ISSN: 0128-7680
Pertanika J. Sci. & Technol. **1(2)**: 225-238 (1993)

Longitudinal Dispersion of Pollutants in Natural Streams – The Aggregated Dead-Zone Approach

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Received 6 January 1992

ABSTRAK

Model Agrigat Zon-Tetap (ADZ) memberi gambaran ringkas mengenai dinamik pergerakan dan penyerakan bahan cemar di dalam sungai yang tidak mempunyai sifat pasang surut. Ianya merupakan satu pilihan terhadap model Alirlintang-Penyerakan yang lebih rumit. Artikel ini memeparkan keputusan yang di dapati hasil dari penggunaan model ADZ untuk sistem sungai. Keputusan menunjukkan bentuk umum fungsi perkaitan di antara parameter orde kedua model ADZ dengan luahan sungai. Suhubungan dengan itu juga, analisis hidrologi secara lazim telah menghasilkan maklumat penting mengenai ciri-ciri hidraulik sungai dan memberi ruang dari segi perbandingan cara ini dengan parameter ADZ.

ABSTRACT

The Aggregated Dead-Zone (ADZ) model provides a simple dynamic description of pollutant transportation and dispersion in a non-tidal river system and is an alternative to the well-known but more complicated advection-dispersion model. This paper presents the results obtained from the application of the model in a river system. The study shows the general form of functional relationships between the second order ADZ model parameters and stream discharge. In addition, more conventional hydrological analysis has yielded valuable information about the hydraulic characteristics of the reaches and has allowed for useful comparisons between these and the ADZ model parameters.

Keywords: **pollutants, dispersion, transportation, advection-dispersion model, Aggregated Dead-Zone model, effective volume, ADZ residence time**

INTRODUCTION

Studies on dispersion processes in rivers are widely used by hydrodynamicists, hydrologists and environmental scientists involved in the study of water pollution problems. The time of travel of a pollutant in a river or estuary, the rate at which the pollutant spreads out, the decrease in peak concentration and the resulting concentration patterns of pollutant are the important variables that must be properly understood. Serious pollution may result if the capacity of a stream to transport and disperse a contaminant is overestimated. Underestimation on the other hand may result in valuable resources not being optimally utilised, resulting in unnecessary expenditure on treatment facilities. It has been emphasised that virtually no water quality management study which is aimed at achieving optimum usage of a river or estuarine system can bypass the need for a reliable means of predicting the dispersion characteristics of the water body (Sooky 1969).

There have been many studies on longitudinal dispersion of pollutants in rivers and natural streams. The best-known study, usually quoted in texts on the subject, is the Fickian theory. It was developed for flow in pipes by Taylor (1954) and extended to channels by Elder (1959) and for natural streams by Fischer (1966). Their research involved a mathematical representation in the form of a single dimensional, partial differential equation, usually known as the one-dimensional Fickian Diffusion model. In this model, dispersion is quantified by the effective longitudinal dispersion coefficient, usually termed the "Dispersion Coefficient". Much effort has been extended in order to measure and/or estimate the dispersion coefficient (Harris 1963; Fischer 1968; Bansal 1971; Liu 1977; Fischer *et al.* 1979; Chatwin & Allen 1985). However, the apparent popularity of the Fickian-type model is not fully justified by its performance in practical applications. When used for the characterisation of dispersion in natural streams, it has not always been successful (e.g. Day 1975; Sabol & Nordin 1978; Bencala & Walters 1983; Legrand-Marc & Laudelout 1985). In particular, the temporal profiles observed at fixed locations on the river appear often to have sharper rises times and longer tails than those predicted by the Fickian-type model; while in non-uniform streams, the longitudinal dispersion coefficients, as described by Taylor (1954) and Elder (1959), vary considerably and consistently from those associated with the normal distribution. Subsequently, various studies have investigated alternative models which are better able to represent the observed "non-Fickian" behaviour in channels and natural streams. Amongst the most successful of these alternative models and the most recent is the aggregated dead-zone model (ADZ) developed by Young (1982), Beer & Young (1983), Young (1983) and Young & Wallis (1986). The model argues that, while Fickian-type dispersion is probably taking place to some extent, most of the dispersion observed in natural streams arises because of the dead-zone effects caused by irregularities in river beds and banks. In other words, it is assumed that the cumulative effects of the dead-zones often dominate the observed dispersion and they can be amalgamated in their total effect to yield an "Aggregated Dead-Zone (ADZ)" whose "residence time" then defines the dispersion properties associated with the stretch of river being studied.

