An efficient double order solution of the groundwater contaminant transport problem

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ABSTRACT: The solution of the 1D contaminant transport problem for steady-state flow fields is attained by de-coupling the transport equation in one convective and in one dispersive component. The convective component is solved by a new numerical methodology: moving from the upstream to the downstream elements, the concentration in each element is analytically computed along the time step assuming a spatial zero-order approximation. The average leaving flux is then assigned as entering flux, constant along the time step, at the next downstream element. The global mass conservation is guaranteed and the unconditional stability is proved using Fourier analysis. To reduce the numerical diffusion each element is divided, for the solution of only the convective transport component, in several subelements. The total number of subelements remains constant and each element is fractioned according to the norm of the concentration gradients and to the concentration value.
The dispersive component can be solved by assuming a first order approximation of the previously estimated concentrations and by locating the nodes at the center of each element. The final results are compared with the analytical solutions in well-known bench mark cases.

1 DOUBLE ORDER SOLUTION FOR THE TRANSPORT EQUATION

In diffusion simulation of passive contaminant, the advection-diffusion equation on the mass transport is solved by using calculated results of flow field. The 1D groundwater contaminant transport equation is given by:

$$\frac{\partial c}{\partial t} + U\frac{\partial c}{\partial x} = D\frac{\partial^2 c}{\partial x^2} \qquad (1)$$

where c=concentration of contaminant; U=the velocity component along x; D=diffusion coefficient in x direction. The numerically solution of (1) can be found by splitting the original equation in two components (Komatsu et al. 1997); the first omponent corresponding to D=0, called convective, is described by

$$\frac{\partial c}{\partial t} + U\frac{\partial c}{\partial x} = 0 \qquad (2)$$

and the second component corresponding to U=0, called dispersive, is also described by

$$\frac{\partial c}{\partial t} = D\frac{\partial^2 c}{\partial x^2} \qquad (2)$$

This splitting approach no has physical explanation, but permit to choose the most appropriate scheme for each transport process. The numerical discretization of the equations (1) and (2) is:

$$\frac{c^{n+1/2} - c^n}{\Delta t} + U\left(\frac{\partial c}{\partial x}\right)^{n+1/2} = 0 \qquad (3)$$

$$\frac{c^{n+1} - c^{n+1/2}}{\Delta t} = \left(D\frac{\partial^2 c}{\partial x^2}\right)^{n+1} \qquad (4)$$

where $(.)^n$ is the finite difference approximation of the argument estimated at time level n. The equations (3) and (4) can be solved sequentially respectively from level time time t to time $t + \Delta t/2$ and from time $t + \Delta t/2$ to time $t + \Delta t$.
The solution of the convective component presents several difficulties (Venezian 1984), especially in 2D problems. Methods like up-stream FEM can be used (Gross et al. 1999), but strongly oscillations occur near the zones with high gradients: the method

displays numerical dispersion. To overcame this problem it is possible to use refined elements using Hermite polynomials (Lapidus & Pinder 1982) or Lagrangian-Eulerian approachs (Yeh 1990) or improved FEM (Yu & Singh 1995), but several computational inconvenients occur. In the following, a new methodology for the solution of the advective equation is presented. The methodology has the following merits:

1) It is unconditionally stable and guarantees global mass conservation;
2) It is simple to apply, because is an explicit method and it should be easily extensible to 2D and 3D problems;
3) Never estimates negative concentrations.

The proposed methodology assumes a constant value of the concentration inside each element. After the solution of the convective component, the dispersive one is solved using a standard finite difference method. The method computes fluxes assuming in space a first order approximation of the concentration. For this reason we say that a double order approximation is used. Observe that, if nodes are located at the center of the elements, the change of the approximation order affects the fluxes between elements, but not the global mass conservation. This also implies that a fully implict approximation of the second order derivatives has to be used.

