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Application of River Water Quality Models: The Role of Dispersion in the Model Calibration[3]

ABSTRACT

In solving real-world river water-quality problems, mathematical models at present are used very little at the decisional level. The reason for this is, in our opinion, the existence of unresolved difficulties associated with the collection of the data required for model calibration. Surprisingly, the literature does not contain a consistent description of criteria supporting the design of data gathering campaigns explicitly dedicated to model calibration. In particular little attention is paid to the role that dispersion plays in this context. It is known that plug flow models can be more easily calibrated than dispersion models when the data gathering campaign is suitably organized. But when can a plug flow model substitute a dispersion model? This paper derives a theoretically sound criterion to reply to this fundamental question.

Keywords: water quality modeling, data collection campaigns, environmental monitoring, calibration, parameter estimation.

1. INTRODUCTION

The planning of a river basin and the Environmental Impact Assessment of corresponding actions make immediate demands for models that are simple enough to be handled by technicians from environmental agencies and to be set up at a reasonable cost. These models must however be sufficiently reliable and sophisticated to describe a real- world system with a suitable level of accuracy, detail and flexibility. For a very large number of cases, one-dimensional models are certainly well-suited for these purposes. However, they must be well calibrated.

Although in the literature there are even very detailed descriptions of the available data (see, for instance, *Gunnerson* [1967] who deals with a tidal estuary), or of the results obtained (see for instance *Betty Ng et al.*, 1996), surprisingly, no emphasis has been placed on fully describing the organization and execution of data gathering campaigns aimed explicitly at model calibration. This reflects the fact that models, in practice, are often badly calibrated or fed with inadequate data. As an obvious consequence, their outputs are not reliable enough. This is perhaps the main reason why, in many countries and in Italy in particular, river quality

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models are actually seldom used. More precisely, they are often used by consulting firms as a "façade" in order to achieve a look of seriousness or completeness or just to comply with given Terms of Reference (typically in Environmental Impact Assessment). At the decisional level, however, they are almost ignored.

The difficulties associated with the data gathering phase derive from, on the one hand, the complexity (number of state variables and parameters) of the model, and, on the other hand, much more heavily, from the structure of the transport term. This depends, in particular, on the presence of dispersion. In fact, the presence of dispersion generally requires the collection of a two-dimensional (time-space) information: the initial condition, the boundary conditions and the pattern of all the exogenous inputs affecting the system. How can the initial condition be measured? (Note that in the case of polluted rivers it cannot be assumed to be zero; an assumption generally and correctly made in dispersion experiments with the release of tracers. See, for instance, *Carter and Okubo* [1972], *Day* [1975], *Bencala and Walters* [1983], *Jobson* [1987]). How can the huge number of collected samples be analyzed in a relatively short interval of time (specially in the case of biodegradable organic pollutants)? These questions, as far as we know, have never been clearly addressed (an interesting attempt in this direction can be found in *Shieh and Davidson* [1971], although the approach adopted is very empirical and is only applicable to a very special situation).

It is useful to point out that the problem we deal with in this paper is one of identification in the original meaning of the term, because our final aim is the model calibration. It is not, however, a classical parameter identifiability problem; indeed, we focus on a more operational, but basic issue which has to be faced previously. It can be noted, in fact, that if the water quality model were described by ordinary differential equations, then it would be possible to use powerful results from identifiability theory. However the serious problem is that the basic model, describing the fate of a solute compound in a river, is not originally written in terms of total differential equations (although this may be justified in some cases as, for instance, in *Wilkinson et al.*, 1995), but, instead, in terms of partial differential equations, i.e. it concerns a two-dimensional (time- space) domain, and not a one-dimensional (time) domain. The key issue is, accordingly, to obtain data that are suited to: first, integrate the model partial derivative equations, and, second, calibrate the model (through comparison of the obtained solution with instream measured data). Although it is with no doubts perfectly known in the literature what are the related mathematical requirements, the practical implications seem to have been almost completely disregarded. The dramatic conclusion we reach is that it is practically impossible to collect all the required data.

The role of dispersion

It may be observed that if dispersion is assumed to be absent, then the well known method of characteristics provides a criterion that dramatically reduces the data collection effort, under the condition that the campaigns are suitably organized. Actually, very often data collection campaigns are carried out according to this method, although perhaps the underlying assumption is not made explicit in the model structuring (this is the case, for instance, of *Scott ad Abumoghli*, 1995). The key issue is, then, when such a "drastic" simplification is applica-

ble. This is why much of this paper is devoted to investigate when a "plug flow" model is completely equivalent, from a theoretical and practical point of view, to a dispersion model. *Thomann* [1973] stated that the applicability of a plug-flow model is limited to the stationary case, but we show here that this conclusion is not true in general and we obtain a criterion that allows to discriminate a priori when the equivalence is acceptable for a given river stretch. Our arguments are however restricted, from a rigorous point of view, to one-dimensional spatial systems with linear kinetics, and to the case in which the interactions, if any, of planktonic with benthic variables can be modeled by introducing suitable exogenous inputs. In particular, problems involving a strong role of the sediments, like that dealt with by *Hawkins Writer et al.* (1995), or problems involving estuaries, like that described by *Betty Ng et al.* (1996), do not fit in our framework.

The paper is organized as follows. First, the general structure of (one-dimensional) models is presented. Then the difficulties to be faced in order to collect the data required by model calibration are pointed out. Three basic situations are then considered (stationary, periodic and aperiodic conditions) and possible design approaches are discussed for each. The benefits obtainable by using the method of characteristics are then shown, and the applicability of this method to the three basic situations is discussed in detail in the case of linear models. Finally, criteria for selecting the most suitable approach for the organization of the campaigns are proposed. Concluding remarks complete the paper.

2. STRUCTURE OF RIVER-QUALITY MODELS

Let us consider a river where the pollutants added to the stream spread through its cross section over a distance that is very short in comparison to the distance covered by a typical dynamic response, e.g. the sag in the case of DO. Hence the river can be described by means of one space co-ordinate only, namely the distance l [m] computed along its axis. Indeed, this is a very common case in river quality modelling for planning purposes. Let us also assume that the influence of biochemical phenomena over the hydrological and thermal processes is negligible, so that the flow rate Q [m^3/s], the cross-sectional velocity v [m/s] and temperature T [°C] are externally given functions of time and space (referred to as "exogenous inputs"). Under such assumptions, a biochemical sub-model is in made up of a set of spatial mono-dimensional partial differential equations that quantify the mass conservation principle. These equations describe the changes over space and time of the state vector **p** [gr/m^3] of state variables -water quality indicators- that represent the average cross-sectional concentrations of the chemical compounds and of the populations of the food web assumed to be representative of water quality. By denoting with, and A [m^2] the cross sectional velocity and area, respectively, of the stream, where A=Q/v [m^2], the related general vector equation can be given the following form (see for instance *Rinaldi et al.* [1979]):

$$\frac{\partial \mathrm{p}}{\partial \mathrm{t}} + \mathrm{v}\,\frac{\partial \mathrm{p}}{\partial l} = \frac{\partial}{A\ \partial l}\left(\mathrm{AD}\,\frac{\partial \mathrm{p}}{\partial l}\right) - \frac{S_q}{A}\,\mathbf{p} + \mathbf{S} \qquad \text{(Eq. 1a)}$$

The first and the second terms of the left hand side of Eq. 1a represent the rates of change of **p** with respect to time and space, respectively, as seen by an observer fixed on the river bank. The first term on the right hand side, called the dispersion term, represents the effects due to molecular and turbulent diffusion and to longitudinal dispersion, in a compact (and simplified) form, which in turn arise because the velocity field over a cross-section is generally non uniform (see *Bear* [1972] and *Rinaldi et al.* [1979]). The dispersion term is essential for all of the following discussion. Note that it is zero when the dispersion coefficient D is zero. The second term on the right hand side takes into account the dilution of **p** due to the water inflow S_q (flow per unit of length, [m^3/s m]) which is an exogenous input from the hydrological sub-model and is thus assumed to be given. Finally, **S** [gr/m^3 s] is the average cross-sectional source term that represents all the processes affecting the variable **p**. The term **S** depends, in general, on the whole vector **p**, on the external load (vectorial) function **P**(t,*l*) [gr/s] (simply called "load" in the following), on the hydrological (v, Q) and thermal (T) state variables (inputs), and on a vector θ of the parameters; i.e:

$$\mathbf{S} = \mathbf{S}(t,\ l,\ \mathbf{p},\ \mathbf{P},\ v,\ Q,\ T;\ \theta) \qquad \text{(Eq. 1b)}$$

3. THE INFORMATION REQUIRED FOR MODEL CALIBRATION

It is to be noted that to fully characterize the term **S** in Eq. 1a it is always necessary to specify the vector θ of the unknown parameters. E.g. in the classic Streeter-Phelps BOD-DO model, θ has two components: the deoxygenation and reoxygenation rate coefficients (see *Streeter and Phelps*, 1925). We do believe that, in general, the values of such parameters cannot be correctly measured, or calculated by means of some theoretical hypothesis, or taken from the literature. They can only be determined via a parameter estimation procedure based on field data. In fact, river conditions are always very different from those of any laboratory test where measurements are generally carried out. The values so obtained cannot be, for this reason, representative of reality. (A serious attempt to negate this statement by performing parameter estimation based on laboratory experiments is found in *Mc Cutcheon* [1987]. However, even there, only first order nitrification decay rate coefficients are estimated. Moreover, Mc Cutcheon's approach is applicable only to estimating reaction rates and not true model parameters. Finally, it requires a large number of field measurements. The validity of this approach has been experienced only for a particular type of river). A theoretical calculation is based on some sort of model, so that the calibration problem would arise for this model too. Finally, every river is such a complex system that "a priori" cannot be assumed to be equivalent to any other. This assertion is supported by observing that the range of parameter values given in the literature [e.g. EPA, 1985] is extremely wide. In order to therefore determine the value of the parameter vector θ, a parameter estimation (calibration) problem must be formulated and solved (see *Beck* [1987] for an important review).