In this paper, we describe the results obtained from application of the ADZ model in a river system. It presents the physical interpretation of the model and also explores the relationships between various ADZ parameters and physical variables such as stream discharge and the volume of water in the reach.

The Aggregated Dead-Zone Model

The simplest way of developing the ADZ model is to consider a typical dead-zone with volume V_i in a steady flow field with a rate Q. Then, under the assumption of complete mixing and a conservative solute, the relationship between the input concentration u(t) and the output concentration x(t) of the solute in the dead-zone is obtained from a dynamic mass balance, as follows:

$$\frac{d[V_i\, x(t)]}{dt} = Q\,u(t) \quad - \quad Q\,x(t) \qquad (1)$$

rate of change in the dead-zone	mass in per unit mass	mass out per unit mass

If for simplicity we assume that both V_i and Q are constant, then the equation for a conservative solute can be written,

$$\frac{dx(t)}{dt} = -\frac{Q}{V_i}x(t) + \frac{Q}{V_i}u(t) \qquad (2)$$

Equation (2) describes the dispersion processes of a single dead-zone which may occur anywhere in the stream. Between any two points, there can be a number of such dead-zones with different volumes, all contributing to the total dispersive properties of the stream as a series of interconnected processes. Thus, in the aggregated dead-zone model, it is assumed that the aggregated effect of all these processes can be described by a small number of "effective" dead-zones. In the simplest case, only one such aggregated dead-zone is necessary for the reach. If its volume is V_e, the effective volume, then the ADZ model for the reach would be:

$$\frac{dx(t)}{dt} = -\frac{Q}{V_e}x(t) + \frac{Q}{V_e}u(t) \qquad (3)$$

where x(t) and u(t) now represent the overall input and output solute concentrations associated with the ADZ for the whole reach.

The ADZ provides the basic mechanism for dispersion in a given reach of a river. However, advective effects also play a major role in the transport of solute down a river (Young 1984). In the Fickian Diffusion model these are introduced by the advective term and controlled by the stream velocity. In the ADZ model a pure time delay is introduced into the input term to allow for the pure translational effect of the river flow. Equation (3) then becomes:

$$\frac{d\,x(t)}{dt} = -\alpha x(t) + \alpha\, u(t-\Gamma) \quad (4)$$

where Γ is the pure time delay and $\alpha = Q/V_e$.

Equation (4) represents a basic equation for a single aggregated dead-zone. It is a first order differential-delay equation. Using Laplace Transforms (Schwarzenbach & Gill 1984), the unit impulse response of Equation (4) is in the form of a simple, time-delayed, exponential decay function as follows:

$$x(t) = -\alpha\, e^{-\alpha}(t-\Gamma) \quad (5)$$

where the time constant $T = 1/\alpha = V_e/Q$ is called the ADZ residence time.

Equation (4) describes the transportation and dispersion properties of a given reach. In order to describe a complete river system it is necessary to combine an appropriate number of such elements in a pattern defined by the physical nature of the river under study. To determine the number of ADZ elements required to represent the specified length of river in a multi-reach model it is convenient to consider the alternative discrete-time, sampled data version of the ADZ model. This not only allows for an objective evaluation but also helps in the implementation of the model and the construction of a stochastic framework around the model, i.e. a framework which has considerable advantages for use of the model in applications such as planning, management, forecasting and control. Also, data obtained from pollution monitoring are often in sampled form and as such, the discrete-time model provides its most natural characterisation.

