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Revisiting the Relationship of Transient-storage and Aggregated Dead Zone Models of Longitudinal Solute Transport in Streams

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ABSTRACT: Theoretical relationships between the one-dimensional distributed transient storage solute transport model (TS, Bencala and Walters, 1983; Runkel and Chapra, 1993) and the lumped, aggregated dead zone model (ADZ, Beer and Young, 1983; Young and Wallis, 1993; Camacho and González, 2008) were obtained. The moment matching technique proposed by Lees *et al.*, (2000), based on the theoretical temporal moments developed by Schmid (2002, 2003), was applied. These relationships allow ADZ model parameters to be reliably derived from TS model parameters and vice versa. They were extended to describe the dispersive fraction in terms of the physical-based model parameters and to analyze its behavior as a function of discharge. Assuring the equivalence between ADZ and TS model parameters a close representation of advection, dispersion and biochemical processes in rivers and streams under both frameworks is demonstrated in this work.

Keywords: Solute Transport, Water Quality Modeling, Data Based Mechanistic, Aggregated Dead Zone Model

1 INTRODUCTION

Data based mechanistic, DBM, environmental models able to accurately reproduce input-output behavior of natural and man-made systems are still required in practical water quantity and quality real-time control applications, due to their low computational cost and high efficiency. DBM models are also efficient and sufficient accurate tools to be used as the basis of complex decision support systems for the integrated management of water resources at the catchment scale.

According to Young and Garnier (2006), the best known transfer function derived using a DBM approach for solute transport and longitudinal dispersion in streams, is the Aggregated Dead Zone, ADZ, model introduced by Beer and Young (1983). The lumped ADZ framework, represented by an ordinary differential equation (Young and Wallis, 1993; Lees *et al.*, 1998), allows effective and efficient use of powerful methods of system identification, parameter estimation and uncertainty analysis to be carried out. An additional advantage relies on the ADZ measurable and observable parameters using data of field tracer experiments, and therefore its underlying potential application to indirectly estimating the space-average parameters of physically-based frameworks as those derived from the advection-dispersion equation, ADE, (e.g. transient storage model TS, Bencala and Walters, 1983; Runkel and Chapra, 1993).

In this work, the relationships between ADZ and TS model parameters obtained by Lees *et al.*, (2000) are revisited to include the TS temporal moments deduced by Schmid (2000, 2003) and verified by Veling (2005). Though this study does not address the current model theory inconsistency to represent observed constant skewness over time (Nordin and Troutman, 1980; Schmid, 2002; González-Pinzón *et al.*, 2013), it covers some issues of the dispersive fraction's physical meaning and its dependence on dead zone transport mechanisms. In addition, it is demonstrated that both modeling frameworks closely reproduce reactive behavior if conservative transport equivalence is guaranteed.

1.1 Solute transport models

1.1.1 Transient storage TS model

The TS model was introduced by Bencala and Walters (1983) to physically describe long concentration tails observed at breakthrough curves observed from tracer studies in streams. Under steady flow conditions and considering a non-conservative solute with first order decay reaction, the model equations are given by:

$$\frac{\partial c}{\partial t} = -u \frac{\partial c}{\partial x} + E \frac{\partial^2 c}{\partial x^2} + \alpha (c_s - c) - k_1 c \quad (1)$$

$$\frac{dc_s}{dt} = \alpha \frac{A}{A_s} (c - c_s) - k_2 c_s \quad (2)$$

where, c [ML^{-3}] is the downstream solute concentration in the main channel; t [T] is time; x [L] is the reach length; u [LT^{-1}] is the mean velocity in the main channel; A [L^2] is the cross-sectional area of the main channel; E [L^2T^{-1}] is the longitudinal dispersion coefficient; c_s [ML^{-3}] is the solute concentration in the storage zone; α [T^{-1}] is the mass-exchange coefficient between the main channel and the storage zone; A_s [L^2] is the cross-sectional area of the storage zone; and k_1 and k_2 [T^{-1}] are the first order decay rates of the main channel and the storage zone, respectively. The mean velocity u is given by the ratio between the stream discharge Q [L^3T^{-1}] and the cross-sectional area A . This model requires the definition of boundary conditions at the entrance and exit of the reach as well as initial conditions at each calculation cell for performing the numerical solution of the differential equations.

