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Evolution of Conservative Tracer Plumes in Turbulent Flows: A Thermodynamic Description

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***Abstract*— Due to exponential growth of water contaminations, the understanding the formation and evolution of tracer plumes is of first importance in environmental practice, either to model or predict these events. However, not all involved mechanisms are clearly described in the state-of-the-art approaches. For this reason, the aim of this article is to review some key concepts about the origin and development of dispersion, especially from a thermodynamic point of view, which allows a compact and general treatment. The developed equations have the advantage of an easy and congruent application. Finally, it is presented an experimental case.**

***Index Terms*—Dispersive transport, Thermodynamics, Tracer theory.**

I. SUDDEN POURING OF A TRACER IN FLOW: A LE CHATELIER-BRAUN MECHANISM

A. *Basic concepts*

Since long time ago, it is well known the response mechanism of a chemical system to an external perturbation that breaks the equilibrium condition. This mechanism is named the Chatelier-Braun Principle. These two scientists observed in 1888 that the direction of reaction of the system may be predicted a simple way as follow [1][2].

"Any system in chemical equilibrium undergoes, as a result of a variation in one of the factors governing the equilibrium, a compensating change in a direction such that, had this change occurred alone it would have produced a variation of the factors considered in the opposite direction"

This general principle may be used as well in the case of pouring a tracer in flow, in order to discover the evolution features of the resulting plume Fig. 1. In this case, when a conservative solute is injected suddenly in water, the factor that is varied is the mass concentration of the tracer, and then the reaction should be in the opposite direction. If the first process is understood as an increase of concentration in a small region, then the response has to be described as a decreasing mechanism of that factor.

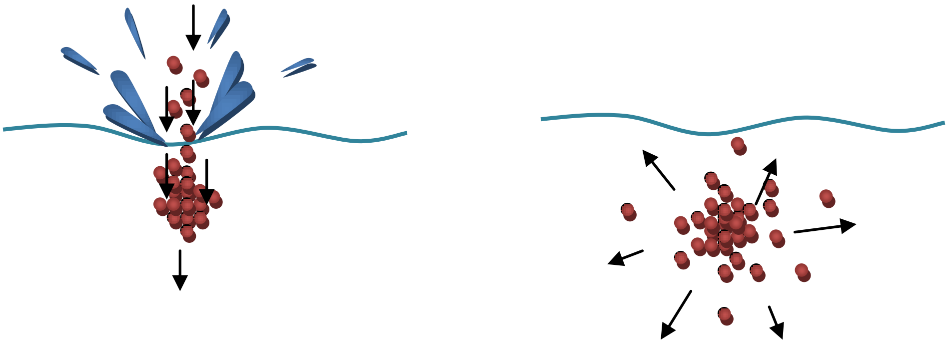

Fig. 1 Perturbation and response due to a tracer injection

This picture means that a *dynamic process* takes place following a sudden injection of tracer, which last until equilibrium is recovered in a finite time. This means that whatever would be the reaction mechanism, there will be a sort of *relaxation* process in which there is a "storage" phase and then an "energy liberation" phase. The difference is that in the case of tracers first phase corresponds to creation of repulsion forces in all control volume, and then the second phase is the mutual separation of particles. Repulsion forces coming from the so called "osmotic pressure" that pushes solute molecules in all directions. Separation effect leads to a *diminution* of this pressure with time. Fig.2.

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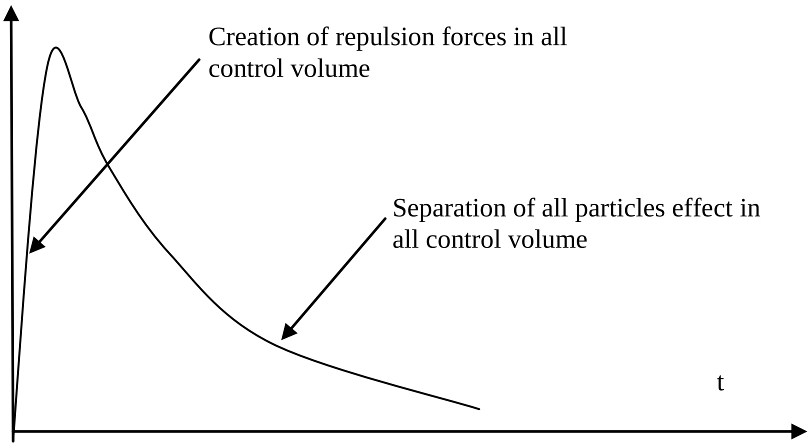

Fig. 2 Relaxation effect in case of sudden tracer injection

Separation phase as was discovered since long time ago [3], is guided by a Brownian pattern, i.e: the characteristic displacement, *Δ*, will grow proportionally to the square root of characteristic, corresponding time, τ. Here, the proportional coefficient in one dimension is the longitudinal transport coefficient, *E*.

$$\Delta = \sqrt{2E\tau} \tag{1}$$

This spreading effect named *dispersion* is mainly due to the shear nature of water in presence of a velocity field, generated by the advective mean velocity *U*. This second mechanism allows to vanishing the tracer motion in a finite time, when equilibrium is restored. Then, to measure the Chatelier-Braun effect when is poured a tracer in flow it is pertinent to define a "dispersion velocity" as follows.

$$V_{disp}(t,x) = \frac{\Delta}{\tau} = \sqrt{\frac{2E}{\tau}} \tag{2}$$

The way to measure either τ or *Δ* is on the Gaussian curve by means of "standard deviation", σ_t, refereed at inflection points of the curve. Fig.3.