As is briefly restated in the following, the estimation problem always requires us to integrate Eq. 1a, and this, in turn, generally requires a large amount of data.

To formulate the estimation problem it is necessary to assume that, for at least some of the I components p_i (i=1,...,I) of the state vector $\mathbf{p}$, n_i measurements $\{\underline{p}_i^k, k=1,..,n_i\}$ can be collected at suitable sampling stations along the river stretch. The simplest and most often used approach for parameter estimation is therefore the following, which assumes that the system model has no process noise. The "distance" between reality and the model (the integration/simulation of which produces the computed concentrations $p_i^k(\boldsymbol{\theta})$ at the same stations) is measured by a given error function $\xi[\boldsymbol{\theta}] = \xi[\boldsymbol{\theta}, \{\underline{p}_i^k\}_{i,k}, \{p_i^k(\boldsymbol{\theta})\}_{i,k}]$. Typically $\xi[\boldsymbol{\theta}]$ is the (weighted) sum, over all the measurements (k=1,..,n_i; i=1,...,I), of the squared deviations between the measured ($\underline{p}_i^k$) and the computed ($p_i^k(\boldsymbol{\theta})$) concentrations (deterministic least-squares estimation). The parameter estimation problem is hence formulated as the problem of determining a value $\boldsymbol{\theta}^*$ that minimizes the error function $\xi[\boldsymbol{\theta}]$. To solve it, perhaps the most common method is simply "by trial and error", in which an empirical iterative search is performed in the parameter space. More refined methods are typically Quasilinearization [*Bellman and Kalaba*, 1965; *Lee*, 1968; *Stehfest*, 1973], or Mathematical Programming algorithms [*Yih and Davidson*, 1975; *Rinaldi et al.*, 1979]. In both the cases, it is evident that the integration (simulation) of Eq. 1a is required at each iteration in order to evaluate $\xi[\boldsymbol{\theta}]$. When a system model is adopted in which the process and measurement noises are formally introduced, the previous method is no longer directly applicable because the state is now a stochastic variable. The approach most often used in this case is to linearize the system model and to then apply the results of the probabilistic linear least-squares parameter-state estimation. The result is the Extended Kalman filter [*Bellman et al.*, 1966; *Beck*, 1974, 1975, 1976, 1980, 1987; *Ikeda et al.*, 1974; *Lettenmaier and Burges*, 1976; *Bowles and Grenney*, 1978]. Even with this technique, a system simulation is (indirectly) required (see *Beck* [1987], Eq.14a), in order to compute the expected state value. Note, that this technique requires a lumped system model, so that, strictly speaking, it is not applicable when the system is described by Eq. 1a. Such an equation is, however, usually transformed into a lumped equation through space discretization or, alternatively, by assuming that dispersion is absent as is well clarified in the following sections. More generally, no matter what the particular approach adopted, parameter estimation requires the integration (simulation) of Eq. 1a directly or indirectly. Thus the information needed to carry out the parameter estimation problem comprises not only the set $\{\underline{p}_i^k\}_{i,k}$ of measurements, but also all the data necessary for the simulation itself. To point out the burden of such a data requirement, let us consider the simulation phase in greater detail.

In order to integrate the model Eq. 1a no matter the particular numerical scheme adopted [*Schoellhamer*, 1987; *Sobey*, 1984; *Bride and Rutherford*, 1984; *Cunge et al.*, 1980; *van Genuchten and Gray*, 1978; *Varoglu and Finn*, 1978; *Gray and Pinder*, 1976], one has to specify, in a suitable domain D of space and time, the inputs [$\underline{Q}(t,l)$, $\underline{v}(t,l)$, $\underline{S}_q(t,l)$, $\underline{T}(t,l)$] and the load function [$\underline{\mathbf{P}}(t,l)$] that "cause" the measurement set $\{\underline{p}_i^k\}_{i,k}$. The domain D is commonly a rectangular domain $T \bullet L$ defined by the cartesian product of the modeled river stretch L and the observation interval T. Moreover, two "conditions" must be given: the *initial* and the *boundary conditions*. The first condition is a "picture" of the concentrations that are present all along the river stretch at (initial) time t=0 and corresponds to specifying $\mathbf{p}(0,l)=\underline{\mathbf{p}}_i(l)$

for all $l \in L$. The second condition corresponds, in the simplest case of the absence of dispersion (D=0), to assigning $\mathbf{p}(t,0)=\mathbf{p}_u(t)$, i.e. to assigning the time evolution of $\mathbf{p}$ in the upstream (initial) section. In the opposite case (i.e. when dispersion is not negligible) the concentration $\mathbf{p}(t,L)=\mathbf{p}_d(t)$ in the downstream (final) section must also be specified.

Here is the crux of our problem: the practical difficulties associated with the collection of the data necessary in specifying all that information. Let us illustrate these difficulties by means of a very simple example. We wish to model a river stretch L of 100 km in length, affected by (only) 15 significant loads (tributaries and/or sewage discharges), with a very simple BOD-DO model (i.e. $\mathbf{p}$ is two- dimensional). The parameter vector $\boldsymbol{\theta}$ of such a model be six-dimensional. In order to obtain a representative image of system conditions, it is reasonable to observe it for at least one day (i.e. T equals 24 hours), so that it would be possible to observe the daily load cycle. To define the initial condition $\mathbf{p}_i(l)$ then one certainly needs no fewer than 15 instream samples which are collected at stations spaced along the river stretch. To specify the upstream boundary condition $\mathbf{p}_u(t)$ at least 12 samples (one every 2 hours) are required. When dispersion is not negligible, 12 additional samples (one every 2 hours) must be collected to define the downstream boundary condition $\mathbf{p}_d(t)$. The load function $\mathbf{P}(t,l)$ can be estimated by collecting at least 12 samples (one every 2 hours) at each of the 15 inflow points. This means that (without considering what is required to specify the input functions $Q(t,l)$, $v(t,l)$, $S_q(t,l)$, and $T(t,l)$) in order to carry out the model simulation a total of 223 samples must be collected. Two measurements must be carried out on each sample: one for BOD and one for DO. Moreover, by assuming a minimum of 10 data for each parameter to be reliably estimated, at least 30 instream samples must be collected to produce the measurement set $\{p_i^k\}_{i,k}$. The total requirement then for the estimation problem is about 500 measurements. It is apparent from this figure, which is definitely a lower bound for the case at hand, that huge practical difficulties would arise in collecting and quickly analyzing such a large number of samples (the measurement of biochemical indicators, like BOD, must take place within a few hours after sample collection). A laboratory is rarely able to afford such a stringent task. Moreover, it is to be noted that the collection of samples that specify the initial condition $\mathbf{p}_i(l)$ requires the availability of many skilled personnel who are distributed along the river stretch, and who act simultaneously at time t=0. Last, but not least, the effort required for the definition of the input functions $[Q(t,l), v(t,l), S_q(t,l), T(t,l)]$ should not be neglected. They must be given in the domain $T \bullet L$. In particular, the determination of the hydrological input $S_q(t,l)$ implies a huge number of costly measurements. In conclusion, it can be seen that it is practically impossible to solve the parameter estimation problem correctly when adopting the general unsteady-dispersion model described by Eq. 1a (except for the case of the release of tracers or pollutant spillover, since in that case the initial condition and the downstream boundary condition are null, the upstream boundary condition is a known impulse function, and the load is null).

It is now evident that, on the one hand, the number of state variables and parameters (i.e. the complexity of the model) should be kept as low as possible and that, on the other hand, any possible reduction in the information required to carry out the simulation is of great importance. In order to understand whether and how such a reduction can be carried out, three basic situations are analysed in the following section.