1.1.2 Aggregated Dead Zone ADZ model

After Young and Wallis (1993) and Lees *et al.* (1998), the continuous form of ADZ model, considering steady flow conditions and first order decay reaction is given by:

$$\frac{dc}{dt} = \frac{1}{T_r} [c_{in} (t - \tau) e^{-k\tau} - c] - kc \quad (3)$$

where, c_{in} [ML^{-3}] is the solute concentration boundary condition at the input or upstream location; τ [T] is the time delay describing solute advection due to the bulk flow movement; T_r [T] is the ADZ residence time at the dead zone representing the component of the overall reach travel time associated with dispersion; and k [T^{-1}] is the first order decay rate.

The residence time T_r is the ratio between the active mixing volume V [L^3] (where dispersion mechanisms take place) and the stream discharge Q . The mean travel time \bar{t} is defined as the time taken while the solute undergoes pure advection, followed by dispersion in the active mixing volume. It is expressed too as the ratio between the overall reach volume V_a and the discharge Q ,

$$\bar{t} = n(T_r + \tau) \quad (4)$$

where n represents the number of identical ADZ elements serially connected. Conceptually, the ADZ model consist of a linear channel with time delay $n\tau$ followed by n completely mixed cells in series with identical residence time T_r .

The most representative parameter of the ADZ model is known as the dispersive fraction DF and it represents the fraction from the overall reach volume that is completely mixed, or the overall time fraction in which the solute is dispersed:

$$DF = \frac{V}{V_a} = \frac{nT_r}{\bar{t}} = 1 - \frac{n\tau}{\bar{t}} \quad (5)$$

Results reported by Wallis *et al.* (1989), Young and Wallis (1993) and Camacho (2000) suggest that the dispersive fraction is constant under broad discharge intervals in alluvial streams. Also, Camacho and Lees (2000) show that DF can be estimated from field hydraulic data and velocity profiles, through the physical relationship of transport parameters \bar{t} and $n\tau$ with the mean velocity u and the maximum velocity u_{max} , respectively, and reach length,

$$DF = 1 - \frac{u}{u_{max}} \quad (6)$$

2 REVISITED RELATIONSHIPS BETWEEN ADZ AND TS MODEL PARAMETERS

Lees et al. (2000) developed mathematical relationships between ADZ and TS model parameters using the moment matching technique. Those authors applied explicit equations found by Czernuszenco and Rowinski (1997), who considered the upper boundary condition defined by $C(0,t) = A_0(t)$, where A_0 is a concentration-time distribution measured at the reach entrance. Later, Schmid (2002, 2003), bearing in mind the same boundary condition, obtained different expressions that were confirmed by Veling (2005) for the first three moments.

The results showed by Lees et al. (2000) comparing longitudinal profiles of simulated temporal moments from TS and ADZ models (cf. Lees et al., 2000, Figure 7), are reproduced here in Figure 1 to compare the performance of theoretical expressions found by Czernuszenco and Rowinski (1997) and Schmid (2002, 2003).

