Concentration profiles of pollutants in a river basin: an application to the Sarno river

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**Abstract**

A simplified numerical model to evaluate the concentration profiles of reactive pollutants in a natural river system is presented.

The model, subdivided in several calculation forms, provides, first of all, of a geometrical schematisation of the system in a linear branch and basins with an elementary shape, in such a way as to deduce easily the flows per unit width in the system, in the flood, low level and ordinary conditions.

Assuming the hypothesis of hydraulic flux in uniform motion, and subdividing each branch of the system into stretches of elementary length, every stretch is regarded as a chemical dispersion flux reactor, for which a simplified analytical expression of concentration profile is deduced.

An example of application of the proposed model for the case of the Sarno River is also proposed.

**Introduction**

Control of water quality in natural hydraulic systems can be made either directly using an adequate monitoring set-up which measures physical, chemical
and biological parameters at fixed points in the system, or else using numerical models, which have to be properly calibrated.

In the first case, to obtaining reliable results over the whole system it is necessary to use sophisticated and expensive equipment, because of the large number and the wide variability of parameters involved and because of the difficulties of managing a system of sensors operating at such a large scale.

In contrast, the use of numerical simulation methods is easier and less costly because, by knowing a limited number of parameters measured at characteristic points of the system, it allows sufficient information to be obtained, nearly in real-time, on the evolution of the concentration profile of a particular pollutant, along the branches of the river system.

However, regarding these models, it has to be noted that their development is very complex, because of the numerical aspects related to the equations that govern hydrological and hydrodynamic phenomena, and diffusion and dispersion processes, as well kinetics of both the chemical and the biological reactions which take place.

Furthermore, a highly sophisticated definition of the mathematical model often does not give better results, because some of the several coefficients, have to be estimated, while they play significant roles in the formulation of the model.

The light of these considerations, we propose a mathematical-physical model. It is based on a simplified analysis and allows results to be directly obtained. These results can then be used in technical applications when a large-scale estimation of waters’ quality is sufficient.

In particular the mathematical model, shown here, consists of several “sub-models” connected between them, but developed separately.

This type of referred to us “forms” on are later related to the following aspects:

- Topological schematisation of the system;
- Estimation of water flows for different hydrological regime;
- Calculation of average velocities in the cross sections;
- Simplified integration of the convective-diffusive transport equation;
- Schematisation of chemical-biological kinetics processes in the presence of reactive pollutants.

A detailed description of these forms is given later on. After, to show an example, an application of this simplified model on the Sarno river system is reported, related to different scenarios with regard to hydrological and hydraulic aspects and also to different point sources of pollution.

1 Geometric schematisation of the overall system, the hydrological regime and the hydrodynamic flows characteristics

Form 1: Topological schematisation of the river system

With regard to the topographic scheme of the system, for these purposes, the branches of the river system are considered rectilinear (fig. 1) and the
maximum order of ramification does not exceed 2 or 3, according to the Horton criterion.

Subsequently, every branch is divided into a certain number of elementary segments with constant length $\Delta l_i$, section $\sigma_i$ and average bottom slope $p_i$. Furthermore a hydraulic resistance parameter $K_i$ (e.g. Gauckler-Strickler roughness coefficient, is given to every segment).

**Form 2 Hydrological regime of the basin**

The estimation of the river flow $q_i$ in a generic section $z$ of the system is, as everybody knows, a very complex problem. In this simplified approach the following cases are taken into account: the flood level and the low level (with a fixed return period) and the ordinary flow (related to annual mean flows).

a) Evaluation criterion of the maximum flow $q_{\text{max},T}$ in a section $z$.

With regard to fig. 1, the generic section $Z_0$, subtends a hydrographic basin whose area is $S_i$, with a length of the principal branch $L_i$. If the relationship of rainfall quantity $h_{i,T}$ with duration $t$ is known ($h_{i,T}=\alpha t^\beta$, with a particular return period $T$), the flow $Q_{\text{max},T}$ in the section $Z_0$ can be written as:

$$Q_{\text{max},T} = \varphi \frac{h_{i,T}}{t_c} S_i$$  \hspace{1cm} (1)

Where, in addition to the already defined symbols, $\varphi$ is the coefficient of runoff and $t_c$ is the time of concentration of the basin.

