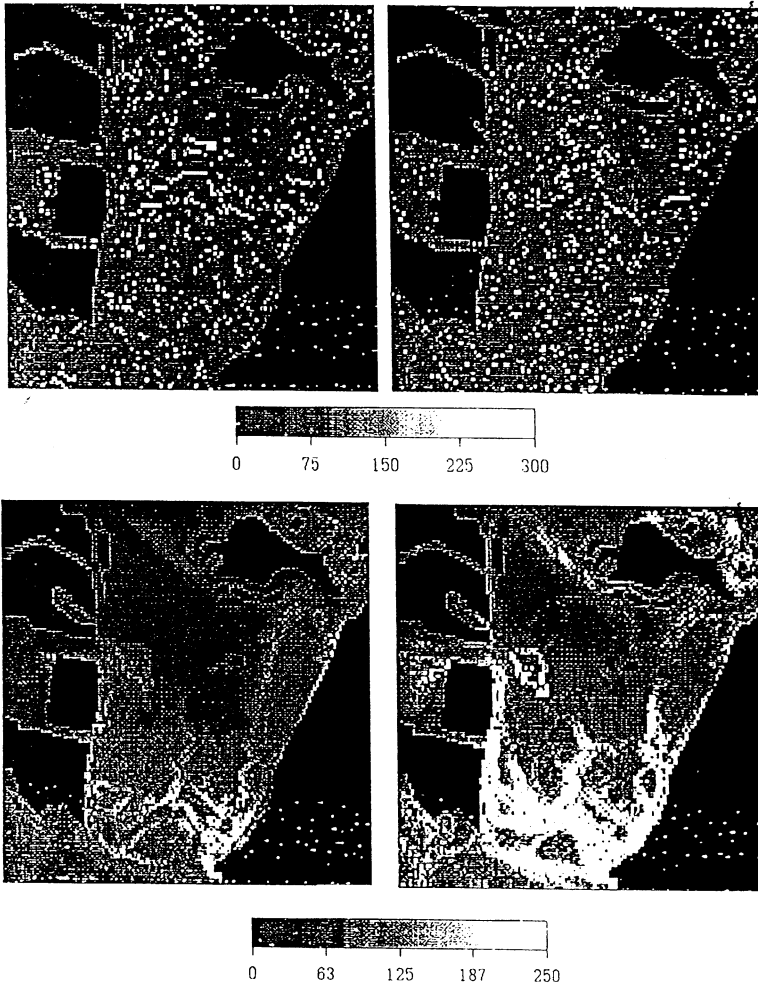


Figure 4: Distribution of the results of von Karman analysis applied a) to the velocity field, b) to the Eulerian components of the diffusivity tensor.