4. THREE BASIC SITUATIONS

Let us consider the following three basic situations (or conditions) which are meant to apply to the entire system (i.e. to the hydrological, thermal and biochemical sub-systems) and to which progressively larger information requirements correspond:

(a) - stationary conditions

(b) - periodic conditions

(c) - aperiodic conditions.

In the first case (a), the partial derivative with respect to time in Eq. 1a is null, so the equation becomes a total derivative which can be integrated by solving a two boundary value problem. Hence the initial condition $\mathbf{p}_i(l)$ is no longer necessary. Furthermore, the boundary condition and the loads can be measured once only in the interval T. The reader can then easily compute that the data requirement is now for only 94 (= [17+30]*2) measurements. Furthermore, the data gathering campaign is quite simple and could be executed by an individual operator. Of course, this is true only if the system is really under stationary conditions, a fact that must be ascertained and that is unfortunately very rarely met in practice.

In the second case (b), we have two alternatives: either (b1) to describe the average behaviour of the system, hence going back to the previous case, or (b2) to consider the time varying, periodic behavior directly. In case (b1), in fact, it is easy to see, provided that the source term **S** is linear with **p** and **P**, that the space dynamics of the average concentrations are governed, as in case (a), by the stationary version of Eq. 1a. (This can be proved easily by applying the Laplace transform with respect to t to both sides of Eq. 1a and by then setting the complex variable s to zero. What one obtains is the equation governing the dynamics of the time averaged concentration $\underline{\mathbf{p}}(l)$.) Even in case (b2) the difficulty of measuring the initial condition $\mathbf{p}_i(l)$ can be overcome: in fact, if the system is asymptotically stable (as it must naturally be) one can assume an arbitrary initial condition $\underline{\mathbf{p}}_i(l)$ and determine the periodic function $\tilde{\mathbf{p}}(t,l)$ to which the solution of Eq. 1a will converge for t approaching infinity. (In practice, this function can be computed by integrating Eq. 1a over an interval of time which is long enough to "forget" the initial arbitrary condition. Note that since the system is by hypothesis under a periodic condition, the boundary condition, the inputs and the load are known for any t, once they are known all across one period.) With respect to the stationary case, in case (b) there is a considerable increase in the number of required measurements. In fact, except for the initial condition (which in the above example is 15 samples), one has to collect the same set of samples required under aperiodic conditions (case c) because the measurements thus obtained are then used to compute a reliable average (case (b1)), or to integrate the general time varying Eq. 1a (case (b2)). In both cases, however, the advantage with respect to the aperiodic condition is twofold: (1) no initial condition has to be determined, and very importantly, (2) the measurements can be spread over time as desired, given that one samples the load and the boundary conditions globally all over an entire period T. Again, of course, it must be true that the system is actually under periodic conditions, but this can be seen in practice much more

frequently than stationary conditions.

We now come to the aperiodic case (c). We have already shown that it is practically impossible to collect all the information required for parameter estimation in such a case. We hence look for an approximate solution such that the information requirements can be reduced. The most attractive alternative is based on the assumption that dispersion is negligible (D=0). The original dispersion model then reduces to a plug- flow model that can be solved by using the old method of characteristics. As is shown in the next section, this approach greatly reduces the amount of data required to carry out the simulation. It is interesting to note that almost all the (few) cases presented in the literature, where a data gathering campaign is described, refer to this assumption explicitly or implicitly. See, for instance, *Jakeman et al.* [1989], *Mc Cutcheon* [1987], *Todd and Bedient* [1985] and *Edeline* [1981]. The size of the error introduced by neglecting the dispersion effect is, however, obviously questionable, and it is interesting to wonder if it can be reduced by means of some technique. The analysis of these questions is the subject of Section 5.

The findings of this section are synthesized in Tab. 1.

Tab. 1 - How to deal with the initial and boundary conditions and the loads in the three basic situations

Situation	Initial condition	Boundary condition, and loads
a) Stationary	not necessary	only one measure
b) Periodic	not necessary or computable	measure over a cycle
c) Aperiodic		
- negligible dispersion	not necessary	only one measure
- not negligible dispersion	necessary	measure over the interval *T*

5. APPLICABILITY OF THE METHOD OF CHARACTERISTICS

When the method of characteristics (see Appendix 1) can be applied, data gathering campaigns can be designed with a very simple and elegant criterion: *the samples* (and the input measurements) *have to be collected as if they had been collected by an observer moving downstream at the same velocity as the flow*.

To point out how the use of the method of characteristic affects the data gathering phase, let us again consider our example (once more, only the measurements related to quality indicators are considered). In order to obtain the 60 measurements necessary for parameter estimation, by means of samples (two measurements for each sample) collected at the 15 instream sampling stations, it is necessary to carry out two different data gathering campaigns. The data necessary for simulation must also be collected in each campaign, that is 16 samples: 15 to quantify the loads and 1 for the initial condition. (Note that this requirement is analogous to that found for the stationary case (a), with the exception that the downstream condition is no

longer necessary since in the absence of dispersion no signal can propagate upstream.) In conclusion, a total of only 62 samples must be collected for the two campaigns, and hence only 124 measurements (against 500) have to be carried out. It must be noted that besides a consistent reduction in the data requirement other considerable advantages arise:

- there is no longer any need for simultaneous sampling because the initial condition $\mathbf{p}_i(l)$ is no longer required;
- the effort required by the analysis laboratory is less than 1/8 that of the previous case because the 124 data are collected in two independent campaigns which can be well spread out over time;
- as the two campaigns can be carried out under different hydro- thermal and load conditions, more insight into the system is obtained and so the model can be more representative of reality;
- the number of measurements can be even further reduced by increasing the number of in-stream sampling stations so that fewer campaigns are required.

In this section we search for a criterion that indicates when the error induced by adopting the solution to the plug-flow model Eq. 1a with D=0) instead of the solution to the dispersion model Eq. 1a with D≠0), is negligible: i.e. we look for a criterion that indicates when a plug-flow model can be adopted to model real-world conditions where dispersion is actually present. Under stationary conditions the criterion we look for is the Dobbins' Criterion (DC). Even if this criterion is well known we present a non-classic way of proving it since this helps us in deriving an analogous criterion in the periodic case (more precisely, for a particular periodic case). This criterion, in turn, helps when dealing with the aperiodic case. From these criteria we derive a technique that, when adopted, always produces a reduction in the approximation error.

5.1 Stationary conditions

From a comparison of the numerical solutions to a simple plug-flow BOD-DO model and of the corresponding dispersion model, *Dobbins* [1964] concluded that dispersion can be assumed to be zero when the following inequality holds:

$$\frac{2\ kD}{v^2} < 10^{-2} \qquad \text{Eq. 2}$$

where k [s^{-1}] is the greater of the deoxygenation and the reoxygenation parameters. Condition Eq. 2 is known as the Dobbins' Criterion (DC). (Sometimes, as in EPA [1985], the criterion is credited to *Ruthven* [1971], but we prefer to credit it to Dobbins, since, as far as we know, he first proposed it).

When the DC is fulfilled, dispersion is negligible in the sense that a natural plug-flow

model is as good operationally as a dispersion model. The data gathering campaign can therefore be organized along a characteristic line defined by equations Eq.5a and Eq.5ab (*natural characteristic line*). This was since now a known result in the relevant literature.

When the DC is not fulfilled, one would intuitively expect that this opportunity would be lost and a dispersion model compulsorily adopted. The intuition is however wrong. As demonstrated in detail in the Appendix 2, when the corrected velocity v^*, given by Eq.13a, is substituted into the natural river velocity v in the definition of the characteristic line (see Eq.5a), the corrected plug-flow model produces the same answer as the dispersion model. In conclusion, under stationary conditions we can always adopt the corrected velocity v^*, then collect data along the corresponding (corrected) characteristic line and finally calibrate a plug-flow model. Moreover, since the natural value k for the reaction rate coefficient through Eq.13a is assumed for both the corrected plug-flow and the dispersion models, it follows that the best estimate for k^* computed in the plug-flow model is also the best estimate for k in the dispersion model.

The reader may observe that, from the point of view of the design of data gathering campaigns, all the techniques we have explained in Appendix 2 are useless. He (she) would be right. In fact, in the stationary case the number of data required by model calibration is not affected by the design criterion one adopts, for the simple reason that concentrations do not vary over time. However, the entire technique is not irrelevant from a conceptual point of view, since it clarifies the relationships between the two types of models (the dispersion-stationary model and the plug-flow model). The knowledge of these relationships is of great help in the analysis of the non-stationary (aperiodic) case.