These parameters are estimated with standard criteria commonly used in hydrology. Particularly, as regards to time of concentration $t_c$, the modified Kirpich expression $t_c \equiv \beta \cdot L_i^{\alpha_1} \cdot C^{\alpha_2}$ can be used, in which $C$ is the altitude difference between the farthest point of the basin and the closure section, and coefficients $\beta$, $\alpha_1$, $\alpha_2$ are assumed to be equal, respectively, to $\beta=0.0662$, $\alpha_1=0.0662$, $\alpha_2=0.0662$. 

![Fig. 1. Geometric schematisation of the river system](image)
$\alpha_1 = 0.385, \alpha_2 = -0.385$, expressing $L$ in kilometres and $C$ in meters [Ven Te Chow et al., 1988].

Once the flow $Q_{\text{max},T}$ in the section $Z_0$ has been defined, it is necessary to estimate the flow $q_{\text{max},T}$ in the generic section $z$, whose branch length is $L_i$.

With regard to this problem, the following simplified criterion can be suggested. It starts from the assumption that the shape of the basin $S_i$ above $Z_0$ can be schematised by a regular geometric figure, and that it is possible to evaluate $q_{\text{max},T}$ from $Q_{\text{max},T}$, as a function only of the length $l$ corresponding to the section $z$.

Considering the (1), it is easy to verify that it results:

- Rectangular basin (width $b$)

$$Q_{\text{max},T} = \varphi a \left( \beta L^{\alpha_1} \cdot C^{\alpha_2} \right)^{n-1} L b = K_1 L^{[\alpha_1(n-1)+1]} \quad (2)$$

$$q_{\text{max},T} = \frac{Q_{\text{max},T}}{L} l = K_1 l^{[\alpha_1(n-1)+1]} \quad (3)$$

in which,

$$K_1 = \varphi a b \beta C^{\alpha_2}$$

- Triangular basin (base $b$)

$$Q_{\text{max},T} = \varphi a \left( \beta L^{\alpha_1} \cdot C^{\alpha_2} \right)^{n-1} \frac{L}{2} b = K_2 L^{[\alpha_1(n-1)+1]} \quad (4)$$

$$q_{\text{max},T} = K_2 l^{[\alpha_1(n-1)+1]} \quad (5)$$

in which,

$$K_2 = \varphi a b / 2 \beta C^{\alpha_2}$$

- Isosceles trapezium shape basin (bases $B$ and $b$)

$$Q_{\text{max},T} = \varphi a \left( \beta L^{\alpha_1} \cdot C^{\alpha_2} \right)^{n-1} \left[ \frac{(b + B) \cdot L}{2} \right] = K_3 L^{[\alpha_1(n-1)+1]} \quad (6)$$

$$q_{\text{max},T} = K_3 l^{[\alpha_1(n-1)+1]} \quad (7)$$

in which,

$$K_3 = \varphi a \left( \frac{b + B}{2} \right) \beta C^{\alpha_2}.$$

b) Evaluation criterion of the low-level flow $q_{\text{min},T}$ in a generic section $z$.

This case is rather more complex and in this simplified treatment the following patterns will be considered:
• Perennial regime basin with hydrometrographic measurement stations. When the basin to be examined is provided with flow measurement stations it is possible to consider the historical data of the lowest annual flows \( Q_{\text{min}} \) and to estimate the probability function \( P(Q_{\text{min}}) \). Considering the well-known Gumbel function, written in the explicit way with regard to variable \( Q_{\text{min}} \), it is [Gumbel, 1973]:

\[
Q_{\text{min}} = e^{-\frac{1}{\alpha} \ln \left( \frac{T}{T-1} \right)}
\]

in which the distribution parameter \( \varepsilon \) and \( \alpha \) are equal to:

\[
\varepsilon = \left( \mu(Q_{\text{min}}) - 0.45\sigma(Q_{\text{min}}) \right)
\]

\[
\alpha = 1.283 / \sigma(Q_{\text{min}})
\]

Once the value of \( Q_{\text{min}}(T) \) in the measurement sections is defined, in order to characterise a criterion well enough to estimate \( q_{\text{min}}(T) \) in a generic section \( z \), it is suggested that the correlation be analysed among the values of \( Q_{\text{min}}(T) \) and \( L_T \) related to the different available stations, in such way as to determine a regression law which makes it possible to estimate \( q_{\text{min}}(T) \) as a function only of the parameter \( l \).