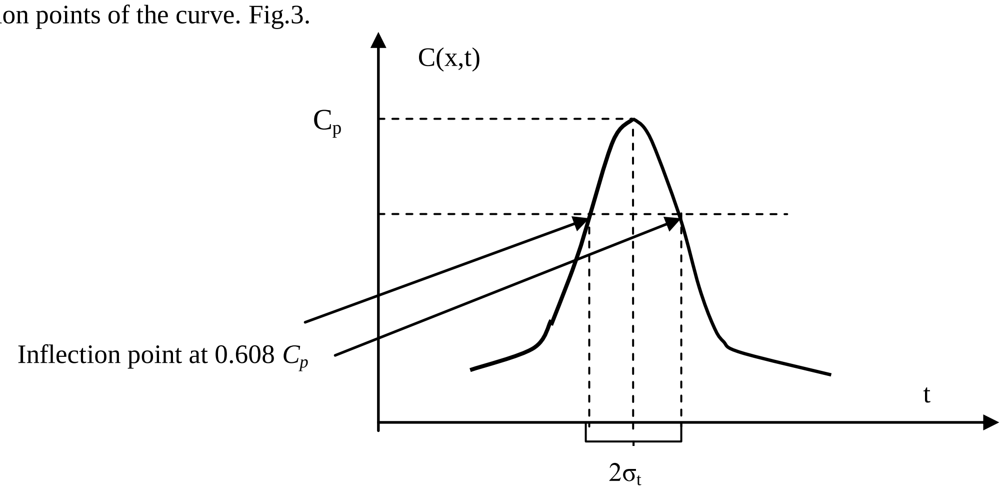

Fig. 3 Key points to make calculations

This curve for the case of dispersion in a flow is described by the Fick´s one-dimension, classical definition for concentration of tracer:

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$$C(x,t) = \frac{M}{A\sqrt{4\pi Et}} e^{-\frac{(X-U\,t)^2}{4E\,t}} \quad (3)$$

It is important to remark that the Gaussian curve is drawn as time function, but in (3) the standard deviation is in space

$$\sigma_X = \sqrt{2\,E\,t} \quad (4)$$

To find the proper standard deviation in time, σ_t, we have to operate this expression by the advective velocity, as follows:

$$\sigma_t = \frac{\sigma_X}{U} \quad (5)$$

But, this is not the only concern about this expression because t is not the same variable than τ, whereas t is the time of transport of flow (related with the peak motion) and τ is the special time that takes the dispersion to spread particles (related with the motion of inflection points) Fig.4.

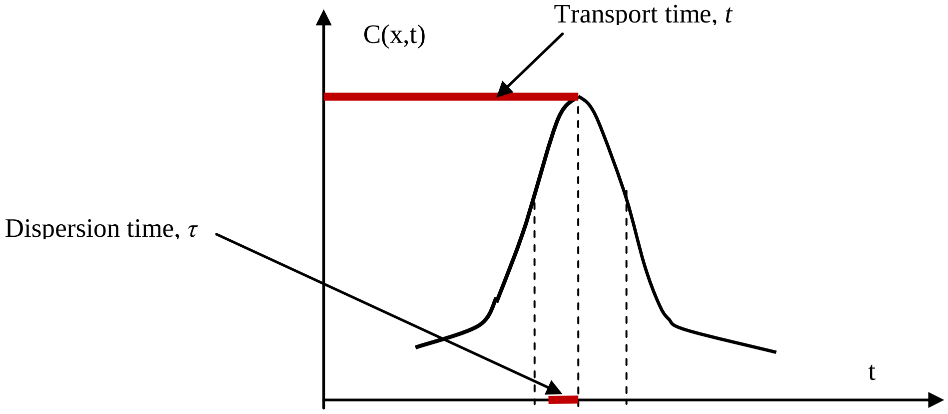

Fig. 4 Difference between *t* and *τ*

The way in which are related these two times is by means of Poisson´s distribution, because the motion of each tracer particle is Brownian itself (i.e: uncommon and pure random in nature) so the whole transport time, t, is the infinite addition of these discrete times, which by their nature are function of key time, τ: [4][5]. This limit is justified as long as there are a very large number of atoms in each molecule-gram of solute.

$$t = Lim_{n\to\infty}\tau(1 + a + \frac{a^2}{2!} + \frac{a^3}{3!} + ... + \frac{a^n}{n!}) \quad (6)$$

By the other hand, the mean value, of this distribution for the case of Brownian motion, $a\approx 1.54$, is well–known since the pioneering researches of T. Svedberg in early years of XX century [6][7][8].
Then:

$$t \approx Lim_{n\to\infty}\tau(1 + 1.54 + \frac{1.54^2}{2!} + \frac{1.54^3}{3!} + ... + \frac{1.54^n}{n!}) \approx 4.67\tau \quad (7)$$

