CONSTITUENT TRANSPORT

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Contents

Summary

Physics of the transport of various constituents in flowing surface waters is discussed in this article. All the mixing mechanisms such as advection, molecular diffusion and turbulent diffusion are considered. Since actual river flows are always turbulent, some attention is paid to the influence of turbulence on the transport processes. Mathematical models that account for all the transport processes and which reflect the principle of conservation of mass are shown. Various versions of such models are presented depending on how detailed output from the model is expected. The description starts from the most general three-dimensional version. Then various averaged versions are shown. The two-dimensional model is obtained from the 3D version with the aid of the depth-averaging operator. One of the results of averaging is the appearance of a new term representing some additional transport of the constituent depending on the non-uniformity of velocity and called dispersion. Further simplification of the transport model is admissible at far distances from the point of release of the constituent and the governing equations may be then averaged over the cross-section, which results in a one-dimensional model. Although such longitudinal-dispersion models are widely used in practice, an alternative model, which accounts for the effects of transient storage due to irregularities in channel geometry, is also presented. Examples of solutions of the models and the results applied to real rivers are briefly presented. In this article attention is also paid to dye tracer studies which are experimental techniques allowing for

estimation of the speed of constituent transport, travel time, and mixing processes in an actual river environment.

1. Introduction

Evaluation of potential impacts on public health or aquatic organisms from contaminants in surface waters is related to estimation of travel time and the concentration of the contaminants migrating from the input zone to the accessible environment. The input zone can be some known source (e.g. an accidental spill, continuous discharge from an industrial plant or farmland) or a result of biological and chemical transformations in the stream. In the described cases the sources of pollution may usually be easily and precisely located along a watercourse. Very often we deal with non-point sources of pollution, i.e. with sources distributed in space and time, like for example run-off from cultivated lands or acid deposition. Any constituent transported downstream by flowing water can constitute an interest for practitioners and researchers. Such constituents like septic waste, pesticides, fertilizers, and hydrocarbons contribute to the deterioration of surface waters and are therefore are very important for the studies. Traditionally, the problems of the transport of, for example, BOD, nitrogen, phosphorus, suspended solids and pH, are often addressed since they can be readily identified from measurements, population equivalent values, production technologies etc.

Classical descriptions of the transport of a constituent in a stream and the prediction of point concentrations in space and time require a detailed knowledge of hydraulic and morphometric conditions and also of some conceptual model, initial and boundary conditions and a method for estimation of parameters. The concentration point values are consequently subjected to irregular variations and to large uncertainty. A famous mathematician John von Neumann used to say, “Truth is much too complicated to allow anything but approximations”. It is exactly the case when one wants to find the concentration field of an admixture in such complex environment as a river. A well-grounded theory exists for mass transport in open channels, but when one deals with an actual river environment, the results derived from those theories are very often not satisfactory. One can easily imagine an alluvial channel splitting into a multitude of channels like in the case of a braided stream. Imagine also a river of a connected network type with characteristic multiple riverbeds, which divide and reunite repeatedly at various points. Among the riverbeds and small channels of various sizes, which connect particular riverbeds, flooded islands are situated and they can be covered by marsh plants, and in some cases by bushes. Such riverbeds are usually sinuous, with small longitudinal declivity, and during high water levels they are unable to store inflowing water and create large broads. Such a description suits for example the Okavango Delta in Botswana or a part of Upper Narew River, the largest tributary of the Wisla River in Poland. One can build up a variety of such descriptions when observing real river systems all over the world and it is not surprising then that the description of mass transport in such systems is not a trivial task. It is definitely the case that the extreme complexity of rivers means that a purely mathematical approach does not work for them.

The continuous interest in constituent transport in natural streams results from the extreme importance of the subject for a still expanding multitude of applications and also from the lack of a comprehensive and satisfactory theory of the subject, despite much important work that has been done. The understanding of the transport of constituents is important not only for solution of river water quality problems. Rivers govern the main export of contaminating substances from a watershed and therefore constitute an important link with the water quality of lakes and seas. An attempt at understanding in the form of a model framework applicable to analyze transport of soluble pollutants in rivers and streams is at the forefront of research programs in the field. Models used for analyses of solute transport can be of “emergency type” and used to analyze the short-term transport of accidental spills. Another type reflects the long-term changes in water quality that occur on a large length scale due to continuous release of a pollutant or disturbance in the cycling of natural substances. For the purpose of this study the first type of model will be presented in more details.