There are many ways of deriving a discrete-time version of the ADZ model (i.e. equation 4), but the simplest and most straightforward is obtained by assuming that the input $u(t)$ is constant over the discretisation interval T_s. With this assumption about $u(t)$, the discrete-time version of the equation takes the following form,

$$x_k = -a\, x_{k-1} + b\, u_{k-\delta} \quad (6)$$

where the subscript k indicates the value of the associated variable at the kth sampling instant and δ, the nearest integral of T/T_s, is the transportation time delay in sampling intervals. In the simplest case, the parameters 'a' and 'b' in Equation (6) are related to the continuous-time model parameters by the following equation,

$$T = V_e/Q = -T_s/\ln(-a);\; b = 1 + a \quad (7)$$

It should be noted however, that both these equations and the definition of the discrete time delay in Equation (6) introduce approximations which may necessitate some alteration in the basic model form to allow for additional parameters and a modification of the relationships in (7).

Equation (6) can be transformed into operator form by the introduction of the backward shift operator z, i.e.

$$z^{-1} x_k = x_{k-1}$$

In this manner, it is straightforward to develop the following discrete-time transfer function form of equation (6).

$$x_k = \frac{b}{1 + a z^{-1}} u_{k-\delta} \tag{8}$$

A general, multi-order form of this model can be written as follows,

$$x_k = \frac{b_o + b_1 z^{-1} + ... + b_m z^{-m}}{1 + a_1 z^{-1} + ...+ a_n z^{-n}} u_{k-\delta} \tag{9}$$

where n and m are integers whose values will be determined by the nature of the transportation and dispersion in the river systems (Young 1984). In general, n represents the number of first order ADZ elements required to describe the observed dispersion properties of the reach, while m will depend on factors such as the presence of non-integral pure time delay or the presence of additional parallel dead zones.

A general approach to modelling water quality in rivers is described by Beck (Orlob 1983). He discussed all aspects of model calibration and verification within a useful unified framework. More specific time series models such as equation (10), and their application to general hydrological problems, are discussed by Young (1983, 1984) and Young & Wallis (1986). For the research described in this paper, computer programs exist for processing data obtained from tracer studies carried out on the river in order to statistically "identify" the k=model order (n and m) and the associated time delay, and to then "estimate" the parameters a_i, i = 1 to n, and b_j, j = 0 to m, as in equation (9).

The particular computer program employed in this study is the micro-CAPTAIN program, which uses recursive Instrumental variable (IV) methods of identification and estimation (Young 1984). This process of identification and estimation can be considered as the statistical equivalent of the better-known, but more closely defined, "calibration" procedures used in the construction of non-conventional water quality simulation models such as QUAL II (Orlob 1983). They have the advantage of allowing model builders to objectively evaluate the model structure which is most appropriate to the characterisation of their field data. In other words, the time-series helps to obviate the construction of a model which may have a reach structure which is more complicated than necessary.

In order to apply statistical identification and estimation procedures to any dynamic model, it is necessary to consider the model in stochastic terms. The major advantages associated with such a stochastic formulation are that (a) it allows the power of statistical methodology to be applied to model calibration, and (b) it provides a means of quantifying the uncertainty associated with both the model parameter estimates and any forecasts made with the help of the model. As regards (a), the microCAPTAIN program provides two main statistics for assessing model adequacy (Young *et al.* 1980). First, the ability of the model to explain the data is evaluated by a Coefficient of Determination (R_T^2) which represents a normalised measure of model fit, with a value of unity indicating a perfect explanation of the time-series data and zero specifying modelling errors of the same order of magnitude as the output data. Second, the precision of the model parameter estimates is indicated by an Error Variance Norm (EVN), which represents an overall measure of the error variance associated with the model parameter estimates and tends to increase sharply in value when the selected model order (the number of ADZ elements in the multi-order ADZ model) is greater than that justified by the data.

The modelling procedure used in microCAPTAIN is based on the repeated evaluation of these two statistics for different order models (i.e. for different values of n, m and δ): the best identified model is then selected as the model which simultaneously provides a good explanation of data, as indicated by a low relative value of R_T^2, and well defined parameter estimates, as indicated by a high relative value for the EVN. In particular, as the number of model parameters is increased so R_T^2 tends towards a "plateau" with very little improvement markedly when the model has too many parameters, illustrating the large increase in uncertainty that accompanies over-parameterisation. Because it may increase by several orders of magnitude following the onset of over-parameterisation, the EVN is normally represented by its natural logarithm, ln EVN.