This constant relationship is named as $1/\beta$:

$$\tau \approx \beta\, t \approx 0.2143\, t \quad (8)$$

Regarding this and (2) it is clear that once system has passed the initial perturbation of equilibrium, the dispersion velocity will vanish as time increase, as required by Le Chatelier-Braun principle. Finally, (4) and (5) hold like that:

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$$\sigma_X = \sqrt{2E\frac{\tau}{\beta}} = \frac{\Delta}{\sqrt{\beta}} \qquad (9)$$

$$\sigma_t = \frac{\sqrt{2E\frac{\tau}{\beta}}}{U} = \frac{\Delta}{U\sqrt{\beta}} \qquad (10)$$

B. Relationship between V_{disp} and U

It is possible to define a relationship between advective and dispersive motions (cause and effect) by means of a function ϕ:[9][10].

$$\phi = \frac{V_{disp}}{U} \qquad (11)$$

Using (2) it holds a new definition for mean advective velocity:

$$U = \frac{1}{\phi}\sqrt{\frac{2E}{\tau}} \qquad (12)$$

This equation has the same mathematical structure than Chezy´s equation for uniform flow regime. Here *C* is the Chezy´s resistance coefficient, *R* the hydraulic radius and *S* the friction slope.

$$U = C\sqrt{RS} \qquad (13)$$

C. A new Fick´s equation

If we clear *E* from (12), it holds:

$$E(t) = \frac{\phi(t)^2 U^2 \beta\, t}{2} \qquad (14)$$

This relationship has a great importance because, against current conception, the transport coefficient is a time function, allowing that several observers may describe the plume evolution congruently. Then a complete (and congruent) application of Galilean transformation in Fick´s definition (3) is as follows. *Q* is discharge as *U*A* [11].

$$C(X,t) = \frac{M}{Q\times\phi\times t\times\sqrt{2\pi\beta}}\, e^{-\frac{(X-U\,t)^2}{2\beta\phi^2 U^2 t^2}} \qquad (15)$$

The wrong application of classical relativity principle has leaded to a serious distortion of theoretical tracer curves that do not fit the experimental shape, especially about the asymmetry of tails. [12].
This equation (15) is useful to model correctly the experimental tracer curves, allowing checking the congruence of used data. Also, according with (2), (10) and (11), ϕ may be redefined as follows. Most right member accounts for time elapsed between the two inflection points in Gaussian curve, very useful for numerical computations.

$$\phi = \frac{\sigma_t\sqrt{\beta}}{\tau} = \frac{\sigma_t\sqrt{\beta}}{\beta\, t} = \frac{2\sigma_t}{2t\sqrt{\beta}} \qquad (16)$$

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II THERMODYNAMIC NATURE OF PROCESS

A. Irreversibility of considered process

Considering the evolution of a conservative tracer in a system isothermal and isobaric, as usual in the case of chemical systems, the irreversible nature of tracer "relaxation" leads to a generation of "internal" entropy (according Second principle of Thermodynamics) [13] which has to be ejected to environments, whereas the temperature in the system should be maintain constant as was stated. This fact implies that *simultaneously* than evolution of tracer plume, especially in the second phase of spreading of tracer particles, there is a transport of irreversible heat from the plume to its boundaries. Then we cannot speak of dispersion process without speak of heat production and transmission. Formally they are the same thing, because the dissipation of osmotic forces is converted *all* in ejected heat. Fig. 5

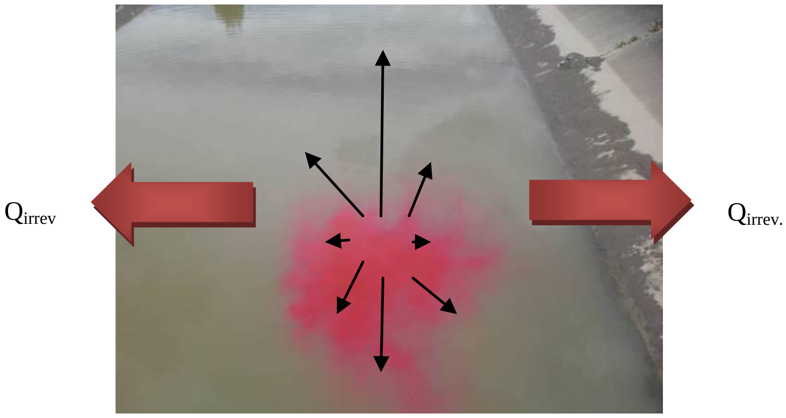

Fig 5. Dispersion and heat transmission as the same thing

B. Thermodynamic nature of ϕ function

If the process itself is thermodynamic in nature, the same thing may be stated for the function that guides its evolution, ϕ. Actually, if we define a linear partial differential expression for this variable as follows:

$$d\phi = \frac{\partial \phi}{\partial U} dU + \frac{\partial \phi}{\partial E} dE \qquad (17)$$