It is important to note at this point that the description of mass transport will be given without the discussion of the momentum transport and the continuity principles in the river itself. Understanding of a river flow and its mathematical treatment is usually a necessary input for mass transport equations and the information on the relevant discharges, water velocity distributions and water levels will be treated as known. More information on these matters may be found in *River Flow*. Some justification for separate treatment of these problems can be that in some cases mathematical equations representing the mass transport can be decoupled from momentum and continuity equations. The reader should however realize that it is not always the case and such an approach is obviously a significant simplification of the reality.

2. Physics of constituent transport.

The main concerns of the present study are the physical processes that govern the fate of constituents in surface waters. Therefore much less attention will be paid to the description of biological and chemical processes. To make the presentation simpler for the reader, herein we will focus on neutrally buoyant substances only. The analysis of such micropollutants like heavy metals (e.g. mercury, cadmium, lead) would go along different lines. The reason is that these substances may be present in three states in the system considered: in dissolved form, in solid phase (mostly present in the suspended solids), and in the sediment below. When these pollutants are in the solid form the relevant description of their transport should appeal to the dynamics of two-phase flows. The solid grains may move in the form of rolling, saltation and suspension. The manner of their motion depends on many factors, like the position at which the particle initiates a move, its size, shape, density relative to the carrier fluid, and turbulent properties of the flow. In general the way in which a particle moves is a direct effect of the role and significance of particular forces acting on a grain and also the variability of other solid particles concentration in its neighborhood. When considering the motion of such a particle in a Lagrangian frame, all the relevant forces would have to be considered, namely the drag force, the drifting force due to turbulence, lift force and the combination of the weight and buoyancy of the particle. Additionally some supplementary model of a stochastic nature, responsible for the collision of the considered particle with solid boundaries would have to be built. For solids, analyses similar to those for sediment transport would have to be conducted and one may learn about basic physics in this respect in *Transport of Sediments*.

Additionally we will assume that the considered mixture is passive, that is one in which the fluid-particle interaction does not affect the dynamics of the flow. Otherwise one would have to include momentum considerations in order to properly represent certain two-phase flows.

We will limit our considerations in the rest of this article to the fate of solutes, i.e. the substances that are dissolved in the water. Throughout the article, we use the macroscopic treatment, i.e. the theory of continuum. Because of practical importance, we do not care about the motion of individual particles of the matter and are interested only in the resultant effects due to the motion of a large number of particles. This is possible because in practical problems the smallest length scales of interest are much larger than the distance between molecules.

When one deals with a quiescent aquatic environment the transport of mass occurs due to the so-called molecular diffusion. It is an easily observable phenomenon in every day experience, for example when an infusion of tea mixes with water in a glass even without stirring. It reveals the tendency of the system to equalize the concentrations of a dissolved substance and results from random molecular motion within the fluid. This motion (so-called Brownian movement) was described for the first time by the botanist Robert Brown in 1828. In investigating the pollen of different plants he observed that this became dispersed in water in a great number of small particles, which were perceived to be in uninterrupted and irregular “swarming” motion.

The molecular diffusion may be described quantitatively with the use of the phenomenological law proposed in 1855 by German physiologist Adolf Fick (1829-1901):

$$\vec{j}_D = -D grad\, c \tag{1}$$

where $\vec{j}_D(x, y, z, t)$ is the diffusion flux density defined so that the inner product $\vec{j}_D dS$ is equal to the mass (or the number) of the diffused particles through the surface element dS during 1 sec time period. D is the diffusion coefficient, usually expressed in [m^2/s] and $c(x,y,z,t)$ – particles concentration, i.e the mass of particles in the unit of volume. The Cartesian coordinate system is used throughout this chapter. In the case of an open channel, the x-axis along the longitudinal direction is parallel to the average bottom slope, the y-axis along the lateral direction is horizontal and the z-axis along the depth direction is normal to the channel bottom. The molecular diffusion coefficient is a property of the fluid and for a given solvent, solute, concentration and temperature D is constant. An important feature of molecular diffusion is its irreversibility. Molecular diffusion occurs also when water moves but its significance, in comparison to other processes, decreases with the increase of the flow velocity or the size of the stream and when velocity variation becomes important.