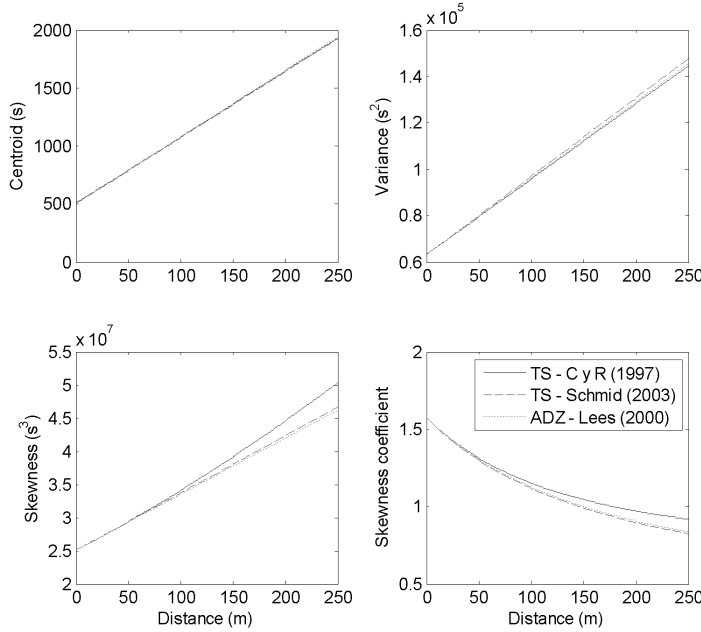


Figure 1. Theoretical temporal moments profiles comparison

Note that the obtained results applying Schmid's (2002, 2003) equations reveal a better graphical fit than those of Czernuszenco and Rowinski (1997), particularly for the third central moment (skewness) and the skewness coefficient profiles. Though it is not displayed here, the moments obtained directly from model simulations each 50 m, according to Lees et al. (2000), show an excellent fit to ADZ theoretical moment curves. These results demonstrate that TS model's temporal moments expressions found by Schmid (2002, 2003) are more accurate than Czernuszenco y Rowinski's (1997) for the moment matching technique performed by Lees et al. (2000). Schmid's (2002, 2003) temporal moments equations are presented below:

$$\bar{t}(x) = \bar{t}(0) + \frac{x}{u}(1 + \varepsilon) \quad (7)$$

$$\sigma_t^2(x) = \sigma_t^2(0) + 2\frac{x}{u} \left[\varepsilon \cdot T + \frac{E}{u^2}(1 + \varepsilon)^2 \right] \quad (8)$$

$$g(x) = g(0) + 6\frac{x}{u} \left[\varepsilon \cdot T^2 + 2\frac{E}{u^2} \varepsilon \cdot T(1 + \varepsilon) + 2\frac{E^2}{u^4}(1 + \varepsilon)^3 \right] \quad (9)$$

where, the first temporal moment \bar{t} , i.e. the centroid, is about the origin, while the second (variance σ^2) and third (skewness g) are central moments; and ε and T are given by:

$$\varepsilon = \frac{A_s}{A} \quad (10)$$

$$T = \frac{A_s}{\alpha \cdot A} \quad (11)$$

If the terms containing TS model parameters, which reflect storage zone effects, are neglected (i.e., $\varepsilon=T=0$), temporal moment equations for the ADE model are obtained. These expressions only depend on the parameters u and E and the distance x (Nordin and Troutman, 1980),

$$\bar{t}(x) = \bar{t}(0) + \frac{x}{u} \quad (12)$$

$$\sigma_t^2(x) = \sigma_t^2(0) + 2 \frac{x}{u} \cdot \frac{E}{u^2} \quad (13)$$

$$g(x) = g(0) + 12 \frac{x}{u} \cdot \frac{E^2}{u^4} \quad (14)$$

Following Lees et al. (2000), ADZ model parameters could be estimated according to,

$$T_r = \frac{1}{2} \left[\frac{g(x) - g(0)}{\sigma_t^2(x) - \sigma_t^2(0)} \right] \quad (15)$$

$$n = \frac{\sigma_t^2(x) - \sigma_t^2(0)}{T_r^2} \quad (16)$$

$$\tau = \frac{\bar{t}}{n} - T_r \quad (17)$$

Beyond the parameter estimation from one modelling framework to another, one practical use of the equations obtained above, is the study of the physical meaning of the lumped model parameters. Combining Eq. (5) and Eq. (7) with Eq.(17), the following relationship for the dispersive fraction can be derived,

$$DF = \frac{4}{3} \frac{\left[\varepsilon \cdot T + \frac{E}{u^2} (1 + \varepsilon)^2 \right]^2}{(1 + \varepsilon) \left\{ \varepsilon \cdot T^2 + 2 \frac{E}{u^2} (1 + \varepsilon) \left[\varepsilon \cdot T + \frac{E}{u^2} (1 + \varepsilon)^2 \right] \right\}} \quad (18)$$