EXPERIMENTAL TECHNIQUES AND DATA PROCESSING

Experimental Sites

The ADZ model study involved dilution gauging methods in selected reaches in Crimple Beck (Beven 1976). It is a catchment area near Harrogate, Yorkshire, comprising small, rocky, steep and rough channels. Flow in selected streams is characterised by slow pool segments, past riffle and rapid segments, waterfalls, and other irregularities in the channel bed creating rapid changes in flow depth and width.

In the experiment, common salt in solution was injected as a single input (slug) at a selected upstream point in the reach. The concentration of salt was subsequently measured at the downstream stations using a portable electrical conductivity meter. The conductivity measurements were then converted to an equivalent concentration of salt by a calibrated dilution of a sample of the input solution with distilled water.

The distance between the point of injection of salt and the sampling point downstream was 30 metres and because of the relative roughness of the stream this offered complete mixing of the tracer. Studies conducted by Beven (1976) showed that the Darcy-Weisbach roughness coefficient (f) was seen to decrease with increasing discharge but at low flows the values are very high. The highest f value recorded was 12 and this is equivalent to a Manning n of > 1. Eighteen experiments were carried out with discharges varying between 4 and 190 litres/second.

Data Processing

In order to describe the transportation and dispersion of pollutant using the ADZ model, two types of observed data were required: the upstream (input) and the downstream (output) data. The measured downstream data were taken from the salt concentration-time data gathered in the dilution-gauging experiments. The output data was compiled at a sampling interval of 15 to 30 seconds.

In the experiments, the upstream (input) data are not the real observed data since Beven (1976) only documented the downstream (output) observations. However, as the common salt solution was injected as a pulse, it is possible to synthesise the input data in the form of an "impulsive" response. This was carried out in the following manner:

(1) At $t = 0$, the input concentration is U g/l. We will see that the U value is, to some extent, arbitrary. However, it was assumed for the moment that it is larger than the maximum observed output data.
(2) When $t > 0$, then the input concentration is zero.

In addition to ADZ model parameter estimation, the data analysis also includes more conventional hydrological calculations. These include the mean travel time $\bar{t}$ which is obtained as the real time difference between the centroid locations of the input data and the observed output concentration-time profiles. Knowing the value of $\bar{t}$ and the discharge Q, other hydraulic parameters related to the ADZ model can be calculated. They are the reach volume (V), ADZ residence time (T), ADZ effective volume (V_e) and the V_e/V ratio.

RESULTS AND DISCUSSION

The results of the study are presented and discussed in two parts: estimation of the ADZ model i.e. the identification and estimation of the ADZ model order; and the physical description of the ADZ.

Estimation of the Aggregated Dead-Zone Model

The results of best model order for the whole series of experiments are summarised in Table 1. *Fig. 1* is an example of the modelling results obtained from the analysis, showing the input (upstream) concentration-time profile and compares the second order (n = 2, m = 2) ADZ model output with the measured output data from the downstream site. The identification statistics in this case (R_T^2 = 0.9941 and 0.9932; ln EVN = -7.5067 and -8.4438) indicate a good, well-defined model. It will be noticed that the model satisfactorily explains the whole of the concentration profile, including the tail. Similar results are also obtained from other experiments in terms of model order (n=2 and m=2) and the identification statistics (R_T^2 are generally greater than 0.9860 indicating that the ADZ model explains the observed data with greater than 98 per cent accuracy).

TABLE 1
Results of best identified model for Crimple Beck

Experiment	No. of 'a' Parameters	No. of 'b' Parameters	Time Delay (sec.)	RT^2	lnEvn
703	2	2	135	0.9932	-8.4438
704	3	1	270	0.9986	-8.7989
705	2	2	105	0.9976	-8.7842
706	2	2	120	0.9923	-8.6133
707	2	2	105	0.9888	-6.5690
708	3	1	75	0.9798	-6.0572
709	2	2	75	0.9798	-6.3054
710	3	1	90	0.9860	-5.9083
711	2	2	120	0.9941	-7.5067
712	2	2	240	0.9955	-8.2270
713	2	2	120	0.9941	-7.5066
714	3	1	60	0.9999	-10.8412
715	2	2	240	0.9974	-7.6762
716	3	1	360	0.9981	-8.6582
717	2	2	180	0.9983	-9.3467
718	2	2	75	0.9961	-8.7723
719	3	1	450	0.9951	-7.2254
720	3	1	480	0.9988	-9.0192