And applying definition (12)

$$\frac{\partial \phi}{\partial U} = -U^{-2}\sqrt{\frac{2E}{\tau}} \qquad (18)$$

$$\frac{\partial \phi}{\partial E} = E^{-\frac{1}{2}} \frac{\sqrt{\frac{2}{\tau}}}{2U} \qquad (19)$$

Then calculating crossed partial differentials:

$$\frac{\partial}{\partial E}\left(-U^{-2}\sqrt{\frac{2E}{\tau}}\right) = -U^{-2}E^{-1/2}\sqrt{\frac{1}{2\tau}} \qquad (20)$$

And:

$$\frac{\partial}{\partial U}\left(E^{-\frac{1}{2}}\frac{\sqrt{\frac{2}{\tau}}}{2U}\right) = -U^{-2}E^{-1/2}\sqrt{\frac{1}{2\tau}} \qquad (21)$$

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We have that (20) and (21) are identical. Hence, according with Schwartz´s criterion, equation (17) is a Pfaffian function which may be integrated as follow: [14].

$$\phi = \int_1^2 d\phi = \phi(U_2, E_2) - \phi(U_1, E_1) \qquad (22)$$

And in a closed trajectory, C:

$$\oint_C d\phi = 0 \qquad (23)$$

Then, ϕ is a state variable that does not depend on trajectory. By the other hand, the behavior of this function is similar than that of V_{diff}, in Fig. 2, assuming an approximate constant value for advective velocity. Fig.6

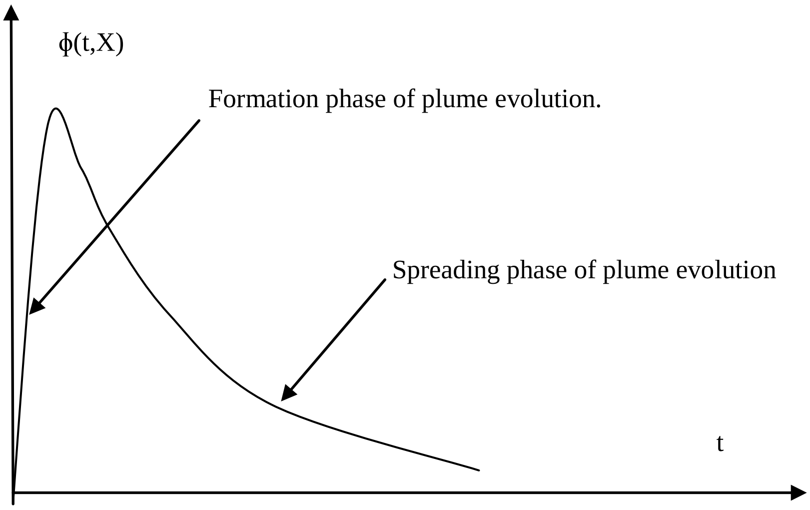

Fig. 6 Relaxation effect in case of sudden tracer injection

III EXPERIMENTAL APPLICATION OF THEORY

A. The used measurement tool

To apply the equations developed in this article, It will be used a hardware-software tool named “Inirida Deep Flow” (IDF) designed in Colombia. This tool allows measuring tracer evolution in a “real time” fashion, and then models theoretically the experimental curves. In next photos we can see the parts of the equipment: Left: conductivity probe, center: digital interface, and right. Hand computer, where is stored the special software. The conductivity probe has integrated a temperature sensor allowing compensation of experimental data. The software also converts conductivity in concentration of tracer. The use of this tool and the theory developed in this article allowing a set of calculations very easy, based all of them in a very straightforward time measurements, as will be shown in an experimental journey. Fig.7 (Authors ´files).

Conductivity probe **Interface** **Hand computer**

Fig. 7 IDF tool used for field measurements

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B. The measured stream

This is a small cannel in ground of about 105 liters/sec., and a width of *W= 1.0 m*, Named “Guaymaral” is located in Bogota, Colombia. Some pictures of the flow are presented in Fig. 8. (Authors ´files). It was done three pouring of ionic tracer, using 139.4 grams of common salt. The distances of measurements were: 15 m, 25m, and 50 m.

Fig. 8 Some aspects of measured small stream “Guaymaral”.

Next it is presented the screen of IDF tool showing the three tracer curves. The red arrow is the instant of pouring. The first curve in sequence was at 25 m, second at 50 m while the third was done at 15 m. As the IDF may measure simultaneously Rhodamine WT or common salt, it has two grids in screen, one in conductivity ($\mu S/cm$) and the other in fluorescence*(x100ppb).* In this field journey only was used the conductivity probe. The stream showed a background conductivity of $C_o=365.0\ \mu S/cm$. Fig. 9. (Authors ´files). This background data should be added in (15) to get a realistic representation of experimental curves in modelation exercises.