When the mass-exchange coefficient between the main channel and the storage zone α acquires a value near to zero (i.e. $T \rightarrow \infty$), the DF is defined by,

$$DF = \frac{4}{3} \left(\frac{\varepsilon}{1 + \varepsilon} \right) \quad (19)$$

This is equivalent to say that the trapped solute in the storage zone takes much time leaving it and the concentration tail of the downstream breakthrough curve becomes longer. Eq. (19) indicates that, under the outlined conditions, DF is exclusively a function of the ratio between the cross-sectional area of the storage zone and the cross-sectional area of the main channel. As it will be shown later, when α decreases, the DF variation as a function of stream discharge is less evident, until reaching a limit value given by Eq. (19). This result can partially explain experimental results about a constant dispersive fraction value under broad discharge intervals.

Otherwise, it is possible to demonstrate that when the cross-sectional area of the storage zone is negligible (i.e. $A_s \rightarrow 0$), or the α coefficient is larger ($\alpha \rightarrow \infty$), DF acquires a constant value equal to $2/3$, without any dependence on the channel geometry. Both conditions described above are equivalent to applying the ADE model. With DF constant and equal to $2/3$, the expressions to obtain ADE model parameter as a function of ADZ model parameters become:

$$u = x / \bar{t}_{ADZ} \quad (20)$$

$$E = \frac{2}{9} \frac{u \cdot x}{n} \quad (21)$$

According to the expressions presented above, to obtain ADE model parameters, it is necessary to set \bar{t} and n as ADZ model calibration parameters with DF fixed and equal to $2/3$. These relationships were ap-

plied to field data obtained from a tracer study in a reach of the Subachoque River, a mountain stream located at the Colombian Andes Mountains, South America. The measured discharge during the field study was $0.270 \text{ m}^3/\text{s}$ and the reach length (distance between NaCl concentration-time breakthrough curves) was 106 m. Using 10,000 Monte Carlo Simulations (MCS), parameters \bar{t} and n were obtained. The convolution method with non-integer n values was applied for the numerical solution of the ADZ model (Camacho, 2000). On the other hand, u and E were obtained directly from ADE model calibration using SCE-UA algorithm (Duan *et al.*, 1994). The optimal model parameters values obtained were: $\bar{t} = 509.57 \text{ s}$, $n = 10.29$ (Nash-Sutcliffe efficient coefficient $R^2 = 0.9988$) and $u = 0.202 \text{ m/s}$, $E = 0.55 \text{ m}^2/\text{s}$ ($R^2 = 0.9974$). Applying Eqs. (20) and (21), ADE model parameters were estimated from ADZ model parameters as $u = 0.208 \text{ m/s}$, $E = 0.48 \text{ m}^2/\text{s}$ ($R^2 = 0.9984$). The comparison between the ADZ calibrated solution and the ADE solution using the parameter relationships is shown in Figure 2. Note that parameter values obtained for ADE model through the two methods described above are very close.

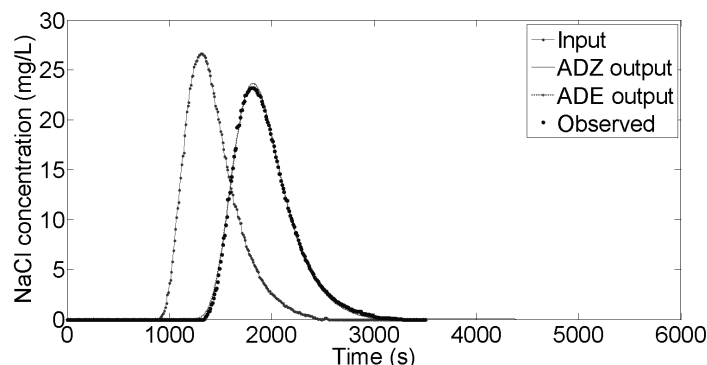


Figure 2. Comparison between ADZ calibrated solution and ADE solution using parameter relationships

3 COMPARISON BETWEEN NON-CONSERVATIVE SOLUTIONS

3.1 Methodology

Several numerical tests using synthetic data under different flow and longitudinal dispersion conditions and channel geometry data were conducted to compare the dynamic response of the lumped ADZ model with the distributed TS model. Tested channel types and characteristics are presented in Table 1.

