The Calculation of Turbulent Diffusion Coefficients in Aquatic Ecosystems

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The paper deals with the issues related to the pollution of aquatic ecosystems. The influence of turbulence on the transport and dispersion of pollutants in the mentioned systems, as well as the calculation of the turbulent diffusion coefficients are studied. A case study on the determination of turbulent diffusion coefficients for some sectors of the Prut River is presented. A new method is proposed for the determination of the turbulent diffusion coefficients in the pollutant transport equation for specific sectors of a river, according to the associated number of Péclet, calculated for each specific area: the left bank, the right bank and the middle of the river.

Keywords: aquatic ecosystem, turbulence, pollutant transport, turbulent diffusion coefficients.

Nowadays, pollution of aquatic ecosystems with different chemical, physical and biological substances is becoming more and more frequent. This has a negative impact on the flora and fauna of the ecosystem, and, last but not least, on human health.

A major problem is the pollution of aquatic systems with petroleum products. This has been recorded for several aquatic systems in different parts of the world. The environmental impact of this problem constitutes an essential issue for environmentalists, natural resource professionals and pollution researchers [1].

In order to determine the pollution degree of the studied ecosystem, including the prevention of exceptional situations, the researchers are increasingly using information systems based on the mathematical and numerical modeling of complex aquatic phenomena. Choosing the mathematical model and the appropriate simulation program will allow proper assessment of water quality [2 - 5].

In order to transform the mathematical model into a numerical model, they use CFD techniques, whereby partial-derivative equations are transformed into algebraic equation systems, the solutions of which represent an approximation of the state quantities in the defined nodes of the computation domain [6, 7].

The numerical models obtained must be calibrated and validated in order to be used in practice. The calibration of numerical models concerning the simulation of pollutants is difficult, the accuracy of the model being affected by the complexity of the physico-chemical phenomena occurring in the river-type systems. The turbulent diffusion coefficients reflect the influence of the turbulence in the convective field, the details of which are often difficult to observe. These coefficients can also be determined using empirical formulas for which many empirical models are developed. If an inappropriate model is applied, we will get an inaccurate estimation of the parameters. Based on the above, each studied sector needs to be individually treated for the choice of method in order to accurately estimate the turbulent diffusion coefficients.

Researches on the turbulence influence on pollutants evolution in aquatic systems

The movement and spreading of pollutants in aquatic systems arise because of a complex process called dispersion, which can be explained by the simultaneous action of the molecular diffusion phenomenon of the pollutant and of the convection-advection phenomenon. Because of the above-mentioned processes, an uneven velocity field appears, which the American physicist O. Reynolds (1883) studied, establishing a turbulent flow regime. The main consequence of this regime is the increase in the velocity of the fluid particles, which leads to mass transport of the fluid. The main characteristics of the turbulence phenomenon are the following: non-static, irregularity, diffuse character, large Reynolds number, three-dimensionality, dissipative character, independence from the nature of the fluid [8, 9].

The fundamental advection-dispersion equation describes the phenomenon of dispersion

$$\frac{\partial C}{\partial t} + \frac{\partial (u_i C)}{\partial x_i} = D\,\frac{\partial^2 C}{\partial x_i^2}\,, \qquad (1)$$

where C is the concentration of pollutant, u_i-transverse flow velocity, t-time, x_i - direction, D - diffusion coeficient.

For incompressible fluids, equation (1) has the form

$$\frac{\partial C}{\partial t} + u_i\,\frac{\partial C}{\partial x_i} = D\,\frac{\partial^2 C}{\partial x_i^2}. \qquad (1')$$

The dimensional number Peclet determines the relation between the parameters *t, D* and u .

$$Pe = \frac{D}{u^2 t}\,. \qquad (2)$$

For some sectors, L=ut, where *L* is a characteristic length. In this case, the relation (2) becomes

$$Pe = \frac{D}{uL}\,. \qquad (3)$$

For Pe>>1 the diffusion processes dominate, but forPe<<1 - the advection processes.

Taking into account the turbulent flow mechanism, in 1894 Reynolds proposed to decompose the instantaneous values of all hydrodynamic quantities that characterize this flow as the sum of the mediated and fluctuating components. In this case, we can limit ourselves to studying the median values, which relatively easily vary in time and space and often present the greatest interest in practice. Based on the above, Reynolds proposed to introduce: t_1- the integral time scale, which represents the

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time frame in which random velocity begins to occur, u_1- the full scale for speed, l_1 -the integral length scale.