2 THE PROPOSED METHODOLOGY FOR THE CONVECTIVE EQUATION

2.1 *Introduction*

Assume a steady-state flow field. The 1D convective transport equation is:

$$\frac{\partial c}{\partial t} + U\frac{\partial c}{\partial x} = 0 \tag{5}$$

During an infinitesimal time interval dt the entering mass is $F_k^e(t)dt$ and the leaving mass is $Qc_k(t)dt$, where $F_k^e(t)$ is the entering flux in the *k*-th element, $c_k(t)$ the concentration value and Q the flow rate. Mass conservation provides:

$$F_k^e(t)\,dt - Q\,c_k(t)\,dt = w\,dc_k \tag{6}$$

in which w=Adx is the volume of each element, with section area A. Dividing by dt, the governing equation for the *k*-th element is

$$\frac{dc_k}{dt} = \frac{F_k^e(t)}{w} - \frac{Q}{w}c_k(t) \tag{7}$$

with the initial condition $c_k(t=t_0)=c_k^*$. If we assume $F_k^e(t)= F_k^e$ to be constant in time, the Cauchy problem has easy solution , that is

$$c_k(t) = \frac{F_k^e}{Q} + \left[c_k^* - \frac{F_k^e}{Q}\right] e^{-\frac{Q}{w}(t-t_0)} \tag{8}$$

A mixed analytical-numerical solution can be found by solving sequentially equation (6) from the upstream elements to the downstream elements. Fixed a finite time and space step, call t the known time level. The concentration value at time t+Δt is evaluated by (6), that is:

$$c_k(t+\Delta t) = \frac{F_k^{e(t,t+\Delta t)}}{Q} + \left[c_k(t) - \frac{F_k^{e(t,t+\Delta t)}}{Q}\right] e^{-\frac{Q}{w}\Delta t} \tag{9}$$

where $F_k^{e(t+\Delta t)}$ is the average contaminant flux entering in the *k*-th cell between t and t+Δt. The average flux entering in the next cell during Δt can be found through the mass balance, that is:

$$F_{k+1}^{e\ (t,t+\Delta t)} = \frac{F_k^{e(t,t+\Delta t)}\Delta t - w\left[c_k(t+\Delta t) - c_k(t)\right]}{\Delta t}. \tag{10}$$

Evaluated the entering flux in element *k+1*, it's possible to sequentially apply equations (7) and (9) to all the remaining downstream elements. To formulate the algorithm we set t=n Δt, x=k Δx and

$$c_k^n = c(x,t) \qquad\qquad f_k^n = \frac{F_k^{e(t,t+\Delta t)}}{Q} \tag{11}$$

equations (9) and (10) become:

$$\begin{cases} c_k^n = f_k^n\left(1 - e^{-c_{ou}}\right) + c_k^{n-1}e^{-c_{ou}} \\ f_{k+1}^n = f_k^n - \dfrac{1}{c_{ou}}\left(c_k^n - c_k^{n-1}\right) \end{cases} \tag{12}$$

where $c_{ou}=Q\Delta t/w$ is the Courant number.

2.2 *Fourier analysis*

System (12) is linear and can be studied through the Fourier analysis (Shapiro & Pinder 1981; Bentley et al. 1990). Due to linearity, we can limit the stability analysis to a single armonic component.
We try to find the solution of system (12) assuming

$$\begin{cases} c_k^n = c_o e^{i\alpha k \Delta x} \rho^n \\ f_k^n = f_o e^{i\alpha k \Delta x} \rho^n \end{cases} \tag{13}$$

in which $\alpha=2\pi/L$ is the wave spatial frequency, L is the domain extension and ρ is a complex unknown number. Substitution in (11) provides the following algebraic system, with unknown coefficients c_o, f_o:

$$\begin{cases} c_o(\rho - e^{-c_{ou}}) + f_o \rho (e^{-c_{ou}} - 1) = 0 \\ c_o \dfrac{1}{c_{ou}}(\rho - 1) + f_o \rho (e^{i\alpha \Delta x} - 1) = 0 \end{cases} \tag{14}$$