Another important transport process is the macroscopic movement of the mixture (water and pollution) displacing the mixture parcels as a whole without affecting the concentration of the solute. This (reversible) process is called advection and it transports the considered constituent away from the source without any change in concentration within the solute cloud (a small parcel of fluid whose dimensions are comparable with the smallest length scale of interest which may be represented by such characteristics as velocity and solute concentration). The advection flux, i.e. the amount of solute transported per unit time per unit area perpendicular to the current (direction of movement), may be determined by the product of the velocity of the medium and its concentration:

$$j_{ax} = uc \qquad (2)$$

where $j_{ax}(x, y, z, t)$ is advective flux in the longitudinal direction, u(x,y,z,t) is the longitudinal velocity and c(x,y,z,t) is the solute concentration.

A vital feature of the flow of all the rivers is the phenomenon of turbulence (see *River Flow*). The river turbulence results in additional, significant mass fluxes appearing in the stream. To define those transport processes let us first pay some attention to the most important features of turbulence in a river. The nature of turbulence and its description is far from being complete at present and is the subject of extensive studies all over the world. For the sake of this article we may assume that turbulence is a stochastic phenomenon, arising from a superposition of individual oscillating fluid motions over a wide range of scales. In a river flow a number of eddies, superimposed on each other, exist. The size of the largest eddies are of the order of flow depth. Larger eddies, continually formed in a turbulent flow, break into smaller and still smaller eddies until they are finally dissipated through viscous shear. Eddies are generated in the region of high shear in the mean flow field, i.e. near the boundary of the channel or in the vicinity of interface between two streams flowing at different velocities and parallel to one another (say at a river confluence or at the edge of the jet created by an inflowing stream). Turbulence in river streams is in principle more complex than in artificial channels. River flows cause changes in the geometry of the channel; they also influence the bed roughness, which is one of the main factors generating the turbulent motion of water. Besides, the river water interacts with the variety of particles existing in the flow (suspended sediment, organic compounds, pollutants).

A criterion known as ‘Reynolds number’ (stability parameter) which is a ratio of inertial force to viscous force, shows if the considered flow is laminar or turbulent. Reynolds number is defined as:

$$\mathrm{Re} = \frac{u_c L}{\nu} \qquad (3)$$

where: u_c is a characteristic velocity, L is a characteristic length scale (in rivers the mean water velocity and mean water depth are usually taken for u_c and L, respectively) and ν is the kinematic viscosity of the fluid. In case of pure water the kinematic viscosity varies depending on the temperature and for example at a temperature of 20 $^\circ$C: $\nu = 10^{-6}$ m^2/s, at 5 $^\circ$C: $\nu = 1.52 \bullet 10^{-6}$ m^2/s; at 30 $^\circ$C: $\nu = 0.8 \bullet 10^{-6}$ m^2/s. The larger the Reynolds number, the less important is the influence of viscosity on the flow pattern and the flow becomes chaotic which is manifested by fluctuations in velocity and pressure. When the Reynolds number exceeds the value of $2 \cdot 10^3$ we usually deal with a turbulent flow. In rivers, the Reynolds number usually appears to be much larger. For example the following Reynolds numbers were reported in relatively small, lowland rivers in Poland (in Wilga River $4.7 \cdot 10^4$ to $5.7 \cdot 10^5$; in Świder River $5 \cdot 10^4$ and in Narew River - $5 \cdot 10^5$ to $7.3 \cdot 10^5$).