For example, the Reynolds decomposition of the turbulent flow concentration is

$$C(x_i, t) = \overline{C(x_i)} + C'(x_i, t), \quad (4)$$

where $C(x_i)$ is the mean concentration; $C'(x_i, t)$ -fluctuation concentration.

The turbulent component has been described as a rapid mixing form, analogous to the molecular diffusion process. Taylor (1921) and Rutherford (1944), Fischer et al (1979), further developed this approach [10].

Taking into account the modifications proposed by Reynolds, by making the corresponding modifications, the fundamental advection-dispersion equation (1) takes the form:

$$\frac{\partial C}{\partial t} + u_i \frac{\partial C}{\partial x_i} = \frac{\partial}{\partial x_i}\left(D_t \frac{\partial C}{\partial x_i}\right) + \frac{\partial}{\partial x_i}\left(D_m \frac{\partial C}{\partial x_i}\right) \quad (5)$$

where χ_i is the direction in which the mass of the fluid is transported in an average time; Dt = $\frac{(\Delta x)^2}{\Delta t} = u_I l_I$ - turbulent diffusion coefficient; D_m - molecular diffusion coefficient.

To determine the magnitude of the turbulence coefficients, it is necessary to determine the dependence of these coefficients on the spatial sizes in which the turbulence occurs. An important property of the three-dimensional turbulence is that the spatial dimension limit large vortices. In river-type systems, the limitation refers to depth. The turbulent properties do not depend on width, but depend on depth,

$$D_t = u_* h, \quad (6)$$

where h is the depth; $u_* = \sqrt{\tau_0/\rho}$ - friction velocity; τ_o - the tangential medium stress on the wall; ρ -the density.

Because the speed is different vertically and transversely, the coefficient D_t is not isotropic in all directions.

Vertical turbulent diffusion coefficients are determined as follows [11, 12]:

$$D_{t,z} = 0.067 h u^*. \quad (7)$$

Transversal diffusion coefficients have been obtained from numerous experiments. It was found

$$D_{t,y} = \alpha h u_*, \quad (8)$$

where the coefficient α=0.6 after Fischer, (1979); after Elder, (1959), α=0.62.

The longitudinal dispersion coefficient reflects the combined effects of turbulent, molecular diffusion and differential convection. It can be determined experimentally or empirically. According to Taylor and Elder,

$$D_L = 5.93 h u_*, \quad (9)$$

According to Fischer et al. (1979),

$$D_L = 0.011 \frac{V^2 B^2}{h u_*}. \quad (10)$$

where *B* is the width of the bed, and V - average velocity in the cross section.

Case study - determination of turbulent diffusion coefficients for some sectors of the Prute River

A survey on the water quality in the Prut River for 4 sectors (Criva, Valea Mare, Leova and Giurgiulesti) was carried out for the period 2011 - 2017.

Based on the analysis of the water quality parameters samples taken by the Environmental Quality Monitoring Division of the State Hydrometeorological Service, it was found that the most frequent exceedings of the Maximum Acceptable Concentrations (MACs) in the studied sectors are for petroleum products, nitrites, phenols and ammonium ions. The sources of pollution of the river are domestic and industrial wastewaters, which are not treated or insufficiently treated, the storage of industrial and domestic waste, fueling stations, petrochemical factories. The nitrites reach the river from farmland after heavy rains [13, 14]. The most frequently encountered pollutants in all studied sectors are the petroleum products, the MACs being 0.05 mg (Figures 1 - 4).