System (14) has non-zero solutions only if its determinant is zero, that is:

$$\begin{vmatrix} \rho - e^{-c_{ou}} & \rho\left(e^{-c_{ou}} - 1\right) \\ \dfrac{1}{c_{ou}}(\rho - 1) & \rho\left(e^{i\alpha \Delta x} - 1\right) \end{vmatrix} = 0 \tag{15}$$

Equation (15) has only one non zero solution for the unknown ρ:

$$\rho_1 = 1 + \frac{(e^{-c_{ou}} - 1)(e^{i\alpha \Delta x} - 1)}{e^{i\alpha \Delta x} - 1 - \dfrac{e^{-c_{ou}} - 1}{c_{ou}}} \tag{16}$$

The first of equations (13) becomes:

$$c_k^n = c_o e^{i\alpha k \Delta x} {\rho_1}^n \tag{17}$$

We now compare this numerical solution with the analytical solution of the convective problem for armonic initial condition

$$c(x,t) = c_o e^{i\alpha(x - Ut)} \tag{18}$$

For $x=k\,\Delta x$ and $t=n\,\Delta t$ we obtain

$$\tilde{c}_k^n = c(k\Delta x, n\Delta t) = c_o e^{i\alpha k \Delta x} (e^{-i\alpha c_{ou} \Delta x})^n \tag{19}$$

it is easy to demonstrate that

$$c_k^n / \tilde{c}_k^n \to 1 \quad \text{if} \quad c_{ou} \to 0\,. \tag{20}$$

This implies that the algorithm is consistent when Δt goes to zero faster than Δx. Call T the time required for an armonic component with frequency α to pass its wavelength and $N=T/\Delta t = 2\pi/(\alpha\, c_{ou}\, \Delta x)$. Define the parameter ξ as

$$\xi = c(x, t+T)/c(x,t) \tag{21}$$

for the analytical solution (18), ξ is equal to:

$$\xi_{ex} = \tilde{c}_k^{n+N} / \tilde{c}_k^n = e^{-i\,2\pi} \tag{22}$$

and for the numerical solution (18) ξ is equal to:

$$\xi_{ap} = c_k^{n+N} / c_k^n = \lambda e^{i\omega} \tag{23}$$

where

$$\lambda = \left(u^2 + w^2\right)^{\frac{\pi}{\alpha c_{ou} \Delta x}} \qquad \omega = 2\pi \frac{\operatorname{arctg}(w/u)}{\alpha\, c_{ou}\, \Delta x} \tag{24}$$

with

$$\begin{cases} u = 1 + \left(2 + \dfrac{e^{-c_{ou}} - 1}{c_{ou}}\right)\left[1 - \cos(\alpha \Delta x)\right] f(c_{ou}) \\ w = -\dfrac{e^{-c_{ou}} - 1}{c_{ou}} \operatorname{sen}(\alpha \Delta x)\, f(c_{ou}) \end{cases} \tag{25}$$

where $f(c_{ou})$ is a function defined as (26):

$$f(c_{ou}) = \left(e^{-c_{ou}} - 1\right) \Big/ \left\{ \left[\cos(\alpha \Delta x) - 1 - \frac{e^{-c_{ou}} - 1}{c_{ou}} \right]^2 + \operatorname{sen}^2(\alpha \Delta x) \right\}$$

For stability analysis, the modules ratio and the phase difference between ξ_{ap} and ξ_{ex} are important. The first one is λ and the second one is $\omega+2\pi$. The functions $\lambda(\alpha\Delta x = 2\pi/s)$ and $\omega(\alpha\Delta x = 2\pi/s) + 2\pi$ for $c_{ou}=1.2$ and $c_{ou}=0.1$ are plotted in figures 1-2.