5.2 Periodic case

In the analysis of the periodic case there is a precedent in *Thomann* [1973], who stated that the applicability of a plug-flow model is in practice limited to the stationary case (in which case there would obviously be neither any need nor benefit in organizing the data gathering campaign along a characteristic line). To reach this conclusion he started from the observation that when a system, described by the simplified version of Eq. 1a presented in Sect. 5.1, is driven in the initial section (l=0) by a periodic sinusoidal load of amplitude U and frequency ω, it supplies an output concentration p(t,l) which, in every section l>0, is a sinusoid of amplitude $R_D(\omega,l)U$ and phase $\Psi_D(\omega,l)$. (This is a well known result from System Theory where the couple [$R_D(\omega,l)$, $\Psi_D(\omega,l)$] is called frequency response.) Then he showed that, under the same load condition, the corresponding plug-flow model also supplies a sinusoidal output concentration p'(t,l). In this case the frequency response [$R_P(\omega,l)$, $\Psi_P(\omega,l)$] is, however, significantly different, both in amplitude and in phase, from the dispersion model frequency response. He demonstrated these results through a series of dimension-less graphs in order to explore a wide range of possible values of the key variables, namely: v, D, k, ω, l. The conclusion was that "...when waste load inputs vary with period of about 7 days or less, the effects of small amounts of dispersion on the amplitude of the water quality response may be significant. For large, deep rivers the effect of dispersion can generally not be neglected in time-varying studies". From such statements one concludes that the area of applicability of a

plug-flow model (and therefore of the method of characteristics), is very narrow since in the majority of cases either the dispersion is not small enough or the load frequency is too high (typically with a period of one day for urban waste).

In the Appendix 3, we show that this conclusion is partially false. In fact, contrary to Thomann, we prove that in the simple sinusoidal load condition he considered, a plug-flow model always exists which is completely equivalent to the dispersion model. Moreover, and more importantly, we derive an "Extended Dobbins' Criterion" which provides a guideline to evaluating the applicability of a plug-flow model when the load is not sinusoidal.

It is perhaps worth anticipating intuitively why we will reach different conclusions to those of *Thomann* [1973]. The reason is not a mistake in his deductive reasoning, but an incorrect positioning of the problem he considered: Thomann compared a dispersion model and a plug-flow model characterized by *the same* value of the coefficient k. As already pointed out, the reaction rate coefficient k, or more generally the model parameter vector θ, is not a priori known and must be calibrated on the basis of field data that are collected in dedicated campaigns. Hence here is the new key idea: it is possible to use a plug- flow model in cases where, according to Thomann's analysis, it would be not applicable, because the calibration itself will produce a value k^* for the reaction rate coefficient that may be, in general, different from the natural value k (that which would be obtained by adopting a dispersion model), but it is such that the output response of the plug- flow model be as close to the observed concentrations as would the output response of the dispersion model. More precisely, in the absence of process and measurement errors, the input-output relationship of the plug-flow model (parameterized with k^*) and that of the dispersion model (parameterized with k) are identical. One might claim that the value obtained for the reaction rate coefficient is not the "true" value. This objection, however, could give rise to endless metaphysical discussions over the meaning of "true". Moreover, if the purpose is to develop a model for decision-making, the only thing that really matters is that the model supplies the right response, even if by using a "fictitious" coefficient.

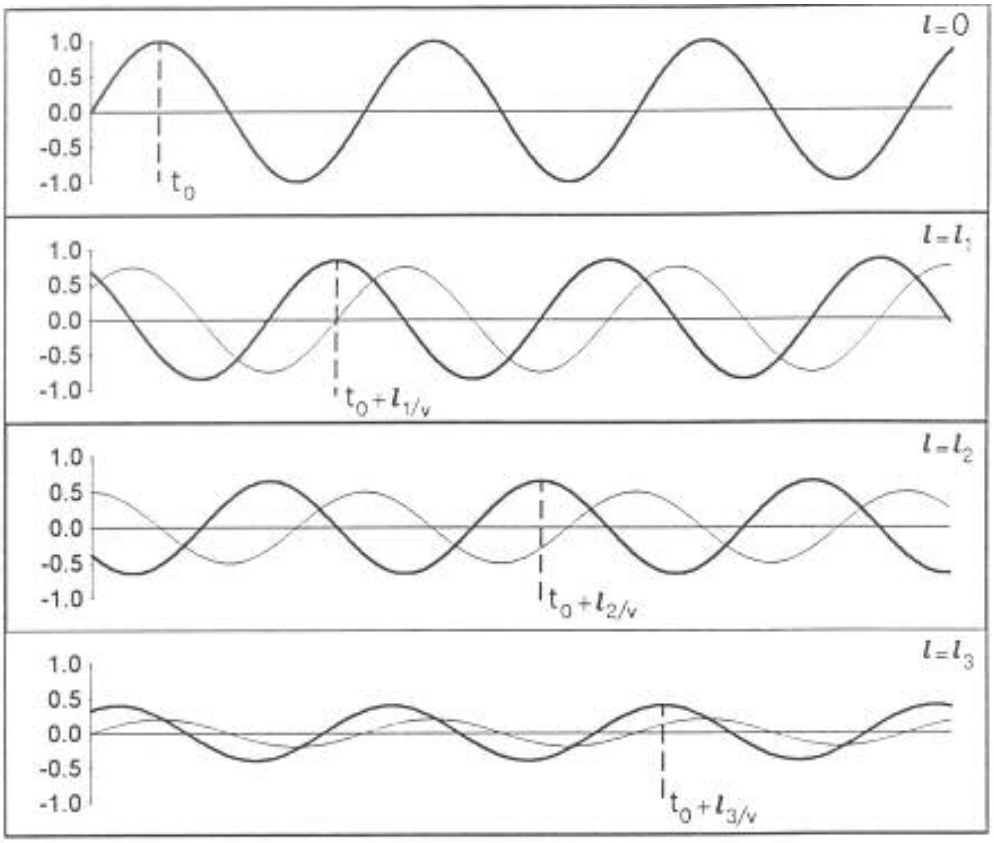

Fig. 1. Distortion effect due to the phase difference (re-worked from *Thomann* [1973], arbitrary scales).

At first glance the above fairly simple idea seems to be destroyed by the following observation: consider Figure 1 (re-worked from Figure 7 of *Thomann*'s paper). This figure reproduces (see window l=0) the fluctuations $\Delta p_u(t)$ of the upstream concentration $p_u(t)$ (boundary condition) with respect to a reference level. It also shows the corresponding fluctuations $\Delta p(t,l)$ of the water quality responses $p(t,l)$ in three downstream sections l_1, l_2 and l_3, for both the dispersion (dashed line) model and for the natural plug flow model (solid line). (Remember that this latter is obtained by setting D=0 in the dispersion model, hence note that the coefficient k is given the same value in both models). By observing the figure, one notes that the responses of the two models differ not only in wave amplitudes but also in phase. One may accept intuitively that the difference in amplitude could be eliminated by a suitable calibration of the plug-flow model (i.e. by using k^* instead of k), but the difference in phase is a more difficult phenomenon. Let us highlight the implications. According to a plug-flow model, a "concentration wave" travels downstream at river velocity v, since, by assumption, there is no longitudinal dispersion effect. Hence, according to this model, when one samples in section l at time $t=t_0+l/v$ (i.e. when one samples along a characteristic line defined by Eq.5a, Eq.5a and Eq. 6a), one samples the effects of the decay process on the water plug that left the starting section

(l=0) at time t_0. Then, if that plug is associated with a concentration peak (i.e. if $p_u(t_0)$ is a maximum) the sampled value in section l is analogously a maximum (see solid line). On the contrary, this is false according to the dispersion model (observe the dashed line). Indeed, the sampled value may be an intermediate value as in section l_1 or even a nearly minimum value as in section l_2. This change of phase is justified intuitively by the fact that the dispersion effect mixes the water plugs as they travel downstream. A question is raised immediately: how can the calibration of the plug-flow model reproduce this phenomenon? Furthermore: the calibration of a plug-flow on data sampled along a characteristic line would be simply impossible. Observe, in fact, that the value of Δp is positive in section zero (at time t_0), nearly zero in section l_1 (at time t_0+l_1/v), while it comes back to being positive in section l_3 (at time t_0+l_3/v). No real value of the coefficient k exists that can reproduce these data.

Analogously to the stationary case, this difficulty can fortunately be resolved by substituting the stream velocity v with a *corrected velocity* v^*: the velocity at which the concentration wave travels downstream. In fact, when water samples are collected by an observer that moves downstream at velocity v^*, the concentrations look as if the samples were collected from the same water plug.

The result obtained in the Appendix 3 is of great interest for the design of data gathering campaigns. In fact, it says that, in the case of a river characterized by an upstream condition that varies sinusoidally with frequency ω, we can collect data along a characteristic line defined by Eq.5a and Eq.5a, where the velocity v is given the value v^* computed by means of Eq. 23. So a plug-flow model calibrated by using these data is completely equivalent to a dispersion model. Moreover, the estimate of the coefficient k for this latter model can be obtained from the estimate k^* by solving Eq. 24 with respect to k. In conclusion, it seems we have reached the goal we posed since we have calibrated a model that correctly describes a non-stationary condition. At the same time, we have also greatly reduced the number of samples to be collected since we have to collect data only on the characteristic line.