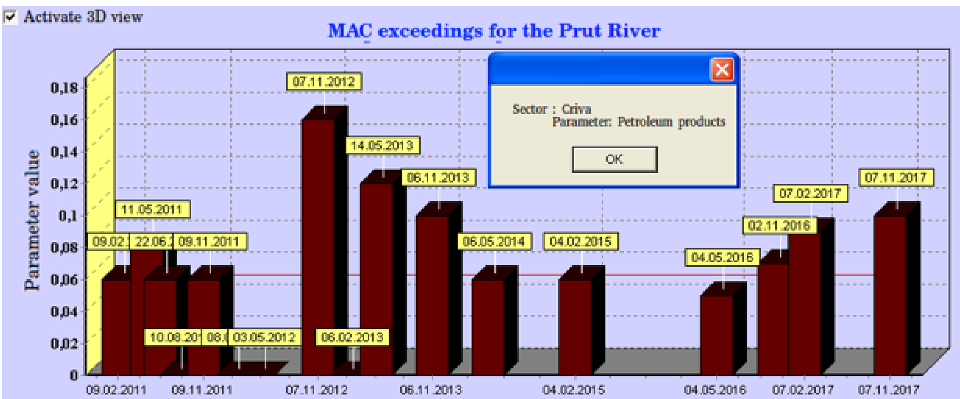

Fig. 1. MAC exceedings for the Prut River, the Criva sector

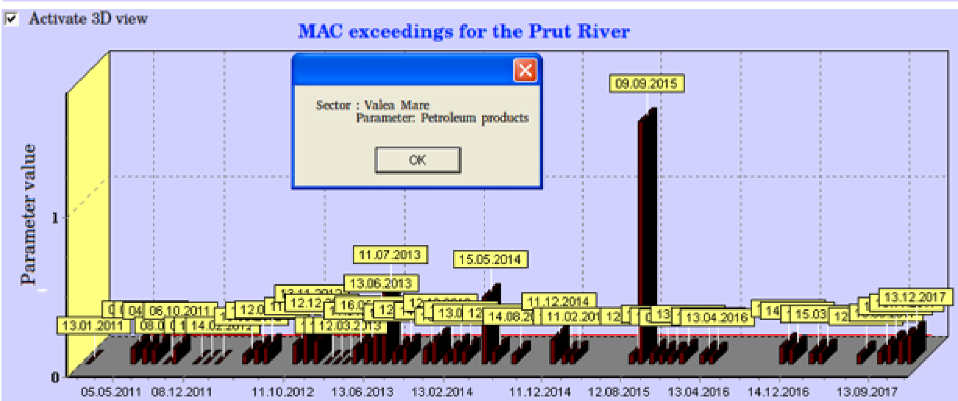

Fig.2. MAC exceedings for the Prut River, the Valea Mare sector

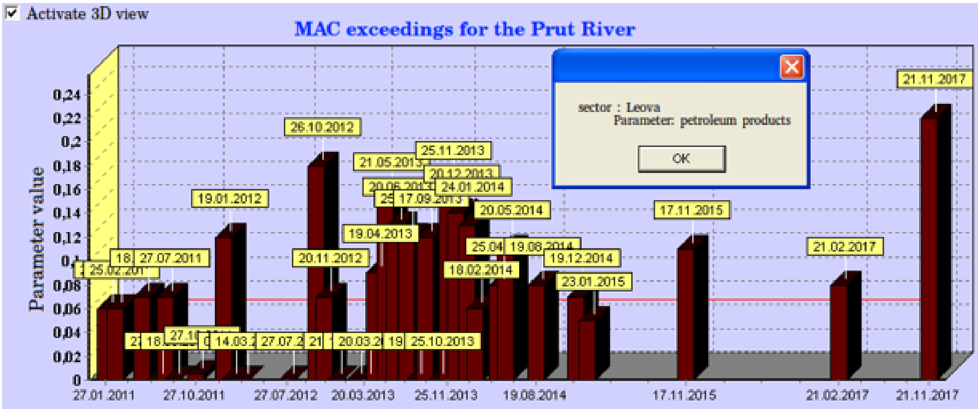

Fig. 3. MAC exceedings for the Prut River, the Leova sector

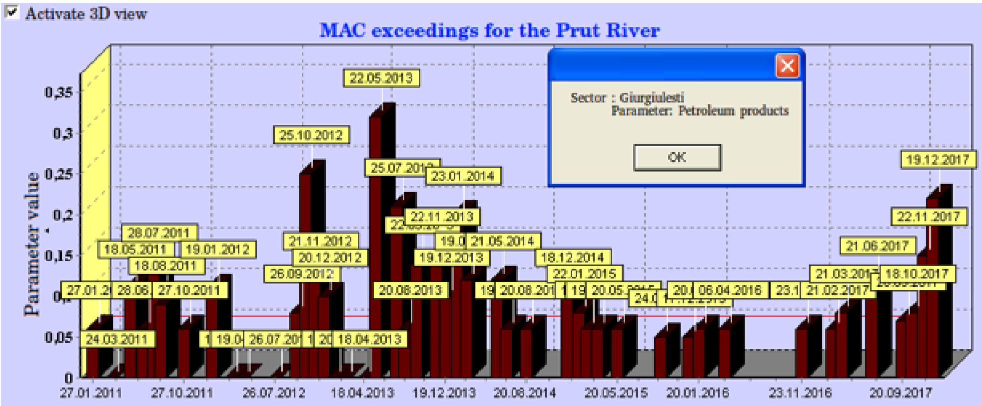

Fig. 4. MAC exceedings for the Prut River, the Giurgiulesti sector

Considering that the most frequently encountered pollutant in all studied sectors is petroleum products, the numerical modeling was carried out for the mentioned pollutant.

In order to obtain the numerical models for determining the pollutant concentration field, some scenarios have been chosen regarding the exceedings of the CMA of petroleum products.

In order to solve the proposed problem, the Surface-Water Modeling System (SMS) was used [15]. Each studied sector of the Prut River was discretized directly in the SMS system in finite elements and was divided into three specific areas: the left bank, the right bank and the middle of the river. For example, from the picture shown in Figure 5 one can see the discretization of the Prut river, the Criva sector:

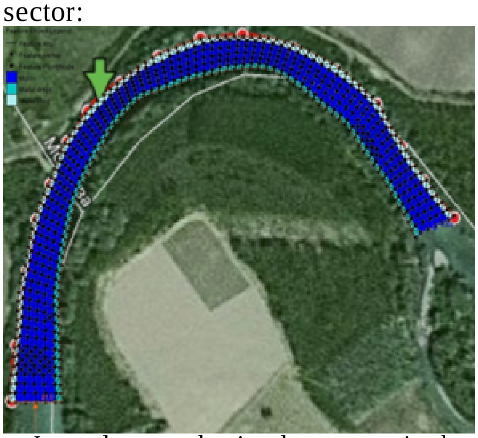

Fig. 5. Calculation network for the Prut River, the Criva sector

In order to obtain the numerical models for the determination of transport and dispersion of pollutants, the RMA4 program in the SMS system was used. Depending on the input data for this program, the results obtained with the RMA2 program in SMS were used.

To describe the phenomenon of the pollutant dispersion, the fundamental advection-dispersion equation was used:

$$h\left(\frac{\partial c}{\partial t}+u\frac{\partial c}{\partial x}+v\frac{\partial c}{\partial y}-\frac{\partial}{\partial x}D_x\frac{\partial c}{\partial x}-\frac{\partial}{\partial y}D_y\frac{\partial c}{\partial y}-\sigma+kc+\frac{R(c)}{h}\right)=0, \quad (11)$$

where c is pollutant concentration (mg/L); D_x and D_y - coefficients of turbulent diffusion in the x and y directions; *k* - the degradation constant (s^{-1}); σ -local source of pollutant term (unit of measure of concentration/s); h-water depth (m); R(c) - precipitation/evaporation (unit of measure of concentration x m/s). The first term of the equation means the local variation of the concentration; the second is the advective term in the direction x; the third - advective term in the direction y; the fourth - the term of dispersion in the direction x; the fifth - the term of dispersion in the direction y; the sixth term means the local source of pollutant; the seventh term shapes the exponential degradation of the pollutant; the last, the eighth term, takes into account the effect of precipitation/evaporation [16].

Turbulent diffusion coefficients, D_x in x and D_y in y directions can be measured experimentally, but because the cross section of the stream is seldom uniform in depth, this measurement is often complicated. In river-type systems, these coefficients can be determined using the empirical formula (9),

$$D_x = 5.93hu_*. \quad (12)$$

The D_y coefficient can be determined using the formula (8),

$$D_y = \alpha hu_*, \quad (13)$$

where α is a coefficient (after Fischer, 1979, α= 0.6; after Elder, 1959, α = 0.2) [17]. Unlike works that typically use formulas (12) and (13), this paper proposes other formulas for D_x and D_y depending on the *Pe* number.