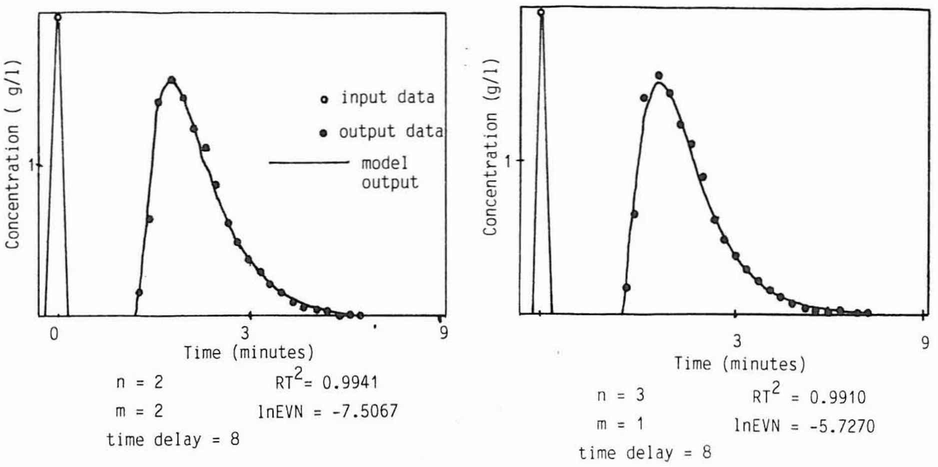


Fig. 1. Modelling results for Crimple Beck

The second order model implies that the reach consists of two individual reaches which may be either in series or parallel. This phenomenon was analysed further. Taking the results from *Fig. 1(b)* as an example, the model can be simplified into a transfer function as follows:

$$\frac{X_k}{U_k} = \frac{(0.0783\ Z^{o} + 0.1223\ Z^{-1})\ Z^{-9}}{(\ 1 - 1.4509\ Z^{-1} + 0.5192\ Z^{-2})} \qquad (10)$$

Factorising the denominator, the model can be written as:

$$\frac{X_k}{U_k} = \frac{(0.0783 + 0.1223\ Z^{-1})\ Z^{-9}}{(1 - 0.8107\ Z^{-1})\ (1 - 0.6401\ Z^{-1})} \qquad (11)$$

Splitting equation (11) into partial fractions gives the following equation:

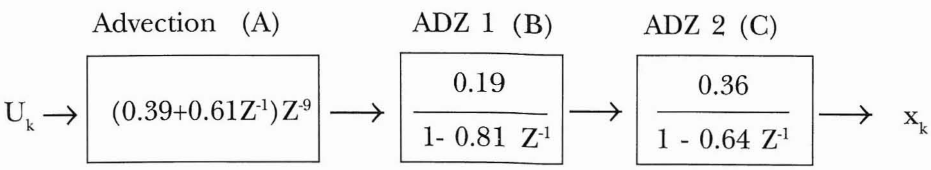
$$\frac{1.0926}{1 - 0.810\ Z^{-1}} - \frac{1.0143}{1\ -\ 0.6401\ Z^{-1}} \qquad (12)$$

Since the two transfer functions in equation 12 are substracted, the possibility of parallel flow is therefore rejected. The roots of the second order denominator and the sign of the two transfer functions of the remaining experiments also indicate that the two ADZ elements have to be in series to satisfy the physical constraints. This can be demonstrated further by normalising equation 12 to unity steady-state-gain in the following form:

$$\frac{1}{2.946} \times \frac{0.0783\ (1 + 1.56\ Z^{-1})\ Z^{-9}}{(1 - 0.81\ Z^{-1})\ (1 - 0.64\ Z^{-1})}$$

$$= \frac{0.0266\ (1 + 1.156\ Z^{-1})\ Z^{-9}}{(1 - 0.81\ Z^{-1})\ (1 - 0.64\ Z^{-1})} \qquad (13)$$

where 1/2.946 is the normalisation allowed by the arbitrary choice of u; the steady-state-gain now is equal to unity (SSG=1). The transfer function can be rewritten as:



where block A represents the advective effects (pure-time delay of 9 sampling periods) and the value 0.39 + 0.61 Z^{-1} is to allow for the additional "non-integral" time delay which gives rise to the requirements for the 2 "b" parameters. Blocks B and C represent 2 unequal ADZ elements in series.