Although the conclusions reached in the previous statements are correct, the optimistic impression they give is partially false for two reasons. First, as in the stationary case, the corrected velocity v^* does depend on the natural value k, which is in turn unknown. Hence, as proposed in the stationary case, we must rely on an a priori estimate k_a of k, or better, determine a criterion that tells us when $v^* \cong v$. A second and more serious drawback affects our result: v^* and k^* depend on the frequency ω ! That means that v^* and k^* have a physical meaning only in the case of rigorously sinusoidally varying conditions, since only in that case does ω have a unique value. In fact, in the non-sinusoidal case, even if periodic, the value of ω is not unique (think about a Fourier's series development). Therefore, our result implies that we should use different velocities for different frequencies! Even if the previous result is fully valid conceptually, it is of no practical use for model calibration, except when the conditions vary sinusoidally.

However, the conclusion would not be so bitter if the dependence of v^* and k^* on ω were weak, i.e. if v^* and k^* did not vary significantly with ω. To overcome both problems, let us determine under what condition $v^* \cong v$ and $k^* \cong k$.

To determine this condition, let us develop the expression Eq. 23 and Eq. 24 of v^* and k^* into a Taylor's series with respect to ω and D in the neighborhood of $D=\omega=0$ as a function of the dimension-less numbers previously introduced, and let us consider only the first and second order terms. We have:

$$v^*(\omega,D) \cong v \left(1 + 2Đ - 2Đ^2 + (2-12Đ + 60Đ^2) W^2 + o^3 \right) \qquad \text{Eq.3a}$$

$$k^*(\omega,D) \cong k \left(1 + Đ - 2Đ^2 + (Đ^{-1} - 2 + 2Đ + 12Đ^2) W^2 + o^3 \right) \qquad \text{Eq.3b}$$

where $W = \omega D/v^2$ and o^3 represents the sum of terms that are infinitesimal of the third and higher order with D and ω. Note that W, as the Dobbins' number Đ, is a pure number and can be formally obtained from Đ by substituting k with ω. Moreover, when the value of W is negligible, the effects of unsteadiness in conditions are negligible. In that case, in fact, the expressions (23a,b) no longer depend on ω and are such that the ratio (k^*/v^*) equals $\delta(k/v)$, with δ given by Eq.13a, i.e. they satisfy the same condition that is valid in the stationary case. Therefore, the number W plays the same role in the periodic case as played by Đ in the stationary case, and we may state the following

Statement 1. Dispersion can be assumed to be null if both Đ and W are negligible (e.g. lower than 0.01). In such a case, a natural plug flow model (i.e. a model with $k^*=k$ and $v^*=v$) is practically equivalent to a dispersion model.

It is interesting to note that, as Statement 1 requires the DC to be satisfied (i.e. Đ < 0.01), and by recalling the definition of W, the same statement can also be posed in an equivalent form:

Statement 1a. Dispersion can be assumed to be null if Đ is negligible and $\omega \leq k$.

That is equivalent to saying that the load must fluctuate "with a period greater than the time 1/k": a condition that has already been found by *Li* [1972a]. Under the conditions of Statement 1, a natural plug-flow model can be adopted and thus the data gathering campaigns can be profitably organized according to the method of characteristics along the natural characteristic lines.

When the DC is not satisfied (i.e. Đ > 0.01) everything is not lost, since we may derive the following statement from Eq.3a:

Statement 2: when only W is negligible (i.e. W < 0.01) a corrected plug flow model can be adopted, where the corrected values k^* and v^* are related to the natural values k and v by expressions (23a,b) with W=0.

Even in that case, therefore, the data gathering campaigns can be organized along the characteristic lines, but these must be calculated on the basis of the corrected velocity v^*, given by Eq.3a. However, as already noted, a vicious loop then arises. It can be resolved by computing the characteristic line on the basis of an a priori estimate of k and by evaluating the validity of the estimate a posteriori. Furthermore, as expected, differently from the stationary case, it is now impossible to calibrate the model by collecting data along the natural characteristic line, except when Statement 1 holds. In fact, we may see from Eq.3a that it is never $v^*=v$, except when $k^*=k$, i.e. when Statement 1 holds.

To conclude the periodic case, we would have to specify how the conditions posed by the previous statements can be tested when the boundary conditions do not vary sinusoidally. In fact in that case the frequency ω is not unique, so that the value of *W* is in turn not unique. Since the solution we have proposed to this problem is also valid for the general aperiodic case, we prefer to consider that case directly.

5.3 Aperiodic case

From the previous discussion it is now easy to derive a criterion that is valid in the general case, that is, when conditions are non- stationary and aperiodic. Let ω' be the maximum frequency, if existing, that is present in the Fourier's transform of the boundary condition, or, when this is infinity, the highest significant frequency in the power spectrum of the boundary condition. Then, from Statements 1 and 2 the following criterion follows that for obvious reasons we propose to call the:

Extended Dobbins' Criterion (EDC). When $\omega' D/v^2 < 0.01$ a corrected plug flow model can be adopted where k^* and v^* are given by expressions (23a,b) with W=0. Furthermore, when the classical Dobbins' criterion is also satisfied (i.e. Đ < 0.01) a natural plug-flow model (i.e. a model with $k^*=k$ and $v^*=v$) is practically equivalent to a dispersion model.

It is interesting to have a practical feeling of when the EDC is satisfied. Dobbins himself, in his 1964 paper, stated that "the highest value that the writer has seen reported for D for a natural stream is 1.57 m^2/s; if this were to apply in a stream where v were as low as 0.1 m/s and k as high as 2 d^{-1}, the value of Đ would be as low as 0.004." On the basis of Dobbins' figures it appears that the DC is hardly violated in the upper and medium parts of a river; and by adopting the same figures it follows that the EDC is satisfied when ω' is lower than 0.00006 s^{-1}, or the period is longer than 4.4 hours. Dobbins based his judgment on *Taylor*'s [1954] and *Elder*'s [1959] formulas for the estimation of D. Later, *Glover* [1964] found that dispersion coefficients in natural streams were likely to be 10 to 40 times higher than predicted by the Taylor or Elder formulas. The lateral variation in stream velocity is the primary reason for the increased dispersion not accounted for by Taylor and Elder. By taking into account Glover's correction, the field of satisfaction of the DC then does not appear as wide as Dobbins thought. It is, however, interesting to note that from Statement 1a it follows that the EDC is satisfied when the DC is satisfied and ω is lower than k. From the values of k re-

ported by *EPA* [1985], it turns out that the time 1/k rarely peaks as high as half a day, thus the condition $\omega \leq k$ appears to be sufficiently easily met. In conclusion, when the DC is satisfied, the EDC is almost always satisfied too. (This is not true, of course, in the highly non periodic case of the release of tracers or pollutant spillover.)

5.4 More complex models

To conclude this section, we must stress that the EDC has so far been derived only in the case of a mono-component system, e.g. BOD alone. *Rinaldi et al.* [1979] showed that the classic Streeter-Phelps BOD-DO model is equivalent to a couple of mono-component systems, the first system governs the dynamics of the BOD concentration b, and the second system that of an "auxiliary" concentration a, defined as

$$a = d + \frac{k_1}{k_1 - k_2} b \qquad \text{Eq. 4}$$

where d is the DO concentration, and k_1 and k_2 the deoxygenation and reoxygenation rate coefficients respectively. Hence we know that the EDC can be generalized to the Streeter-Phelps BOD-DO model with a simple statement: the EDC must be verified for both k_1 and k_2. We do not know what happens in the general case of n-coupled variables. A theoretical development is formally difficult, but we do not see any structural reasons that may cause the failure of the criterion, provided that the corresponding model has linear source terms.

6. A PROPOSAL FOR THE GENERAL CASE

What can be done when the EDC is not satisfied, or the source term is not linear, or more than two variables are considered? One might think that, to be safe, it would be easier to adopt tout court a dispersion model, since it is conceptually "closer to reality". However, as shown in Section 3, it is practically impossible to collect all the data required for the calibration of such a model (except for the case of the release of tracers or pollutant-spillover in which case the use of a dispersion model is generally both feasible and necessary). The correct positioning of the problem is therefore one of a trade-off between a conceptually satisfactory model (a dispersion model), but one which is very likely to be poorly calibrated, and a conceptually less satisfactory model (a plug-flow model), but one which is probably well calibrated.