It must be observed that in a small basin, often, flow measurement stations are not available. In this case we can find that an empirical expression \( q_{\text{min}}(T) = f(l) \) applies the principle of the hydrological similarity at a spatial scale which is bigger than the one of the basin to be examined [Gupta et al, 1986].

• Evaluation of the lowest flows, in a basin with both rainfall and contribution by underground waters and sources.

When the regime of the river depends mainly on rains, the lowest flows are null, if there are not contribution by underground waters and sources.

In this case, the flow \( q_{\text{min}}(T) \) in each section can be evaluated by examining the phenomenon of exhaustion of underground waters [Shaw, 1988].

c) Evaluation criterion of the ordinary flows in a generic section \( z \).

In the \( Z_0 \) section of a generic basin whose area is \( S_i \) and whose main branch length is \( L_i \) (fig. 1), it is possible to estimate the yearly average volume of runoff \( D \) (and so the yearly average flows \( Q \)) that are assumed as ordinary flows.

Once known the value \( Q \) in the \( Z_0 \) section, it is possible to evaluate the one, \( q \), in the generic section \( z \) whose main branch length is \( l \), using, in a simplified way, a linear distribution of \( \bar{q} \):

\[
\bar{q}(z) = (\bar{Q} / L)l
\]
The evaluation of $D$ is obviously very easy when the section $Z_0$ is provided with a flow measurement station, and so the historical data $D_i$ of yearly runoff is known.

In the absence of a measurement station, the value of $D_i$ can be estimated by the calculation of the volume of rainfall $A_i$. These can be determined using, e.g., the well-known Thiessen polygons method, with reference to the historical data of yearly average rain height $h_i$, in the rain gauge stations which are located in the basin to be examined.

Once the values of $A_i$ are known, the relationship will be: $D_i = \varphi_i A_i$, $\varphi_i$ being the coefficient of the runoff which can be generally evaluated directly or by opportune studies at a larger scale.

**Form 3** Hydraulic conditions of the water flow in the system

It is well known that hydrodynamic conditions in a natural water system are represented by a time varying free surface motion. This is described, within the hypothesis of gradually varied motion, by the equations of De Saint Venant [Yen Te Chow, 1959]. These have to be integrated with numerical methods (normally finite-differences) once those boundary conditions have been adequately determined [Cunge et al., 1980].

Instead of this theoretical approach, which can end up rather onerous, according to other simplifications, it is here proposed that, in every element segment, $\Delta l_i$, of the system, whose section $\sigma_i$, slope $p_i$ and roughness $K_i$ are constant, the flow conditions are assumed to be those of uniform flow.

So it is possible, for the generic segment $\Delta l_i$, to evaluate water levels and velocities related to the flows $q_{\text{max},i}$, $q_{\text{min},i}$ and $q_i$.

2 Schematisation of the convective-diffusive transport of reactive pollutants

Within the hypothesis of mono-dimensional flow, the conservation equation for a generic pollutant $A_i$ is the following one:

$$\frac{\partial (\sigma_i C_{A_i})}{\partial t} + \frac{\partial (\sigma_i V_i C_{A_i})}{\partial l} - \frac{\partial}{\partial l} (\sigma_i D \frac{\partial C_{A_i}}{\partial l}) = \sigma_i (G_{A_i} - P_{A_i}) \quad (12)$$

in which, $G_{A_i}$ and $P_{A_i}$ are, respectively, all the sources and sinks of the species $A_i$, $V_i$ the average velocity, $C_{A_i}$ the concentration and $D$ the diffusion coefficient.