Physical Description of the Aggregated Dead-Zones

Fig. 2 summarises the mean travel time (t), pure time delay (Γ) and the ADZ residence time (T) as a function of discharge (Q). It demonstrates

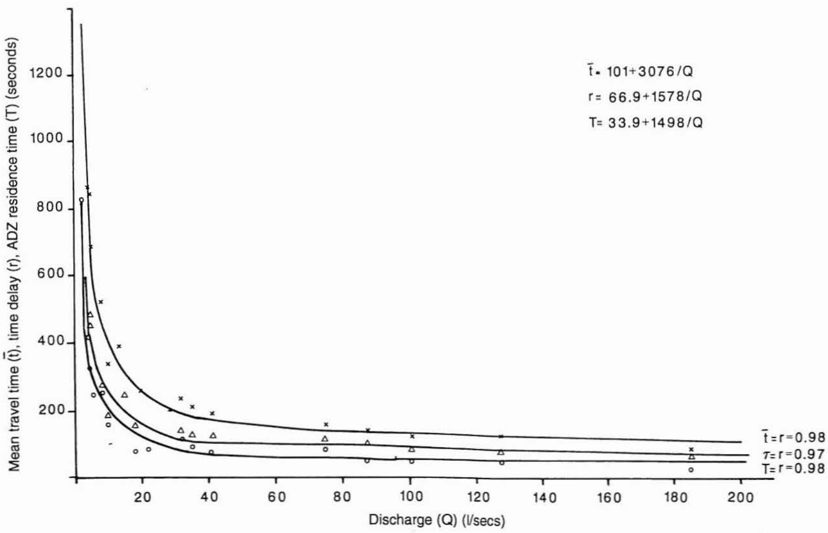


Fig. 2. Mean travel time, time delay and ADZ residence time as functions of discharge for Crimple Beck

that these parameters exhibit a relatively smooth functional relationship with discharge, with the parameters decreasing with Q as might be expected from physical considerations. The curves however, level out as Q increases. Similar relationships have been found by Beven (1976), Beltaos (1982) and Young & Wallis (1986).

The relationship between the reach volume (V) and the ADZ effective volume is also analysed and summarised in *Fig. 3*. It shows relatively linear relationships between the two parameters. The results also show that the volume associated with the dispersion of pollutant (V_e) is less than the reach volume.

Fig. 4 shows the ratio V_e/V as a function of discharge. This is an interesting parameter in physical terms; it is a measure of the importance of the dead-zone effects, as defined by the ADZ volume V_e, in relation to the total volume of water in the reach V. In a more general dead-zone context it has been referred to as the "immobile fraction". It will be noted that since $V_e = Q.T$ and $V = Q.\bar{t}$, the ratio V_e/V is equivalent to $T/\bar{t}$ and so provides a measure of the ADZ residence time. For the channel investigated, the ratio seems relatively independent of discharge. The mean value of the ratio lies between 0.3 and 0.4. The results for the V_e/V ratio are very important. If further studies confirm that the ratio is relatively constant for a particular reach or type of channel, it will have major implications for the modelling of riverine dispersion. The transport and dispersion behaviour of pollutants in a wide range of flow can be estimated from this ratio.