Finding an answer to this dilemma is not an easy task because it is generally impossible, or too cumbersome, to develop an analysis analogous to the one previously exposed. Furthermore, as already noted, the complexity of a model is determined not only by the structure of the transport term, but also by the number of state variables and the form of the source term **S** (see Eq. 1a). Therefore, it seems perhaps more attractive and feasible to develop a Decision Support System (DSS) that can help in selecting the entire structure of the model to be

adopted and, consequently, in planning the necessary data gathering campaigns. The DSS should allow one to specify the physical structure of the system under consideration (hydraulic characteristics, tributary locations, load patterns, etc.), the number and locations of the possible instream sampling stations, the number of samples that can be collected and analyzed in a given time interval due to budget constraints, etc. Then, one could select a model structure to be adopted, for instance a plug-flow model, and *simulate the calibration of the model*. That is, first generate realistic space time patterns of the water quality indicators by means of a dispersion model, for which parameters θ are given a priori values (for instance, taken from the literature). Then, extract the dataset that could be collected in dedicated campaigns from these patterns and calibrate the selected model on this dataset. Hence, the calibrated model could be validated through a series of simulated experiments that consider the planning scenarios that could be analyzed. The above procedure should be repeated over a suitable range of values of the key variables, namely v, Q, D, the a priori estimates of the parameters θ, and the dynamic characteristic of the loads.

On the basis of such analysis, it may be found that given the operational constraints on the feasible campaigns, a complex, conceptually satisfactory model cannot be calibrated well enough, and that therefore it performs worse than a simpler model which, in turn, owing to its simplicity, may be conceptually unsatisfactory, but able to be calibrated satisfactorily. *Wood et al.* [1990] demonstrated how an expert system can help in the calibration and simulation of a river quality model. We have not found, however, examples or proposals explicitly referring to the idea discussed above, i.e. to develop a DSS (or expert system) to support the simultaneous choice of model structure and organization of the necessary campaigns.

7. CONCLUSIONS

It was first noted that data gathering campaigns for model calibration constitute the key aspect in closing the gap between the theoretic development of river quality models and their application to real-world problems. Then, it was shown that the amount of data required to correctly carry out the calibration of a complete dispersion model in unsteady-state conditions is generally prohibitively large to be collected (except for the case of the release of tracers or pollutant- spillover). In order to find out under what conditions the data requirement can be reduced, three basic conditions have been investigated:

a) stationary conditions: such conditions do not present considerable difficulties in the calibration of a general dispersion model, but are rarely met in practice. Although it does not have effective implications in approaches to the data gathering problem, we have shown that a linear plug-flow model always exists that is completely equivalent to a given linear dispersion model. The velocity and/or the parameters of the plug-flow model are to be *corrected* with respect to their *natural* values (i.e. the values they have in the dispersion model) according to given formulas (see Eq.13a). Moreover, when the classic Dobbins' criterion is satisfied, the corrections turn out to be negligible, i.e. the dispersion effects can be ignored.

b) periodic conditions: under such conditions the difficulties presented by the data gathering campaigns, when a dispersion model is used, can still be afforded. However, we have

proved that in the presence of load conditions varying sinusoidally (but under stationary hydrologic conditions) the results found for the stationary case are still valid. It is, therefore, easier to calibrate a corrected plug-flow model (see Eq.3a), by taking advantage of the method of characteristics in the organization of the campaigns.

c) aperiodic conditions: in this case, the difficulties presented by the data gathering campaigns, when a dispersion model is used, cannot be handled at all. We have proved that when a specific condition is met, there is a linear plug-flow model which is completely equivalent to a linear dispersion model. Owing to the formal analogy of this condition to the classic Dobbins' criterion, we proposed calling it the "Extended Dobbins' Criterion" (EDC). When the EDC is met, it is possible and strongly advisable to take advantage of the method of characteristics in the organization of the campaigns.

The EDC has been derived only for the case of a monocomponent, linear model, but we feel it can also be adopted for multicomponent, non-linear models. In fact we do not perceive any structural reasons that prevent it being extended, even if the proof we developed cannot be extended technically to the non-linear case. In any case, in order to deal with more general cases, or with the case when the EDC is not met, it would be helpful to develop a Decision Support System that would allow us to "simulate the calibration" of different models (in particular, dispersion and plug-flow models), given the physical structure of the system at hand and any constraints imposed by the specific problem to be solved.

As a general conclusion, it can be stated that plug-flow models, and thus the method of characteristics, can be easily exploited under a much broader range of conditions than what was previously thought.

Examples of application of the previous theoretical conclusions will be presented in separate papers in this Journal, in order to derive guidelines for action that could help the engineering judgement and the common sense in the analysis of real world cases.

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APPENDIX 1 - THE METHOD OF CHARACTERISTICS

In this section the well known method of characteristics (see, for instance, *Di Toro* [1969]) is briefly restated for the benefit of the reader. By assuming that dispersion is absent, i.e. D=0 (plug-flow system), it is easy to see that Eq. 1a, together with the initial condition $\mathbf{p}_i(l)$ and the upstream boundary condition $\mathbf{p}_u(t)$, is completely equivalent to the following set of total differential equations

$$\frac{dt}{d\tau} = 1 \qquad \text{Eq.5a}$$

$$\frac{dl}{d\tau} = v(t,l) \qquad \text{Eq. 5b}$$

$$\frac{d\mathbf{p}}{d\tau} = -\frac{S_q(t,l)}{A}\mathbf{p} + \mathbf{S} \qquad \text{Eq. 5c}$$

with initial condition (see point A in Figure 2)

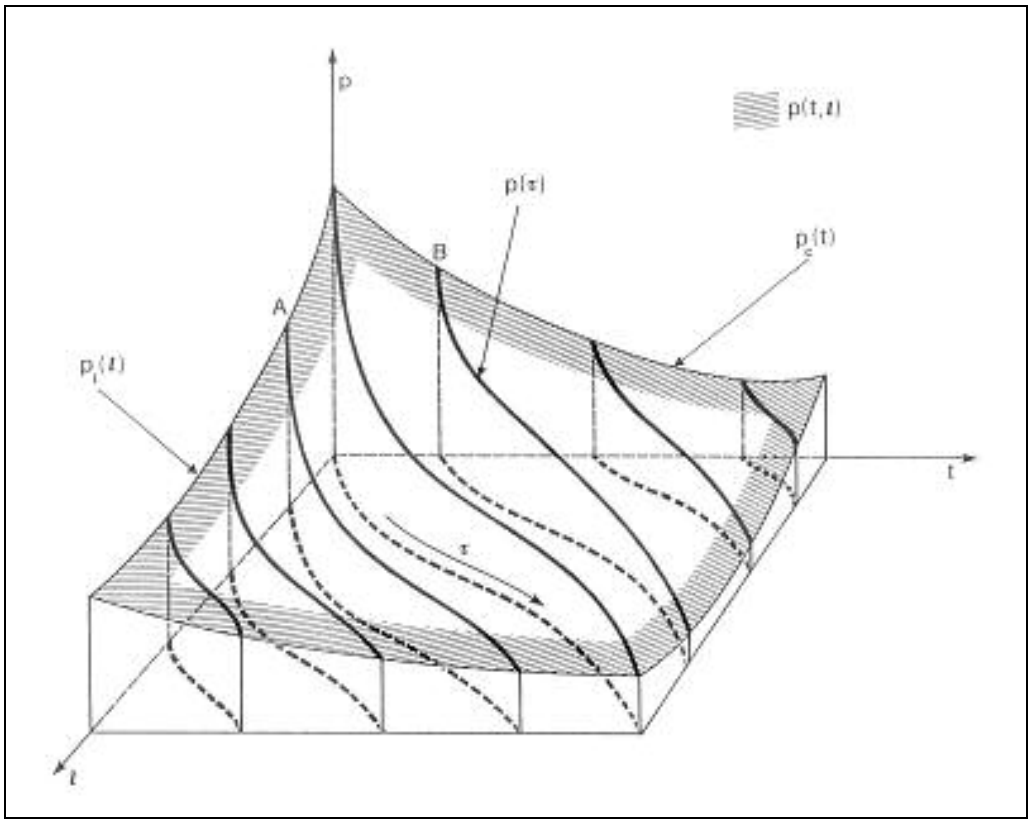

Fig. 2. Representation of the spatial pattern of the (scalar) concentration p and characteristic lines.

$$t(0) = 0, \quad l(0) = l_0, \quad p(0) = p_i(l_0) \quad \text{with} \quad l_0 \in L \qquad \text{Eq. 6a}$$

and (see point B in Figure 1)

$$t(0) = t_0, \quad l(0) = 0, \quad \mathbf{p}(0) = \mathbf{p_u}(t_0) \quad \text{with} \quad t_0 \in T \qquad \text{Eq. 6b}$$

The line $(t(\tau),l(\tau),\mathbf{p}(\tau,l(\tau))$ in the space $(t,l,\mathbf{p})$, solution of Eq.5a, with initial condition Eq. 6a (or Eq. 6b), for a given value of l_0 (or t_0), lies completely on the surface $\mathbf{p}(t,l)$ (see Figure 1 where **p** is assumed to be one-dimensional) and constitutes what is called, in the mathematical literature, a *characteristic line*. In the following, however, we refer by use of this term (as is usual in hydrological literature) to the projection $(t(\tau),l(\tau))$ of the above line on the plane (t,l), i.e. to the solution of Eq.5a and Eq.5a with initial condition Eq. 6a (or Eq. 6b).