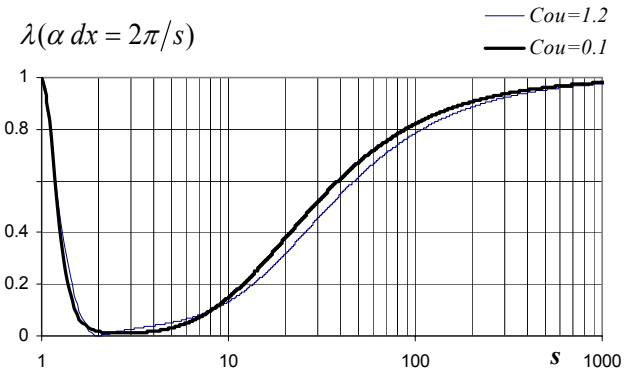

Figure 1.Graph of the modules ratio of ξ_{ap} and ξ_{ex} for $c_{ou}=1.2$ and $c_{ou}=0.1$.

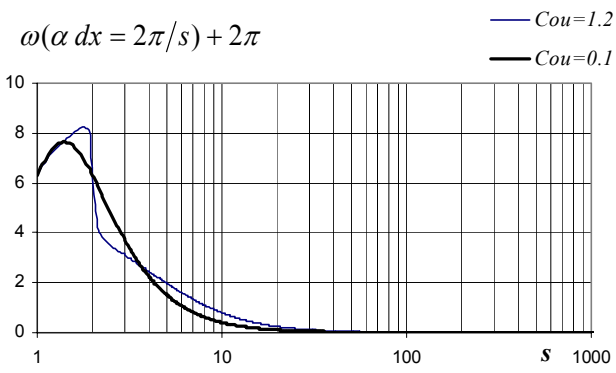

Figure 2.Graph of the phase difference of ξ_{ap} and ξ_{ex} for c_{ou}=1.2 and c_{ou}=0.1.

From figure 1 it can be observed that the method is unconditionally stable: the amplitude of the numerical armonic wave λ is always smaller than one, even if diffusion grows along with the Courant number. From figure 2 it can also be observed that the waves with highest frequency are not in phase with the analytical solution, but dispersion does not occur because the amplitude of these waves is strongly diffused.

2.3 *Breaking up the elements into a fixed total number of subelements*

In the previous section we have shown that the proposed methodology is unconditionally stable, simple and robust, not dispersive. By the Fourier analysis we have observed that for large courant numbers numerical diffusion occurs, especially in cases of strong concentration gradients. To improve the accuracy of the method we proceed with the break up of the elements with stronger concentration gradients. Because the method is basically explicit, in the sense that the computation proceeds one element after the other, the number of subelements can be changed according to the diffusion expected in each element and to the total number of subelements available for the computations. To estimate the expected diffusion in each element, the concentrations at time level n+1/2 are solved twice; a first time without division, a second one using the subelements division estimated with the result of the first iteration. Call $\underline{c}_k^{n+1/2}$ the concentration computed at the first time in a generic element.
The numerical diffusion will be larger in the elements where the concentration $\underline{c}_k^{n+1/2}$ is very different from both the initial value c_k^n and the asymptotic one cm_k^n obtained in (8) using an infinite time step. This is because the concentration, assumed constant in space due to the zero-order approximation, attains in the analytical solution both values, the first at the downstream end, the second at the upstream end of the element. An empirical way to weight the potential diffusion in each element is given by the following formula, that also takes into account the need of using a larger number of subelements in areas with higher concentrations:

$$Dis_k^{n+1} = \sqrt{\min\left(\left|\underline{c}_k^{n+1} - cm_k^n\right|, \left|\underline{c}_k^{n+1} - c_k^n\right|\right) c_k^n} \qquad (27)$$

To use a total fixed number of subelements, a density proportional to the above index could be reached by setting:

$$Nel_k^{n+1} = Int\left(\frac{Dis_k^{n+1}}{\sum_j Dis_j^{n+1}} Nel\right) \qquad (28)$$

where Nel = total number of available subelements, $Nel_k^{n+1/2}$ = number of subelements obtained from element *k*-th and Int = integer part of the argument. It is more convenient, to easily reduce or amplify the number of subelements in each element, to reduce the left hand side of (28) up to (29):

$$Nel_k^{n+1} = \max_j 2^j \text{ subject to } Nel_k^{n+1} \le Int\left(\frac{Dis_k^{n+1}}{\Sigma_j Dis_j^{n+1}} Nel\right)$$