Table 1. Test channels to compare non-conservative solutions of TS and ADZ models

Channel	L= 100 km			
Rectangular	Width (m)	Longitudinal slope	n-Manning	
1	25	0.0002	0.04	
2	25	0.0002	0.02	
3	25	0.002	0.02	
4	25	0.001	0.04	
Trapezoidal	Width (m)	Lateral slope	Longitudinal slope	n-Manning
5	25	1:1	0.0001	0.04

Non-conservative reactive first order decay transport was considered. Both models were executed under the same upstream boundary conditions. ADZ model with non-integer n identical mixed cells in series and first order reaction was programmed and executed using MATLAB (The MathWorks, 2009). TS model equations were numerically solved using OTIS (One-dimensional transport with inflow and storage, Runkel, 1998). In order to guarantee equivalent conservative solute transport parameters, the theoretical relationships developed by Lees *et al.* (2000) using temporal moments for the TS response reported by Schmid (2000, 2003) were applied. The ADZ model parameters were obtained from prescribed TS model parameters $\alpha = 0.001 \text{ s}^{-1}$ and $\varepsilon = A_s/A = 0.30$; main channel velocity u and longitudinal dispersion E were obtained supposing uniform flow and using Kashefipour and Falconer (2002) expression:

$$E = 10.612Hu \left(\frac{u}{u^*} \right) \quad (22)$$

where, $H [L]$ is the water depth and u^* is the shear velocity calculated as $\sqrt{gHS_o}$, with $g [LT^{-2}]$ the gravity acceleration and S_o the longitudinal energy slope. The first order decay rate k was defined equal to 0.5 d^{-1} . Solutions at three different distances ($x = 10, 50$ and 90 km) were computed, considering discharges of $10, 100, 200$ and $400 \text{ m}^3/\text{s}$. The upper boundary condition was synthetically generated using a gamma type distribution with peak time $t_p = 5 \text{ hr}$, background concentration $c_o = 100 \text{ mg/L}$, peak concentration $c_p = 1000 \text{ mg/L}$ and skewness coefficient $\gamma = 1.15$. The time span was defined between 0 and 300 hours:

3.2 Results

Conservative transport parameters for the ADZ model using the relationships (15) to (17) with TS temporal moments obtained by Schmid (2002, 2003) are presented in Table 2 for channels 2 and 3 with discharges of 10 and $100 \text{ m}^3/\text{s}$, respectively. The corresponding graphical results for non-conservative solute are shown in Figure 3.

Table 2. ADZ model parameter values and goodness of fit between the framework responses estimated using the moment matching technique

Channel	Discharge ($\text{m}^3 \text{ s}^{-1}$)	E (m^2/s)	A (m^2)	Distance (km)	\bar{t} (hr)	DF	n	τ (hr)	T_r (hr)	R^2
2	10	61.88	18.17	9.96	6.532	0.75	19.89	0.081	0.247	0.99983
				50.00	32.807		99.89			0.99984
				89.82	58.935		179.44			0.99993
3	100	2123.46	37.06	8.59	1.150	0.74	2.55	0.116	0.335	0.99982
				49.22	6.587		14.60			0.99975
				89.84	12.024		26.65			0.99974