In the eq. (12) the terms on the left side represent, respectively, the variation of concentration of $A_i$ in time, caused by convective motion and by phenomena of molecular and turbulent dispersion.

The term on the right hand characterise phenomena of production and consumption of the species $A_i$ (chemical-biological kinetics).

Either production phenomena, or consumption ones, are often complex and not easy to describe with simple models, particularly in the presence of
biological reactions which requires that a dynamic equilibrium is established between the different species of the trophic system and the substratum of organic pollutants shed in the river. This equilibrium is made more complex and more frail by the interaction with nutrient (phosphorus, nitrogen and carbon) and inhibitory (e.g. heavy metals) substances and dissolved oxygen. Furthermore, the variety of organic and inorganic substances which are directly shed in the water course, or which can be intermediate products of decomposition reactions make the mathematical description of the bio-chemical reactions very complex and difficult to manipulate because of the large number of parameters involved.

The description of the simplified model for the schematisation of convective-diffusive transport in the presence of reactive pollutants and chemical kinetics is reported.

**Form 4 Simplified Integration of the Convection-Diffusion equation in the presence of reactive pollutants.**

In simplified modelling of the reactive pollutants transport here proposed the river is regarded as a chemical reactor, in which pollutants are released at singular points and mix with the water, reacting with this and other chemical elements possibly present.

Particularly the “dispersion flux model” [Levenspiel, 1981] has been regarded. This model represents a valid transformation of the ideal plug flow reactor, for which, in steady flow conditions, the following simplifying hypotheses are valid:

- The conditions of the reacting system (temperature and concentration) do not depend on time.
- The mass flow across the reactor is constant.

The shifting from plug flow reactor model is fundamentally due to the presence of eddies (that can produce a convective mixing), to the non-uniform velocity distribution along the cross-section of the duct and to molecular mixing.

On the grounds of the previous considerations, the redistribution of the substance in the above mentioned model can be assimilated to a flux induced by a local spatial gradient of concentration.

This stated, having discretized the system in stretches of length $\Delta l_i$, constant section $\sigma_i$, uniform velocity $V_i$ and flow $q_i$, in the simplified model each stretch is considered as a single chemical reactor. In the hypothesis that kinetics of the generic pollutant $A_i$ can be written by the relation:

$$r_{Ai} = k_0 C_{Ai}^m$$

in which $k_0$ is the kinetic constant and $m$ a numerical coefficient, the equation (12), which expresses matter conservation inside the generic reactor, becomes:

$$V_i \frac{\partial C_{Ai}}{\partial l} + D \frac{\partial^2 C_{Ai}}{\partial l^2} = k_0 C_{Ai}^m$$

Equation (14), in the case of a first order kinetics ($m=1$), admits the following analytic solution [Wehner and Wilhelm, 1956]:

$$C_{Ai} = C_{0Ai} \exp\left[-k_0 \tau + \left(k_0 \tau\right)^2 \frac{D}{V_i \Delta l_i}\right]$$

In the equation (15) \( C^0_A \) is the initial concentration and \( \tau = V/Q_i \) is the residence time in each single stretch.

By the light of what has been stated, once the coefficients \( D \) and \( k_0 \) has been fixed, it is possible to obtain the concentration contour \( C_A(l) \) along the generic river branch.

### 3 Application

An application of the described criterion for the Sarno river, located in the Gulf of Naples (Southern Italy), is shown (fig. 2). This river, well-known because of its serious state of pollution, has been recently the object of a considerable work of environmental re-qualification, still in course. This intervention includes also the construction of six treatment plants. In the following example the proposed model is applied to determine concentration profiles of COD and Surfactants, within the hypothesis of contemporary operation of all the plants and in the case in which one or more plants is out of order. The flows used for the simulations are the ordinary ones and the flood ones with a return period \( T=100 \) years.

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**Fig. 2. Sarno river basin**

**Form 1 Topological schematisation of the river system.**

The hydrographic system of the Sarno river basin has been schematised taking into account only the principal branch and the two most important tributaries: the Cavaiola and the Solofrana rivers (fig. 3). In this scheme three characteristic sections have been chosen (\( Z_1, Z_2, Z_3 \)). In those sections the determination of hydrological and hydraulic parameters has been made.