The choice of (29) allows to easily assign the concentrations of the subelements defined at time level n at the new subelements defined at time level n+1/2. This can be done by averaging the concentrations of subelements close to each other if $Nel_k^{n+1/2} < Nel_k^n$ and by assigning the same concentration to different subelements if $Nel_k^{n+1/2} > Nel_k^n$.
The new Courant number of the subelements will be much larger of the original one and this can limit the reduction of the numerical diffusion. It is then convenient to reduce, along with the spatial step, also the time step. The next results have been obtained using for the time step the same division of the spatial one.

3 APPLICATION TO SOME BENCH MARK CASES

We simulate the transport of gaussian concentration hill in a one-dimensional uniform flow, (YEH, 1990). Different numerical solutions have been computed, each one with a different number of total subelements *Nel* in (28). The governing equation (1), with upstream and downstream boundary conditions c=0 and initial condition given by:

$$c(x, t = 0) = e^{-(x - x_0)^2 / 2\sigma_0^2} \qquad (30)$$

has analytical solution

$$c(x,t) = \frac{\sigma_0}{\sqrt{\sigma_0^2 + 2Dt}} e^{-\frac{1}{2}\frac{(x-x_0-Ut)^2}{\sigma_0^2+2Dt}} \qquad (31)$$

The examples velocity, spatial and temporal step are equal to U=0.5 m/s, Δx=200 m, Δt=96 s (c_{ou}=0.24). 65 elements have been used and the total number of time steps is 100. Tests are provided for D=0 m^2/s (*case*1), for D=2 m^2/s (*case*2), D=50 m^2/s (*case*3). Observe, in Figure 3, the results obtained for *case*1 using values 435 and 1435 for the *Nel* parameter. The limitation of the pick reduction is, of course, less than proportional to the *Nel* parameter. Observe the improved accuracy with respect to the results of the up-stream FEM.