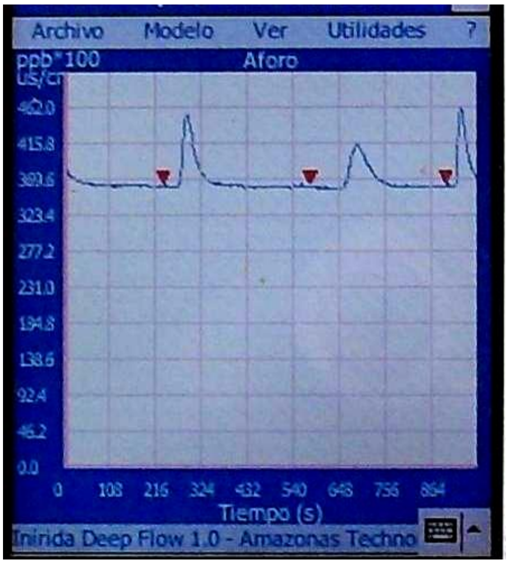

Fig. 9 IDF screen with three ionic pouring.

C. Application of proposed formulas

The aim here is to verify the validity of equations. For this purpose we have down load the experimental curves from IDF tool, put them in Excel format, and then measure the time σt, in order to calculate V_{disp} , ϕ and E. This measurement is done on the inflection points of bell-shaped curves for the three pouring. Figure 10 (a) is for distance $X=15\ m$. Fig. 10 (b) is for a distance $X= 25\ m$. And Fig. 10(c) is for distance $X=50\ m$. The baseline for calculating peak conductivity, C_p is the background conductivity, C_o.

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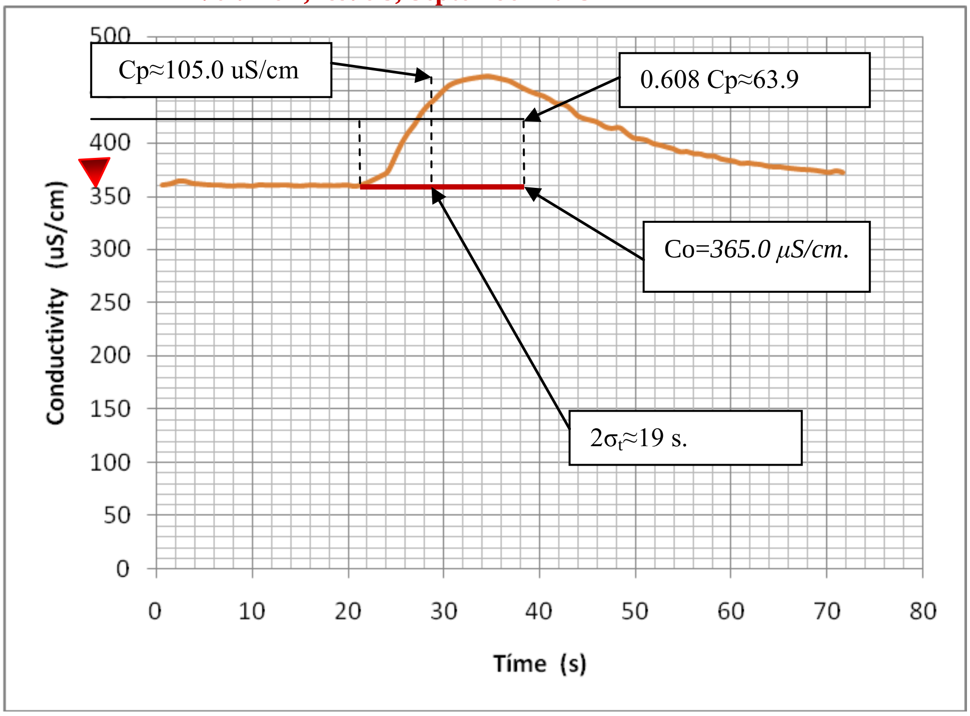
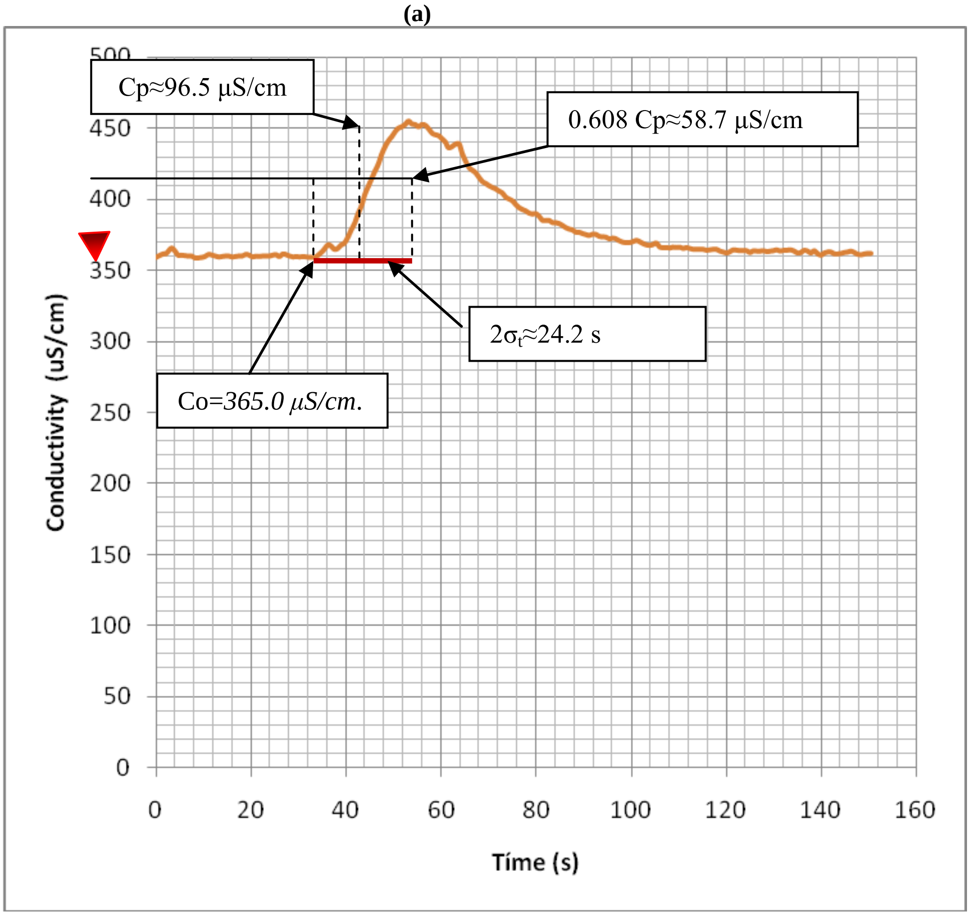