(*) $\alpha=0.001$ and $A_s=0.3A$

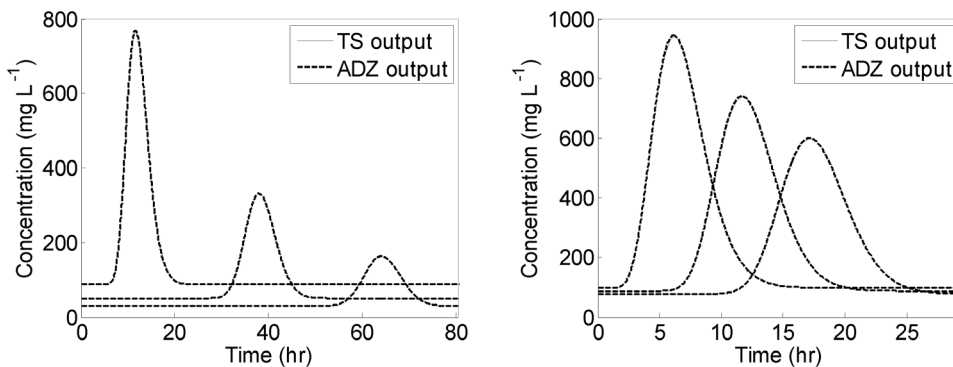


Figure 3. Comparison between model responses with ADZ model parameters estimated using moment matching technique. Left: Channel 2, $Q = 10 \text{ m}^3/\text{s}$; Right: Channel 3, $Q = 100 \text{ m}^3/\text{s}$

3.3 Steady-state solutions

3.3.1 TS modeling framework

It can be demonstrated for well-mixed conditions that the concentration in the main channel is given by:

$$c = \frac{c_{in}}{k_1 T_r^{ts} + 1}; T_r^{ts} = \left[\frac{(k_2/k_1)\epsilon}{(1+k_2T)} + 1 \right] T_r; c_s = \frac{c}{k_2T + 1}$$

The residence time T_r in this modeling framework is computed as the ratio of the main channel volume and the discharge Q . For plug-flow conditions, the following expression is obtained for the solute concentration in the main channel:

$$c = c_{in} e^{-k_1 \bar{t}_{ts}}; \bar{t}_{ts} = \left[\frac{(k_2/k_1)\epsilon}{(1+k_2T)} + 1 \right] \bar{t}$$

Considering mixed-flow conditions and according to Chapra (1997), it is possible to demonstrate the following solution under the TS modeling framework:

$$k' = \left[\frac{(k_2/k_1)\varepsilon}{(1+k_2T)} + 1 \right] k_1; \quad \lambda_1 = \frac{u}{2E} \left(1 + \sqrt{1 + \frac{4E \cdot k'}{u^2}} \right); \quad A = \frac{c_{in} \lambda_2 e^{\lambda_2 L}}{\lambda_2 e^{\lambda_2 L} - \lambda_1 e^{\lambda_1 L}}; \quad B = \frac{c_{in} \lambda_1 e^{\lambda_1 L}}{\lambda_1 e^{\lambda_1 L} - \lambda_2 e^{\lambda_2 L}}$$

$$c = A e^{\lambda_1 x} + B e^{\lambda_2 x}$$

It is worth noting that when the first order decay rate at the storage zone is equal to zero, this zone does not have any effect on the solute concentration at the main channel and the steady-state solutions become equal to the ADE model solutions.

3.3.2 ADZ modeling framework

The general solution for mixed-flow steady-state condition under the ADZ modeling framework, considering n ADZ elements in series, is given by:

$$c = \frac{e^{-k \cdot n \cdot \tau}}{(kT_r + 1)^n} c_{in}$$

Solving for well-mixed conditions, $DF = 1$ (pure dispersion) which means that $\tau = 0$, the corresponding solution is given by:

$$c = \frac{c_{in}}{kT_r + 1}$$

Under plug-flow conditions, $DF = 0$ (pure advection) and $\tau = \bar{t}$, the following expression is obtained:

$$c = c_{in} e^{-k\bar{t}}$$

3.4 Discussion

Comparison between non-conservative TS and ADZ model responses using mathematical relationships between model parameters, show that both frameworks are able to generate the same results. It is possible to conclude that the k parameter has the same physical and mathematical meaning for both modeling frameworks. This verification suggest that a reliable application of complex processes (reaeration, oxidation, hydrolysis, sorption, volatilization, settling, etc.) based on the ADZ modeling framework is possible. These approaches will produce similar responses to mechanistic formulations derived from the traditional advection-dispersion equation if conservative solute transport parameters equivalence is guaranteed. Nash-Sutcliffe efficiency coefficients R^2 found for non-conservative responses under both frameworks range from 0.9961 to 0.9999, with mean value of 0.9993 for the 75 simulated cases. Also, it was observed that the n values monotonically increase with reach length. Furthermore, it was found for the 75 synthetic cases that the corresponding equations produce practically the same results applying the solutions of mixed-flow under both modeling frameworks with equivalent conservative transport parameters.