In some numerical simulation systems, two direct methods are used to determine the respective coefficients, where each element receives the respective values of these coefficients, or automatic, using the Peclet number (the recommended values are between 15 and 40):

$$Pe = \frac{\rho U d}{D}, \quad (14)$$

where ρ -water density (kg/m^3); $U = \sqrt{u^2 + v^2}$ is the average resultant velocity (m/s), d - the length element in the flow direction (m); D - the turbulent diffusion coefficient (m^2/s).

The coefficient of turbulent diffusion in the *x*, direction, proceeding from (14) can be calculated as follows:

$$D_x = \frac{\rho U d_x}{Pe} \qquad (15)$$

in the *y* direction:

$$D_y = \frac{\rho U d_y}{Pe} \qquad (16)$$

The simulations were performed in a dynamic mode. Figure 6 shows the evolution of the pollutant concentration after 3.30 hours.

It is observed that after 3 hours and 30 minutes from the moment of confluence with water the concentration of pollutant has decreased.

The numerical models obtained were calibrated and validated. The calibration was performed by the variation of turbulent diffusion coefficients D_x and D_y, which were calculated in two ways:

-according to empirical formulas (12), (13);

-based on Peclet number (15), (16).

For each studied sector, the coefficients for the left bank, the right bank and the middle of the river were calculated. It has been found that the variant using the Peclet number is better because it allows the variation of the local turbulent diffusion properties according to the variable speed field, as compared to the use of empirical formulas that have been developed based on samples taken from several rivers with different water flow parameters.

In connection with the complexity, not all models can be applied to a particular river because of physico-chemical phenomena occurring in rivers and there are differences even between applying models to the same river segment.

The Peclet number was calculated for each specific area of the sector: the left bank, the right bank and the middle of the river. By performing many simulations, the optimal values of the coefficients D_x and D_y were