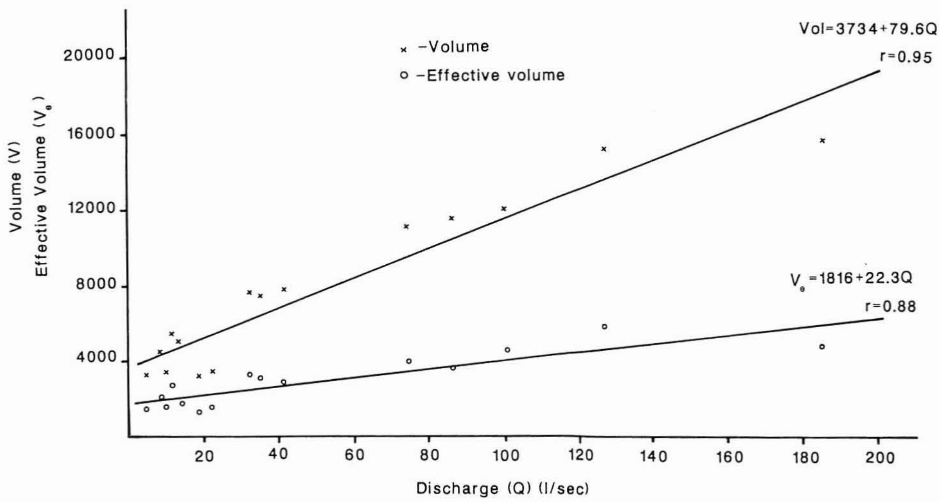


Fig. 3. Reach volume and ADZ volume as functions of discharge for Crimple Beck

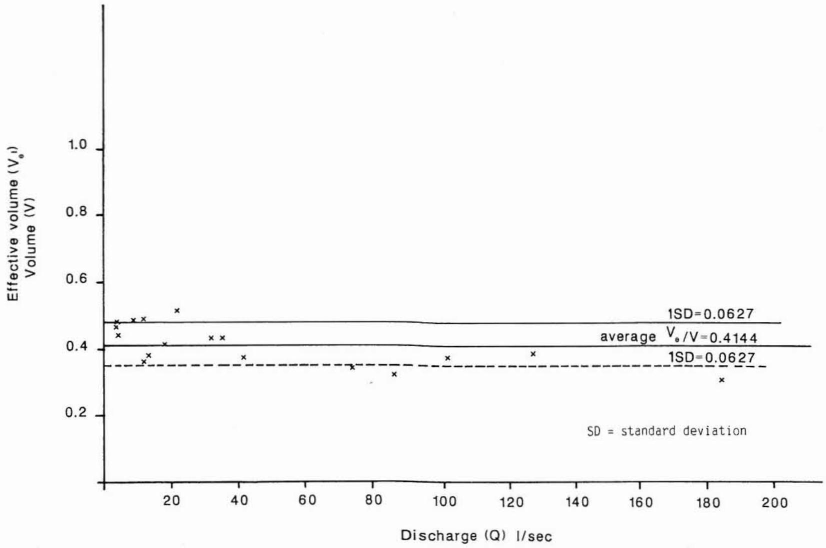


Fig. 4. Immobile fraction as a function of discharge for Crimple Beck

CONCLUSIONS

The recent approach to water-quality modelling reviewed in this paper is based on the assumption that the longitudinal transportation and dispersion of pollution are governed not by the classically assumed mechanisms of the distributed parameter, Fickian-Diffusion model, but by the aggregative effects of the dead-zones in the river whose "residence time" then defines the dispersion properties. These dead zones, which arise from various factors associated with the non-uniformity of the river, tend to characterise natural channels and lead to transient retention of a pollutant and increase of the dispersion processes in the stream. The resultant ordinary differential equation, Aggregated Dead-Zone (ADZ) model can be simplified into discrete form, where the dispersive characteristics are described by the n parameters and the presence of the non-integral time delay or additional parallel dead zones by the m parameters. The model is attractive not only because the dead-zone phenomena are readily observable in natural streams, but also because it provides a much better explanation of the observed data.

The results of the study in Crimple Beck, Yorkshire confirm earlier promise of the ADZ model when fitted to data from a wide variety of river channels in the UK (Young & Wallis 1986). They also indicate that the parameters of the ADZ model (namely the advective transport time delay b, the residence time T and the ADZ volume V_e) are all relatively smooth functions of stream discharge Q. The results also suggest that the ratio V_e/V, which is a measure of the dead-zone effects in relation to the total water volume in the reach at any time, appears to be relatively independent of discharge. This opens up the possibility of calibrating the reach in ADZ terms from the results of only a small number of dilution-gauging or dye- tracer experiments.

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