(a)



(b)

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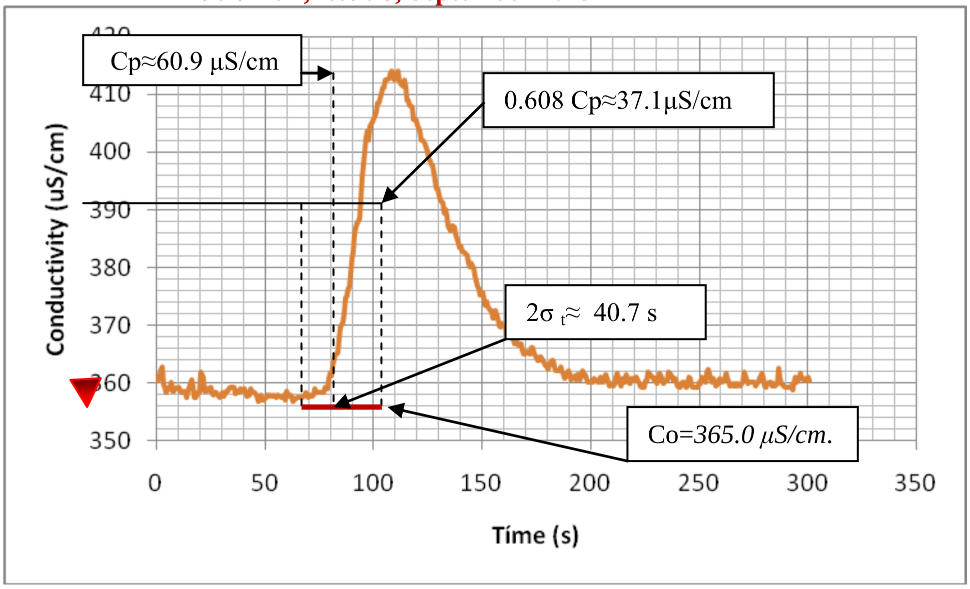

(c)

Fig. 10 Measurement of $2\sigma_t$ times in each experimental curve

Results of the measurements on curves are in Table 1.

X Distance (M)	t Peak transport time (s)	τ Characteristic dispersion time (s)	Ux Mean Advective Velocity (M/s)	2σt Time for inflection points (s)	Cp Peak Conductivity (µS/cm)
15	34.1	7.33	0.440	19.0	105.0
25	54.4	11.7	0.458	24.2	96.5
50	109.8	23.6	0.455	40.7	60.9
Average	-------	------	0.451	------	-------

Table 1 Pouring data from experimental figures

1. - Calculation of ϕ:

Using (16):

X=15 m:

$$\phi \approx \frac{2\sigma_t}{2t\sqrt{0.215}} = \frac{19.2}{2\times 34.1\times 0.464} \approx 0.60$$

X=30 m:

$$\phi \approx \frac{2\sigma_t}{2t\sqrt{0.215}} = \frac{24.2}{2\times 54.4\times 0.464} \approx 0.48$$

X=50 m:

$$\phi \approx \frac{2\sigma_t}{2t\sqrt{0.215}} = \frac{40.7}{2\times 109.8\times 0.464} \approx 0.40$$

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2. - Calculation of *E*:

Using (14):

X=15 m:

$$E \approx \frac{U^2 \phi^2 \tau}{2} = \frac{(0.44)^2 (0.60)^2 \times 7.33}{2} \approx 0.256\, m^2 / s$$

X=30 m:

$$E \approx \frac{U^2 \phi^2 \tau}{2} = \frac{(0.458)^2 (0.48)^2 \times 11.7}{2} \approx 0.283 m^2 / s$$

X=50 m:

$$E \approx \frac{U^2 \phi^2 \tau}{2} = \frac{(0.455)^2 (0.40)^2 \times 23.6}{2} \approx 0.391 m^2 / s$$

3. - Calculation of *Δ*:

Using (1):

X=15 m:

$$\Delta \approx \sqrt{2E\tau} \approx \sqrt{2 \times 0.256 \times 7.33} \approx 1.94\ m$$