The variable τ is called flow time and represents the time elapsed from the instant t_0. From the above it follows that the evolution of the biochemical process starting in the initial section $l=0$ (or $l=l_0$) at the initial time $t=t_0$ (or $t=0$) can be completely described along the corresponding characteristic line independently from what happens along the nearby characteristic lines. From a physical point of view this is quite understandable. Since dispersion was assumed to be insignificant, plugs of water of infinitesimal thickness in the l-direction retain their identity as they flow downstream, so that what happens in each plug is independent from what happens in upstream and downstream plugs. This fact implies that to carry out a simulation along a characteristic line it is necessary to specify the load $\mathbf{P}(t, l)$, as well as the input functions $v(t, l)$, $Q(t, l)$, $S_q(t, l)$, $T(t, l)$, along that line only, and only a point-wise value for the initial condition is needed (this last factor also plays the role of the upstream boundary condition).

APPENDIX 2 - DERIVATION OF THE DOBBIN'S CRITERION BY SYSTEM THEORY

We derive the DC from the structure of the two models by means of a proof that outlines how the criterion applies only to stationary conditions (this proof was originally presented in *Rinaldi et al.* [1979]). The proof can be applied to a complete BOD-DO linear model (see *Rinaldi et al.* [1979]). For simplicity, however, we make reference to a simplified scalar version of Eq. 1a in which, apart from the assumption that the source term S is linear in the concentration p (as in the classical BOD equation of Streeter-Phelps' model) the following positions are taken: the fate of the concentration p is assumed to be independent from other compounds and populations in the ecosystem; the dispersion coefficient D is assumed to be space invariant; no water inflow term S_q is considered; and finally, no loads are present downstream from the initial section. We now proceed as follows. Under a hypothesis of stationary conditions, we transform the simplified version of Eq. 1a into a second order linear lumped-parameter system. We then show that the response of this system to a boundary condition p(0) (that is the initial condition for the lumped parameter system), in the absence of any downstream loads, is identical to the response of a plug- flow model, provided that a *corrected velocity* v^* and/or a *corrected decay coefficient* k^* are used in the latter, instead of the *natural* velocity v and the *natural* decay coefficient k. Finally, we show that when the DC is satisfied, then $v^* \cong v$ and $k^* \cong k$, i.e. the natural plug-flow model, which is the model obtained from the dispersion model by setting D=0, gives nearly correct results (in other words, dispersion can be assumed to be zero).

From the simplified scalar version of Eq. 1ait is evident that one can derive the following system which, under stationary conditions, is equivalent to Eq. 1a:

$$\frac{dp}{dl} = g \qquad \text{Eq.7a}$$

$$\frac{dg}{dl} = \frac{k}{D} p + \frac{v}{D} g \qquad \text{Eq. 7b}$$

where g=g(l) is the gradient of the concentration p(l), and k is the coefficient of the linear source term, i.e.: S = -kp.

From Eq. 1a, it is also evident that one can conclude that the *natural* plug-flow model is given by:

$$\frac{dp}{dl} = \frac{k}{v} p \qquad \text{Eq. 8a}$$

Then a *corrected* plug-flow model has the form:

$$\frac{dp}{dl} = \frac{k^*}{v^*} p \qquad \text{Eq. 8b}$$

Note now that system Eq.7a is a simple linear system of the form:

$$\frac{d\mathbf{x}}{dl} = \mathrm{Fx}$$

Eq.9a

with:

$$\mathrm{x} = \begin{vmatrix} p(l) \\ g(l) \end{vmatrix} \qquad \mathrm{F} = \begin{vmatrix} 0 & 1 \\ k/D & v/D \end{vmatrix}$$

Eq. 9b

The eigenvalues of the matrix F are given by:

$$\lambda_1 = \frac{v}{2D}\left(1 + \sqrt{1 + 4\frac{kD}{v^2}}\right); \qquad \lambda_2 = \frac{v}{2D}\left(1 - \sqrt{1 + 4\frac{kD}{v^2}}\right)$$

Eq. 9c

Remember that, by definition, an eigenvector $x^{(i)}$ associated with an eigenvalue λ_i is a vector such that $Fx^{(i)} = \lambda_i x^{(i)}$. Then, if the state $x(l)$ of the system at a point l is proportional to $x^{(i)}$, i.e. $x(l)=cx^{(i)}$, where c is a scalar constant, we have $dx(l)/dl = \lambda_i x(l)$; that is, in the state space, the tangent to the state trajectory is proportional to the value of the state itself. This implies that in the state space there are two particular straight lines through the origin which are associated with the two eigenvalues Eq.9ac, and which correspond to trajectories of the system. The trajectory associated with λ_1 is directed outwards from the origin, since $\lambda_1>0$, while the trajectory associated with λ_2 is directed towards the origin since $\lambda_2<0$. Thus, the path of p and of its gradient g along the river is that of a *saddle point* in state space.

Since we assumed that there are no loads downstream of the initial section (l=0), the following must hold:

$$lim_{l\to\infty}\ \mathrm{p}(l) = 0$$

Eq. 10

but this can be obtained if and only if the initial state is proportional to the eigenvector associated with λ_2 , which implies that:

$$\mathrm{g}(l) = \lambda_2\, \mathrm{p}(l) \qquad \text{for all } l>0$$

Eq. 11

Thus, from Eq.7a and Eq. 11:

$$\frac{dp}{dl} = \lambda_2\, \mathrm{p}$$

Eq.12

By comparing Eq.12 with Eq. 8ab the following conclusion can be drawn: a corrected plug-flow model (Eq. 8ab) is equivalent to the dispersion model Eq.7a, provided that the ratio k^*/v^* equals $-\lambda_2$. This can be obtained, for example, by setting

$$k^* = k \quad \text{and} \quad v^* = v/\delta, \quad \text{with} \quad \delta = \frac{\sqrt{1 + 4\frac{kD}{v^2}} - 1}{2kD/v^2}$$

Eq.13a

or, equally, by setting

$$k^* = \delta k \quad \text{and} \quad v^* = v$$

Eq. 14b

or by any other combination such that $(k^*/v^*) = \delta (k/v)$. In any case, the correction factor δ is a function of the dimensionless number $Đ = kD/v^2$, that from this point on is called *Dobbins' number*.

A Taylor's series of δ as a series of powers of D then gives

$$\delta = 1 - Đ + 2Đ^2 + o^3$$

Eq. 14c

where o^3 represents the sum of terms that are infinitesimal of the third and higher orders with $Đ$. Eq.13a justifies Dobbins' criterion, since under condition Eq. 2 $Đ$ is negligible and therefore δ nearly equals 1. Thus, when the DC is fulfilled, dispersion is negligible in the sense that a natural plug-flow model is as good operationally as a dispersion model. The data gathering campaign can therefore be organized along a characteristic line defined by equations Eq.5a and Eq.5ab (*natural characteristic line*).

Notice that when the corrected velocity v^*, given by Eq.13a, is substituted into the natural river velocity v in the definition of the characteristic line (see Eq.5a), the corrected plug-flow model produces the same answer as the dispersion model. In conclusion, under stationary conditions, even when the DC is not fulfilled, we can always adopt the corrected velocity v^*, then collect data along the corresponding (corrected) characteristic line and finally calibrate a plug-flow model. Moreover, since the natural value k for the reaction rate coefficient through Eq.13a is assumed for both the corrected plug-flow and the dispersion models, it follows that the best estimate for k^* computed in the plug-flow model is also the best estimate for k in the dispersion model.

It is important to observe, however, that in Eq.13a the corrected velocity v^* does depend on the value of k, but this latter is a priori unknown. It therefore seems that we are in a vicious loop, since on the basis of the value of v^* one can design the data gathering campaign, but it is only on the basis of the collected data that the value of k can be estimated upon which the value of v^* depends. The loop can be broken by calculating $v^*(k_a)$ on the basis of an a priori estimate k_a for k, and by verifying a posteriori that the velocity $v^*(\hat{k})$, computed with the a posteriori estimate $\hat{k}$ of k, does not significantly differ from $v^*(k_a)$. The possible error incurred in such an a priori estimate $v^*(k_a)$ of $v^*(\hat{k})$ is often smaller than the normal error present in any velocity measurement. The reason now emerges for the classic use of the DC: if condition Eq. 2 is satisfied for a sufficiently wide range of a priori estimates of k then we are

sufficiently sure that $v^* \cong v$ both a priori and a posteriori.