The length of the principal branch \( L=L_1+L_2+L_3 \) is equal approximately to 40 km. This branch has been divided into small stretches whose length is about \( \Delta l=100 \) m. The section of the river has been assumed rectangular with a width...
varying between 4 and 10 m. The slope has been taken 1.5% in the branch $L_1$, 0.25% in $L_2$, and 0.1% in $L_3$.

Form 2 Hydrological regime of the basin.

a) Ordinary flows

The yearly average flows $\bar{Q}$, by which the ordinary flows have been estimated, have been determined by the yearly average rain-falls $\bar{A}$, evaluated with Thiessen polygons method, once the data of the rain-gauge located in the basin by S.I.I. (Hydrographic National Service) are known.

The coefficient of runoff $\varphi$ has been estimated equal to 0.23, with regard to the yearly hydrological balance of the station located in S. Valentino Torio. The results of this elaboration are shown in tab. I, where the values of the ordinary flows, estimated from equation (11) are also reported.

<table>
<thead>
<tr>
<th>Sect.</th>
<th>$L$ [km]</th>
<th>Rainfall $\bar{A}$ [$10^3$ mc]</th>
<th>Runoff $\bar{D}$ [$10^3$ mc]</th>
<th>$\bar{Q}$ [mc/s]</th>
<th>$\bar{q}(l)$ [mc/s × m]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Z_1$</td>
<td>39.8</td>
<td>6.531</td>
<td>0.150</td>
<td>2.093</td>
<td>0.052</td>
</tr>
<tr>
<td>$Z_2$</td>
<td>30.2</td>
<td>8.709</td>
<td>0.200</td>
<td>2.790</td>
<td>0.092</td>
</tr>
<tr>
<td>$Z_3$</td>
<td>22.0</td>
<td>15.240</td>
<td>0.350</td>
<td>4.833</td>
<td>0.22</td>
</tr>
</tbody>
</table>

tab. I

b) Flood flows

With regard to simplified model previously described, and taking into account the geometrical shape of the basin the three elementary sub-basins, related to sections $Z_1$, $Z_2$, $Z_3$, have been schematised as simple geometrical figures (rectangles).

In the tab. II the values of the geometrical characteristics ($b$ and $L$) of all the rectangular sub-basins are reported. Furthermore, the coefficients of the rain-time correlation $a$ and $n$, related to a period of return $T=100$ years, are also shown, together with coefficient of runoff $\varphi$. Finally, in the same table the values of the flood flows $Q_{\text{max},T}$ obtained by the (1) and the values of the flood-flows for unity of length $q_{\text{max},T}(l)$, obtained by eq. (3), are also reported.

<table>
<thead>
<tr>
<th>Sect.</th>
<th>$b$ [km]</th>
<th>$L$ [km]</th>
<th>$a$ [mm]</th>
<th>$n$</th>
<th>$\varphi$</th>
<th>$Q_{\text{max},T=100}$ [mc/s]</th>
<th>$q_{\text{max},T}$ [mc/s × m]</th>
</tr>
</thead>
<tbody>
<tr>
<td>$Z_1$</td>
<td>19.5</td>
<td>39.8</td>
<td>20.3</td>
<td>0.37</td>
<td>0.23</td>
<td>155</td>
<td>3.89</td>
</tr>
<tr>
<td>$Z_2$</td>
<td>15</td>
<td>30.2</td>
<td>19.0</td>
<td>0.37</td>
<td>0.18</td>
<td>118</td>
<td>3.91</td>
</tr>
<tr>
<td>$Z_3$</td>
<td>13</td>
<td>22.0</td>
<td>17.2</td>
<td>0.37</td>
<td>0.27</td>
<td>87</td>
<td>3.95</td>
</tr>
</tbody>
</table>

tab. II

Form 3 Hydraulic conditions of the water flow in the system.