X=30 m:

$$\Delta \approx \sqrt{2E\tau} \approx \sqrt{2 \times 0.283 \times 11.7} \approx 2.57\ m$$

X=50 m:

$$\Delta \approx \sqrt{2E\tau} \approx \sqrt{2 \times 0.391 \times 23.6} \approx 4.30\ m$$

4. - Calculation of V_{disp}:

Using (2):

X=15 m:

$$V_{disp} \approx \frac{\Delta}{\tau} \approx \frac{1.94}{7.33} \approx 0.265 m / s$$

X=30 m:

$$V_{disp} \approx \frac{\Delta}{\tau} \approx \frac{2.57}{11.7} \approx 0.22 m / s$$

X=50 m:

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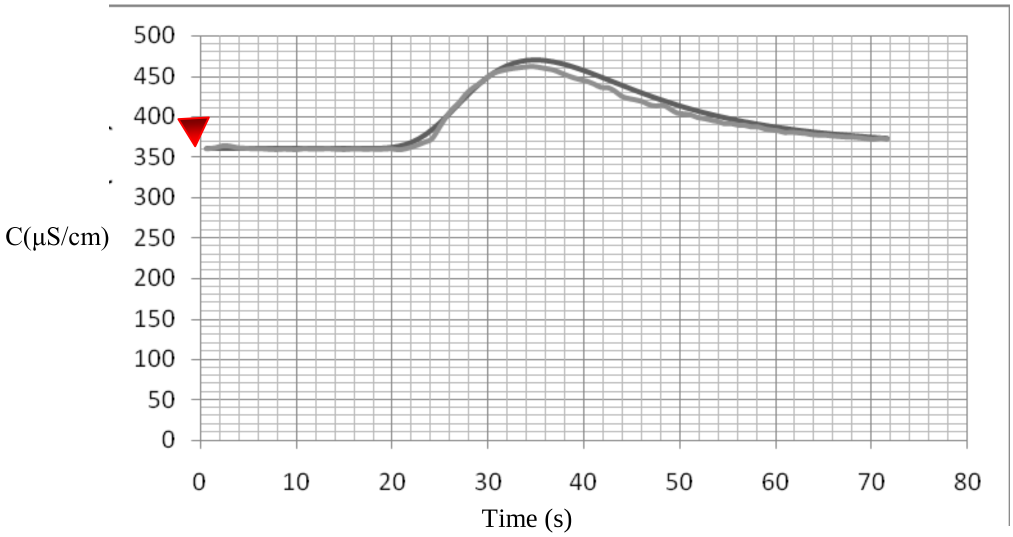
$$V_{disp} \approx \frac{\Delta}{\tau} \approx \frac{4.30}{23.6} \approx 0.182 m/s$$

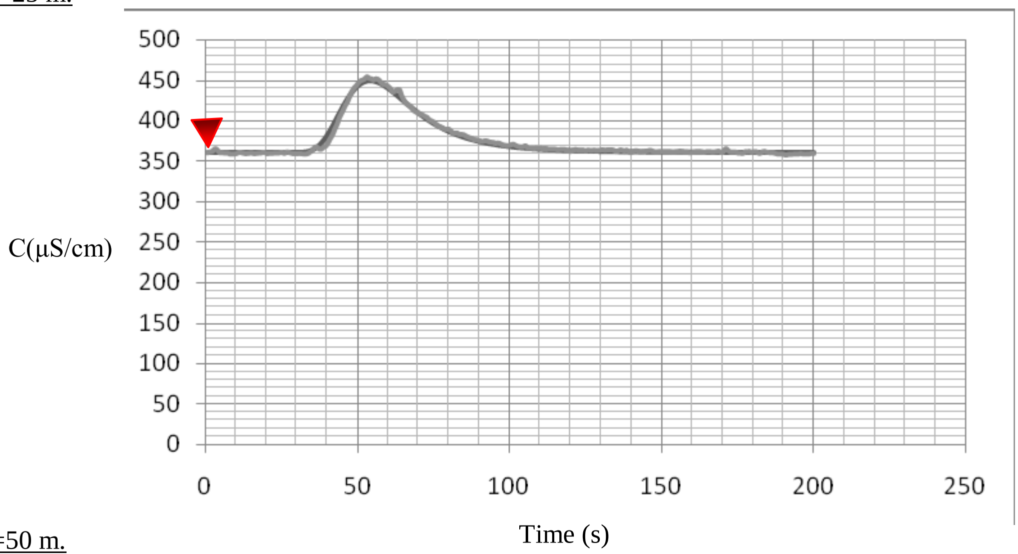
D. Theoretical modulation of experimental curves

Using (15) converted in conductivity, and numerical data obtained before, it is possible to simulate the experimental curves as is shown following. Some small distance corrections were done. Fig. 11:

X=15 m.



X=25 m.



X=50 m.