The cut in the loop is, however, a hasty solution. In fact, if we consider the alternative position expressed by Eq.13ab, we perceive that another, more effective, procedure is available. We may collect data along the "natural" characteristic line (i.e. the line computed using the natural river velocity v) and estimate the corrected coefficient k^*. Then, we can obtain the natural value of k from the first of the Eq.13ab. There is a simple, structural reason for the existence of this alternative procedure: i.e., under stationary conditions the value of the concentrations in a given section does not change over time. Therefore, the actual time of measurement, and hence the adopted value of the velocity, cannot prevent an estimate of k. But the same reasoning already tells us that an analogous procedure cannot hold in the aperiodic case, as we can see in the following.

Incidentally, it may be of interest to evaluate the error one would produce by adopting the concentration $p_p(l)$ computed using the natural plug-flow model instead of the concentration $p_d(l)$ computed by the associated dispersion model. To that end, consider the ratio R of these concentrations. As a function of l it is given by

$$R = 1 - (k/v)l\,Đ + \frac{kl(kl+4v)}{2v^2}\,Đ^2 + o^3$$

As one can see, R is a function of l, but it approaches the unity as Đ approaches zero.

A last point deserves some comment. The reader has probably noted that the structure of the previous analysis is based on the assumption that the initial condition p_0 is the same for both models. However, he (she) may observe that this assumption is incorrect. It is fair to compare the responses of the two models when they are subject to the same load, but the same load does not imply the same initial condition. In fact, the dispersion phenomenon takes place in the downstream as well as in the upstream direction, while the latter is excluded by our assumption. In reality, a given load will produce a lower initial concentration in the presence of dispersion than in the opposite case. Therefore, the previous analysis has to be modified to take account of this phenomenon by considering the model response to a concentrated input. So as not to bore the reader with tedious calculations, the derivation of the right expression of δ is not described here and only its Taylor's series is given:

$$\delta = 1 + \frac{v}{kl}\ln(Đ) - (1+\frac{v}{kl})\,Đ + (2+\frac{3}{2}\frac{v}{kl})\,Đ^2 + o^3$$

Eq.14d

By comparing Eq.13ac with Eq.13ad one can note that the difference between the two expressions of δ decreases hyperbolically with l; i.e. the expression Eq.13ac that is derived by neglecting the dispersion effect on the initial condition (and is therefore independent of l), is nothing but the limit of the valid expression Eq.13ad for l going to infinity. However, this difference vanishes after a few hundred meters (l is in meters and appears in the denominator), so that in this paper we definitively disregard the effect of dispersion on the initial condition.

APPENDIX 3 - TECHNICALITIES CONCERNING THE PERIODIC CASE

To rich the conclusion anticipated in the text, we proceed as follows: under the hypothesis of periodic conditions (more precisely, sinusoidal conditions), we first compute the amplitude and phase for the two models. We then define the corrected velocity v^* as the velocity that makes the plug-flow model phase equal to the dispersion model phase. We then determine the corrected coefficient k^* as that value of the coefficient in the corrected plug-flow model (i.e. the plug-flow model where the value of velocity is assumed to be v^*) that equals the amplitudes of the frequency responses from the two models. Finally, we determine under what conditions v^* and k^* nearly equal the natural values.

Before proceeding with the analytical development, let us clarify that we have restricted the analysis to the same simplified version of Eq. 1a considered in the stationary case (see above). Moreover, it must be recognized that, as Eq. 1a is a partial derivative equation, the associated transfer function and hence the frequency response, depend on the initial and boundary conditions, as well as on the load pattern. This is because the transfer function is a "one- dimensional" (time only) object, while the system under consideration is a "two dimensional" (time and space) object. For simplicity, we therefore consider just the basic situation where the boundary condition $p_u(t)$ is periodic and the load $P(l,t)$ as well as the initial condition $p_i(l,0)$ are null for all positive l and t.

Let us apply the Laplace operator $L[\cdot]$ to the simplified version of Eq. 1a, by denoting the Laplace transform of $p(t,l)$ with $P(s,l)$, where s is the complex variable:

$$sP + v\frac{dP}{dl} - D\frac{d^2P}{dl^2} = -kP$$

Eq.14a

with boundary conditions

$$P(0,s) = P_u(s) = L[p_u(t)]$$

Eq.14b

$$lim_{l\to\infty} P(s,l) = 0$$

Eq.14c

The second order differential Eq.14a can be split into the following two first order differential equations

$$\frac{dP}{dl} = G$$

Eq.15a

$$\frac{dG}{dl} = \frac{k+s}{D}P + \frac{v}{D}G$$

Eq. 15b

where $G(s,l) = L[g(t,l)]$. Note now that the system Eq.15a is formally similar to Eq.7a. Hence from the results obtained for the stationary case:

$$\frac{dP}{dl} = \lambda_2(s)\, P$$

Eq. 16

where

$$\lambda_2(s) = \frac{v}{2D}\left(1 - \sqrt{1 + 4\frac{(k + s)D}{v^2}}\right)$$

Eq. 17

Therefore, the Laplace transform of p(t,l) in section l is given by

$$P(s,l) = P_u(s)\, e^{\lambda_2(s)\, l}$$

Eq. 18

and the transfer function $M_D(s,l)$ that specifies the input-output relationship between $p_u(t)$ and p(t,l) according to the dispersion model Eq.14a, is given by

$$M_D(s,l) = e^{\lambda_2(s)\, l}$$

Eq. 19

Let us now consider the corrected plug-flow model. Deriving the transfer function is straightforward

$$M_P(s,l) = e^{-(k^* + s)\, l/v^*}$$

Eq. 20

System Theory tells us that the amplitude $R(l,\omega)$ and the phase $\Psi(l,\omega)$ of the frequency response are nothing but the modulo and the argument of the transfer function when it is evaluated for $s=i\omega$ (where: $i = \sqrt{-1}$ 1). Because of the presence of the square root in Eq. 17, the complex function $\lambda_2(s)$ may assume two alternative (complex) values which are characterized by the same modulo and arguments but differ by π. Only one of these values has a negative real part (i.e. it is the stable eigenvalue), and since we are interested in only the stable eigenvalue it is this unique value we have to consider (the other one is nothing but the unstable eigenvalue). Then, for the dispersion model, we have

$$R_D(l,\omega) = \exp\left[\frac{vl}{2D}\left(1 - \left(\frac{1}{2}\left((\alpha^2 + \beta^2)^{1/2} + \alpha\right)\right)^{1/2}\right)\right]$$

Eq.21a

$$\Psi_D(l,\omega) = -\frac{vl}{2D}\sqrt{\frac{1}{2}\left((\alpha^2 + \beta^2)^{1/2} - \alpha\right)}$$

Eq.21b

with

$$\alpha = 1 + 4\frac{k\ D}{v^2} \qquad \text{and} \quad \beta = 4\frac{D}{v^2}\,\omega$$

Eq.21c

and for the plug-flow model:

$$R_P(l,\omega) = \exp\left[- (k^*/v^*) l \right]$$

Eq.22a

$$\Psi_P(l,\omega) = - (\omega/v^*)\, l$$

Eq.22b

Now, as stated, we can determine the corrected velocity v^* by imposing $\Psi_P(l,\omega) = \Psi_D(l,\omega)$, thus obtaining

$$v^*(\omega,D) = \frac{2\,\omega\,D}{v\sqrt{\frac{1}{2}\left((\alpha^2+\beta^2)^{1/2} - \alpha \right)}}$$

Eq. 23

The corrected coefficient k^* is analogously computed by imposing $R_P(l,\omega) = R_D(l,\omega)$ and hence

$$k^*(\omega,D) = \omega\, \frac{\sqrt{\frac{1}{2}\left((\alpha^2+\beta^2)^{1/2} + \alpha \right)} - 1}{\sqrt{\frac{1}{2}\left((\alpha^2+\beta^2)^{1/2} - \alpha \right)}}$$

Eq. 24

Let us make some comments on these results. Expressions Eq. 23 and Eq. 24 are necessarily consistent with our previous results. In fact, for D going to zero they give $v^*=v$ and $k^*=k$, and for ω going to zero (i.e. in the stationary case) they are such that the ratio (k^*/v^*) equals $\delta(k/v)$, with δ given by Eq.13a. Moreover, it is of interest to observe that for k=0 (i.e. for conservative substances) $v^*=v$ and $k^*=D\omega^2/v^2 + o^4$ where o^4 represents the sum of terms that are infinitesimal of the fourth and higher orders with ω. That means that the equivalent plug-flow model indicates a corrected coefficient k^* that is not zero when ω is not zero. This slightly surprising result can easily be understood by observing that under non-stationary conditions the concentration of a substance, even if conservative, would not be constant in space. Therefore, the dispersion phenomenon affects the concentration pattern. A corrected plug-flow model can interpret this modification only as corresponding to a non-conservative substance and therefore k^* must result as being different from zero.

We have fully solved the task we posed ourselves at the beginning of this section: to prove that a corrected velocity v^* and a corrected coefficient k^* exist such that, no matter what the values of D and ω, the output response from a corrected plug-flow model equals that of the dispersion model. Moreover, note that v^* and k^* do not depend on l, thus the result is valid for any section.