For every stretch of length $\Delta l_i$, with the Gauckler-Strickler formula the uniform flow velocity $V_i$, related to values of $\bar{q}(l)$ and $q_{\text{max},T}(l)$, has been determined assuming a roughness coefficient $K=30$.

Form 4 Evaluation of the concentration profiles.

In the tab. III the locations of the six treatment plants are reported and, for every plant, the "equivalent" number of citizens that are served, the design flow, and the concentration of COD and Surfactants to be treated.
With reference to fig. 3, the effluxes from treatment plant have been regarded being discharged in a concentrated form. The concentration profiles for COD and Surfactant substances have been deduced by (15), assuming for the kinetic constant $k_0$, respectively, the values [Perry et al., 1997]: $k_{COD}=5.3 \cdot 10^{5}$ s$^{-1}$ and $k_{f.o}=1.8 \cdot 10^{4}$ s$^{-1}$.

These values have been deduced from the values commonly found for these constants in a biological oxidation tank, divided by 100, in such a way to consider the large difference in bio-mass concentration between the tank and the river.

Furthermore, the dissolved oxygen concentration has been calculated on the grounds of the following assumptions:
- the entry flow in each cell $\Delta l_i$ is saturated with oxygen at a temperature of 15°C ($C_{O_2}=10.2$ g/mc), fig. 3a;
- the oxygen concentration $C_{O_2}$ of the concentrated discharge coming from the treatment plant is zero;
- the oxygen flux coming from atmosphere is estimated by: $\delta=(C^*-C_0)V_i$
where $\delta$ is a term equivalent to an exchange coefficient, and can be expressed as [Vesilind et al., 1982]:

$$
\delta = 3.9W_i^{0.5} \left[ 1097 \left( T_0 - 20 \right) \right]^{0.5} / d_i^{1.5}
$$

where temperature $T_0$ has been considered constant and equal to 15 °C, $d_i$ is the water depth, and $W_i$ is the cell volume.

The oxygen consumption has been evaluated by the oxidation rates of COD and surfactant substances.

In the fig. 4-5-6, with reference to ordinary flows, are shown the concentration profiles related to the following operating conditions:

- a) All the plants are operative, and discharge into the river;
- b) Only the “Alto Sarno” plant is operative;
- c) No plant is operative.

Fig. 4. COD, Surfactants and dissolved oxygen [g/m$^3$] concentrations in the Condition a.
Fig. 5. COD, Surfactants and dissolved oxygen [g/m$^3$] concentrations in the Condition b.
In the figures above the continuous line indicates the variation of COD and Surfactant concentration along the river branch, I indicates the point of discharge (plants) and T the confluence points along the principal branch. The dashed line, instead, represents the variation of dissolved oxygen concentration.

It must be observed that in the diagrams the threshold value for dissolved oxygen, equal to 8 g/m\(^3\) [Fogler, 1992] is shown. This value is the vital minimum for survival of river flora and fauna.

The results show clearly the different chemical and biological conditions in the river whether in the presence of treatment plants, and in the partial or total absence of them.

**Conclusions**

The model allows the concentration profiles of the reactive pollutants to be evaluated along the branch of a river system, using four calculation forms, with ease regard to conceptual planning and numerical processing. The above mentioned forms are articulated in this way:

- **form 1**: it allows the system to be schematised geometrically by linear branches, with assigned section, slope and roughness;
- **form 2**: it allows the values of flows \(q_{\text{max},T}\), \(q_{\text{min},T}\) and \(Q\) to be evaluated by simple hydrological models in a generic section \(z\) of a branch of the system, during flood, low level and ordinary flow;
- **form 3**: it uses the uniform motion schematisation to evaluate the hydraulic parameter of each elementary stretch \(\Delta l_i\) of the system;
- **form 4**: it allows the concentration profile to be plotted along the river assuming that each elementary stretch \(\Delta l_i\) is a chemical reactor such as a “dispersion flux”
one, for which, considering a linear kinetics, an analytical solution of convection-diffusion equation has been deduced.

An application of the proposed criterion on the Sarno river has proved its utility in the forecast of eventual critical situations, in relation to different conditions of letting in from treatment plants.

References