From the theoretical relationships found between ADZ and TS models parameters, using synthetic data from the five studied channels for non-conservative solute transport models comparison, curves relating the DF as a function of discharge and α were constructed and are shown in Figure 4. According to Figure 4 (left), the DF is not modified drastically with discharge (maximum change in the order of 0.15 for channel 3 in a range from 10 to 400 m³/s). It is observed that while the discharge increases, DF 's rate of change decreases. It is worth noting that channels 3 and 4 show the greatest change with discharge and have the steepest longitudinal slope. Channels 1, 2 and 5, with slopes similar to those of alluvial rivers, show the lowest DF variation. Figure 4 (right) was constructed with data obtained from channel 3 to show the change of DF with different values of the α parameter. It is shown that while α decreases, the DF curve becomes flatter, until it reaches a constant and discharge-independent value, as it has been observed in natural channels. This constant value is given by Eq. (19). The results shown in Figure 4 are valid if it is supposed that the ratio between the cross-sectional area of the main channel and the cross-sectional area of the storage zone ε is constant over time. The latter must be experimentally investigated because it is not a necessarily a practical condition. If ε is variable with stream flow, the measured constant values for DF possibly respond to interdependence between the water body hydrodynamics and the transport mechanisms in the storage zone.

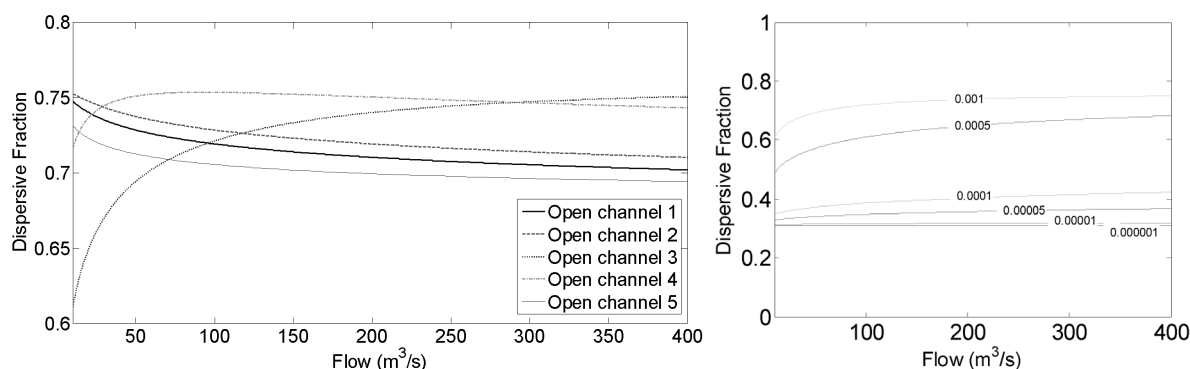


Figure 4. Theoretical behavior of DF in function of discharge. Left: Five channel. Right: Channel 3, different values of α

The observation and results presented above suggest that the order of magnitude of DF responds to the value of ε , and its variation with discharge depends on the α value and the channel's energy slope (hydraulics). The DF increases with the rise of the ε value, which is physically consistent, because it implies a greater active mixing volume or storage zone.

4 CONCLUSIONS

This research work demonstrates that both, steady state and dynamic solutions of reactive transport, using TS and ADZ modelling frameworks are equivalent if correct mathematical relationships between the conservative solute transport model parameters are used first. The latter can be achieved through the relationships proposed by Lees et al. (2000) using temporal moments for the TS model response reported by Schmid (2002, 2003).

These results highlight the aggregated ADZ modelling framework potential to be used as an efficient, effective alternative to traditional distributed approaches based on the one-dimensional advection-dispersion equation. This potential is particularly useful for real time control applications and water quality decision support tools at the catchment scale where computational cost is still an issue. There is an additional advantage, since it has been demonstrated that the data based mechanistic ADZ model parameters are observable, measurable and have physical meaning (Camacho and González, 2008), and the numerical solution of the resulting ordinary differential equation is very efficient.

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