One can imagine that special interest is paid to the characteristics of the flow at a particular point (when for example the value of the concentration of an admixture is sought there). Then the passage of the eddies of various sizes through this point cause velocity fluctuations of small magnitude and large frequency as well as large magnitude and small frequency. It yields a fluctuating velocity field. An exemplary time series of the recorded velocities at a selected point in the River Severn, UK, is shown in *River Flow*.

3. Turbulence in river flow

For mathematical simplification Osborne Reynolds (1842-1912) proposed in 1895 to decompose an unsteady flow into slowly varying mean and rapidly fluctuating parts. Following this idea any quantity like instantaneous velocity, and concentration can be presented as the sum of mean value (time average) and the fluctuating component:

$$\begin{aligned} u &= \overline{u} + u' \\ v &= \overline{v} + v' \\ w &= \overline{w} + w' \\ p &= \overline{p} + p' \\ c &= \overline{c} + c' \end{aligned} \qquad (4)$$

where u,v,w are the instantaneous point velocities in longitudinal, vertical and transversal directions respectively, p is the pressure and c is the instantaneous value of solute concentration; $\overline{u}, \overline{v}, \overline{w}, \overline{p}, \overline{c}$ are the average values, *u’*, *v’*, *w’*, *p’*, *c’* are the fluctuation components. In case of stationary turbulent flows (when statistical parameters related to the flow do not change with respect to time) the time average for any quantity $\overline{\xi}$ is:

$$\overline{\xi} = \frac{1}{2T} \int_{-T}^{T} \xi dt \qquad (5)$$

at a given point in space (x,y,z). The sampling time 2T should be sufficiently large compared to the time scale of small eddies and small compared to time scales of large eddies. According to this averaging, the average of the fluctuating components is equal to zero. However, this is not true for the product of fluctuations. When standard averaging concepts are used in the averaged governing equations, representing water flow, additional stresses, known as Reynolds stresses appear. They result from the turbulent fluctuations and they encompass all phenomena associated with turbulence.

Moreover, these stresses represent the essence of the difficulties associated with the modelling of turbulence because their behavior is not completely understood. The hydrodynamics equations will not be discussed within this article, although they constitute an integral part of the study of mass transport in flowing surface waters.

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Biographical Sketch

Paweł M. Rowiński is currently the Director of the Institute of Geophysics, Polish Academy of Sciences. He studied applied mathematics at the University of Warsaw and earned the M.S. degree in mathematics in 1988. He received the Ph.D. degree in Earth Sciences in 1995 and his Habilitation in 2003 from the Institute of Geophysics, Polish Academy of Sciences. From 1991 to 1992 he was a visiting scholar (Soros Fellow) at the State University of New York at Stony Brook. He was also a trainee of Central European University in Budapest, National Center for Ecological Analysis and Synthesis, University of California, Santa Barbara, USA; University of Minnesota, Minneapolis, USA and Institut für Gewässerökologie und Binnenfischerei im Forschungsverbund in Berlin. His research interests and contributions are in fluvial hydraulics, river turbulence, pollution and sediment transport in rivers, two-phase flows, chaotic dynamics, water balance in a catchment, adaptive environmental assessment and management. He has well over 80 scientific publications in prestigious journals, and numerous presentations to his credit. He has been a co-author and co-editor of 7 scientific volumes. He was awarded a number of recognised prizes, among them the Award of the Prime Minister of Poland for outstanding Ph.D. dissertation and later for outstanding habilitation dissertation, Stipend of the Foundation for Polish Science for outstanding young scientists, scholarship of the Central European University. He is an Associate Editor of Hydrological Sciences Journal (IAHS Press, Wallingford, UK) and a member of numerous professional bodies such as: the Board of Managers of Warsaw Branch of Polish Geophysical Society, Physics of Water Section of the Polish Academy of Sciences, Scientific Council of Institute of Physical Geography at Warsaw University, Founder Member of the Narew Society for Environmental Protection; International Association of Hydraulic Engineering and Research (IAHR), International Association of Hydrological Sciences. He has been an organizer and participant of numerous symposia and workshops; in 2005 he was nominated by the Committee for Water Management of the Polish Academy of Sciences to chair the International School of Hydraulics.