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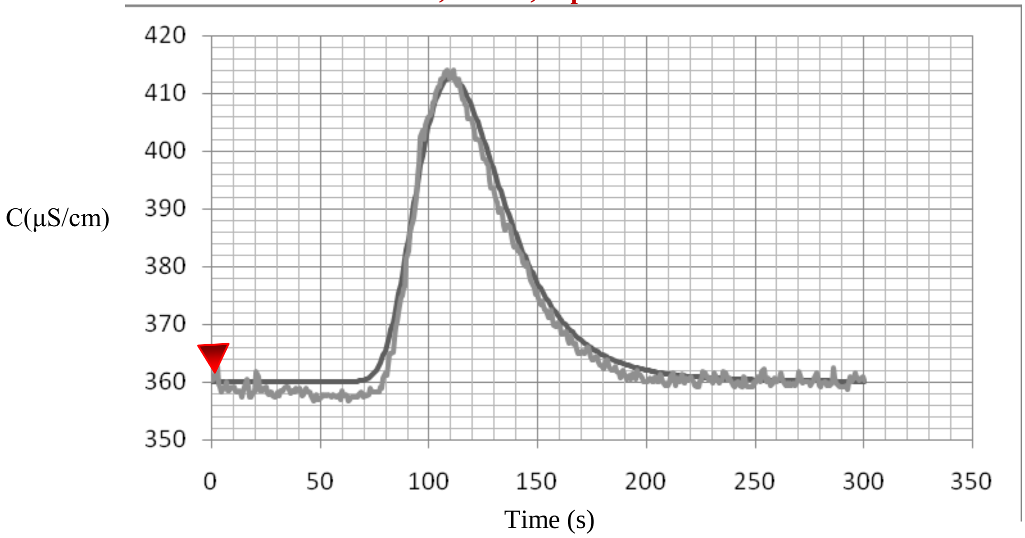

Fig. 11. Theoretical modelation of three pouring in "Guaymaral"

As it can be seen, the modelation of experimental curves is well fitted using the calculated values for parameters, indicating that they are very congruent.

E. Trend curves for ϕ, E and V_{disp}

In Fig. 12 it is shown the experimental trends for trend curves for ϕ, E and V_{disp}. They are congruent with theoretical guidelines as can be seen.

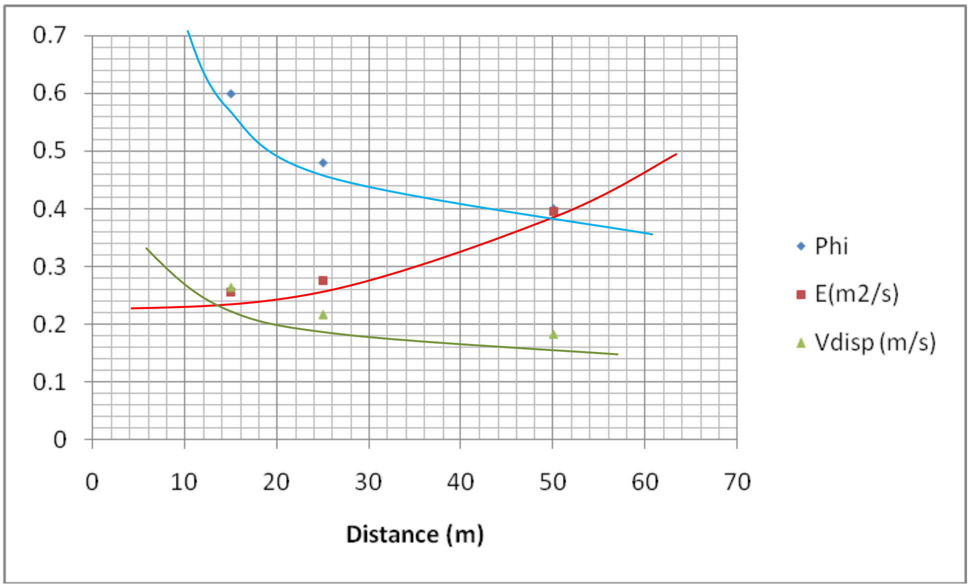

Fig 12 Trends for ϕ, E and $V_{disp.}$

IV. CONCLUSIONS

- It was developed a theory based on time measurements only on experimental tracer curves, i.e.: with a huge experimental foundation. This theory describes the formation and evolution of conservative solute plumes, from interchanges of energy viewpoint. This focus gives us a very general and intuitive sight of these mechanisms. Also this theory would be important for the modelation and prediction of contaminations in streams.

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- Hence, it is applied thermodynamic concepts to the analysis of several stages of tracer plume evolution taken advantages of this sort of approaches, i.e.: huge generality of results and a very compact format of mathematical tools used.
- Features of this new procedure are: A. - Theoretical results are very concordant with experimental observations. B. - It gives right, congruent values for different involved parameters. C. - It gives appropriate shapes for theoretical curves compared with experimental ones. D. - It may be developed with easy mathematical support and with current computational tools as Excel.
- In this theory, ϕ is a very useful function that allows describing when the tracer plume lose freedom degrees, and hence it tell us a very accurate history of irreversible process in streams.
- Experimental measurements were done in a small stream in Colombia. It was used a powerful instrument (IDF) that gives "real time" results using a graphical interface. In this case was used common salt as tracer but the instrument may use also with Rhodamine WT tracer, simultaneously. The use of two tracers at the same time allow to measure very small or very large streams.

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