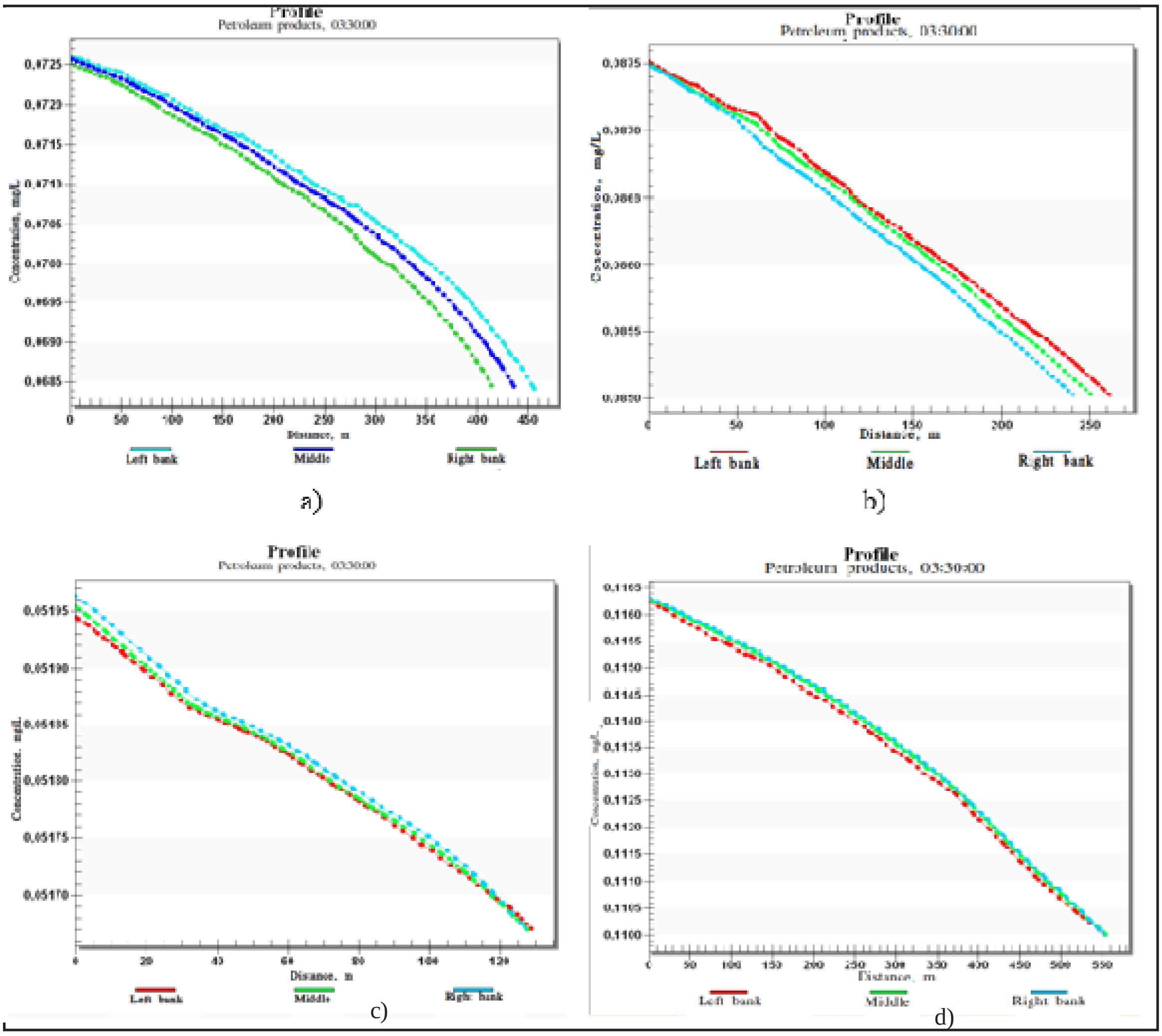

Fig. 6. The concentrations field after 3.30 hours: a) Criva, b) Valea Mare, c) Leova and d) Giurgiulesti

Table 1

TURBULENT DIFFUSION COEFFICIENTS D_x AND D_y

	Criva (Pe = 15)			Valea Mare (Pe = 30)			Leova (Pe = 35)			Giurgiulești (Pe = 25)		
	Left bank	Right bank	Middle	Left bank	Right bank	Middle	Left bank	Right bank	Middle	Left bank	Right bank	Middle
D_x	0.48	0.49	0.48	0.29	0.29	0.28	0.52	0.51	0.53	0.23	0.21	0.20
D_y	1.60	1.80	1.70	1.00	1.20	1.10	1.10	1.00	1.20	0.73	0.72	0.71

Sector of the Prut River	Criva, mg/L	Valea Mare, mg/L	Leova, mg/L	Giurgiulești, mg/L
Measured data	0.080	0.100	0.060	0.130
Calculated data	0.075	0.090	0.056	0.125
Measured data used for calibration	0.160	0.200	0.180	0.120
Calculated data	0.158	0.194	0.178	0.118
Measured data used for validation	0.120	0.260	0.150	0.320
Calculated data	0.119	0.255	0.147	0.318

Table 2
COMPARISON OF MEASURED AND CALCULATED DATA

determined according to the Peclet number, which differs from one sector to another (Table 1).

For the calibration, the same calculation network used for modeling was used, with the same size and roughness. Following the above-mentioned process and performing numerous numerical simulations, the coefficients D_x and D_y D_y.

The comparison of the obtained results concerning the concentration of the petroleum products showed a good correlation between the calculated data and the measured values in the field (Table 2).

Conclusions

A study was conducted concerning the turbulence influence on the evolution of the pollutant concentration field. It has been found that turbulence influence on this phenomenon is taken into account by turbulent diffusion coefficients.

Numerical models for 4 sectors of the Prut River were determined in order to determine the evolution of the pollutant concentration field. The numerical models were calibrated by varying the turbulent diffusion coefficients D_x and D_y.

The calculation of the mentioned coefficients was done by two methods: by a standard method according to the empirical formulas, and a second method proposed in the present paper - by calculating the Peclet number for each specific area of the studied sector: the left bank, the right bank and the middle of the river. It is considered that the second method is more indicated, the errors of the calibrated models based on the Peclet number being smaller, compared to the errors of the calibrated models according to the empirical formulas.

The proposed method concerning calibrating numerical models for simulating the concentration of pollutants over time and space allows the determination of the water quality and the prediction of exceptional water pollution situations with greater accuracy.

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