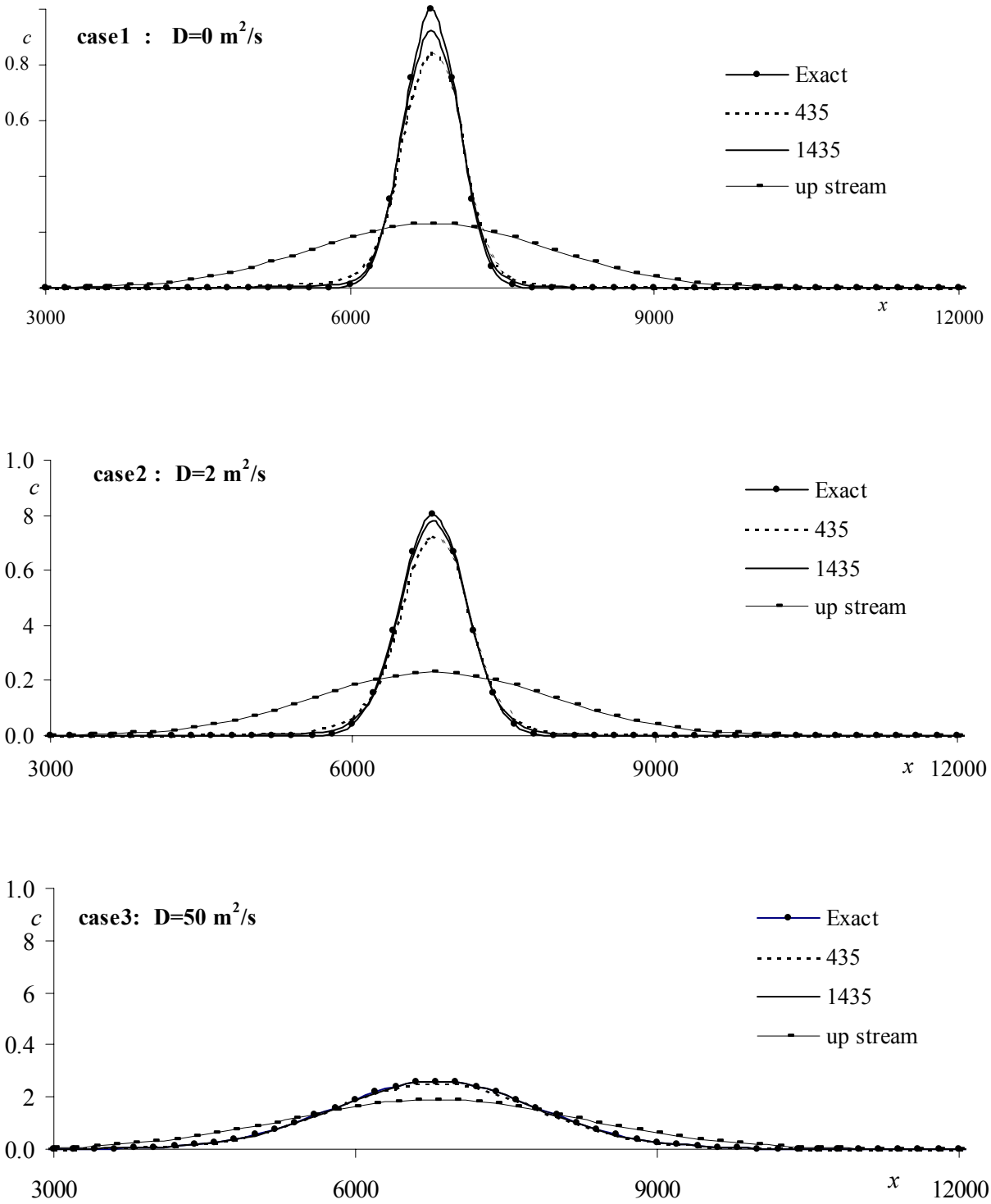

Figure 3. Examples of simulation.

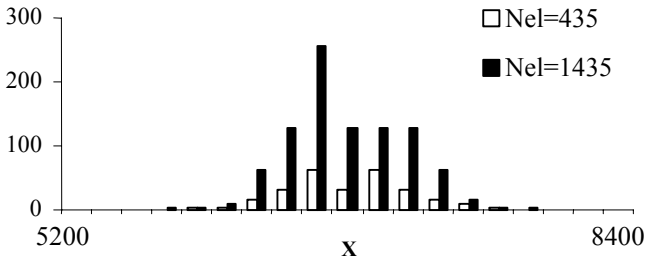

Figure 4. *Case*1: The subelement distribution for 5200<x<8400 (in this zone of domain there are all the elements broken)

Also you can observe the results obtained for the *case*2 and the *case*3. It can be observed that the accuracy of the results increases along with the dispersion, because a compensation of the numerical dispersion obtained in the solution of the convective part of the problem is obtained in the solution of the dispersive part. Finally you can observe, in figure 4, the distribution of the subelements at the final computational time for *case*1. Note that the maximum number of subelements is reached, in the case of *Nel* = 435, in only part of the concentration peak. This is because the numerical diffusion has already caused, in this case, a flat area of high concentration.

CONCLUSIONS

A new algorithm for the solution of the convective component of the groundwater transport equations has been proposed. The algorithm is unconditionally stable, guarantees global mass conservation and does not require any backtracking. The numerical diffusion associated with the solution is treated by dividing each element in several subelements. The number of subelements changes, for each element and for each time step, according to the location of the larger gradients and to the total number of available subelements. The application of the algorithm to 2D and 3D cases should be facilitated by the explicit nature of the algorithm and by its semplicity.

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