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Hydrodynamic interaction between suspended sediments and the transport of contaminants in open channel flow Interacción hidrodinámica entre sedimentos suspendidos y el transporte de contaminantes en flujo de canal abierto

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Abstract

This paper presents a research about the interaction between suspended solids and the pollution transport in streams. It involves the study of the interaction between sediments, reactive chemical substance and stream, in which, the hydrodynamic processes are modeled including the advection, turbulent diffusion, sedimentation, and the effect of kinetics. The main concern is to know how suspended solids can influence in the pollutant concentrations and how they are able of absorbing part of the chemical substances, which generally follow decay processes (Revelli & Ridolfi, 2002). Mathematical models described in this document take account the advection, turbulent diffusion, and the exchange kinetics between the solid phase and dissolved phase.

Key-words: hydrodynamic, sedimentation, contaminants.

Resumen

Este trabajo presenta una investigación sobre la interacción entre los sólidos en suspensión y el transporte de contaminantes en canales abiertos. Esto implica el estudio de la interacción entre los sedimentos, sustancia química reactiva y la corriente, en la cual, los procesos hidrodinámicos son modelados incluyendo la advección, difusión turbulenta, sedimentación, y el efecto de la cinética. La principal preocupación es saber cómo los sólidos en suspensión pueden influir en las concentraciones de contaminantes y la forma en que son capaces de absorber parte de las sustancias químicas, que en general siguen procesos de desintegración (Revelli & Ridolfi, 2002). Los modelos matemáticos que se describen en este documento tienen en cuenta la advección, difusión turbulenta, y el intercambio cinético entre la fase sólida y la fase disuelta.

Palabras claves: hidrodinámica, sedimentación, contaminantes.

Introduction

The hydrodynamic of suspended solids and its effect on the transport of contaminants in a stream is a relevant issue in Environmental Fluid Mechanics. It is known that the transport of dissolved matter in a stream is affected by physical, biological, and chemical processes. Physical processes include the advection, turbulent diffusion and dispersion. When the contaminants are discharged to the stream, the chemical species is partitioned in two aqueous (dissolved) and sorbed (solid) phases with permanent exchange regulated by local gradient concentrations between both phases (NG & Yip, 2001; Revelli & Ridolfi, 2002). Because of the shear process, the dissolved phase follows the advection, turbulent diffusion and dispersion while the sorbed phase is linked to the sediment following the sedimentation process (Revelli & Ridolfi, 2002). Here the questions are how can the solids in suspension alter the transport of chemical substances in a river? and how is the interaction between sediments and contaminants?. For answer these questions, the main objective of this research is to investigate the effect and interaction of suspended solids on substance contaminants in open channel flows. Equations are described take account the advection, turbulent diffusion, and the exchange kinetics between the sorbed and dissolved phase. Three major papers were reviewed to study this process. Additionally, decay process for these two phases, in the chemical pollutant, is included showing the influence of the decay and suspended solids on the alteration of the transport mechanism.

Problem statement

A two-dimensional steady and uniform turbulent flow, with mild slope in the channel are considered to study and formulate the advection-diffusion equation that governs the transport of suspend sediments and chemical substances in the domain considered (in this case 0 < z < h). Figure 1 shows the reference system used for this end, with x-coordinate along the river and a z-coordinated vertical normal to the bed. Also, h is the normal depth, u (z) is the time average stream velocity, q is flow in the river, and φ is the concentration of suspend sediments. Likewise, it is assumed that the channel is carrying a steady uniform suspend load and that the solid particles behave as those of the fluids, with difference that solid particles tend to settle with a fall velocity W_s . In addition to this, mass exchange with the bed is not considered which means the interaction between the groundwater and the river flow is ignored.



Figure 1. Reach of the river showing the profiles of local average velocity and the suspend sediment concentration

Source: Adapted from Revelli and Ridolfi (2002).

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Transport of suspend sediments.

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By the conservation mass, the transport equation for the suspended sediments is expressed as follow:

$$\frac{\partial \mathbf{j}}{\partial t} + u \frac{\partial \mathbf{j}}{\partial x} - w_s \frac{\partial \mathbf{j}}{\partial z} = \frac{\partial}{\partial x} \left(D_x \frac{\partial \mathbf{j}}{\partial x} \right) + \frac{\partial}{\partial z} \left(D_z \frac{\partial \mathbf{j}}{\partial z} \right)$$
(1)

Where j(x, z, t) is the suspend particle concentration, t is time, u (z) is time local flow velocity (advection velocity), Dx(x) and Dz(z) are the horizontal and vertical eddy diffusivity. For this case, the boundary conditions are following:

$$w_{s}j + D_{z}\frac{\partial j}{\partial z} = 0 \text{ at } z = 0, h$$
 (2)

To derive equation 2, steady uniform suspended sediment is considered which implies that the rate of deposition is equal along the depth. A steady uniform load indicates that the local rate of change of the suspend concentration at a given point and the settle gradient horizontal of the particle concentration (the advective derivative, advection in this direction), and the horizontal diffusion are neglected. Where $\varphi = \varphi(z)$ is the suspend sediment concentration, we is the settling velocity. In equation 2, boundary conditions mean that net flux on the bottom and top of the river or channel is zero.

From equation above, it is possible to derivate the vertical profile of the sediment concentration, integrating and applying boundary conditions as follow:

$$w_{s}\varphi + D_{z}\frac{\partial\varphi}{\partial z} = 0 \rightarrow \partial\varphi = -\frac{w_{s}\varphi\partial z}{D_{z}} \rightarrow \frac{\partial\varphi}{\varphi} = -\frac{w_{s}}{D_{z}}\partial z \rightarrow \int_{0}^{z} \frac{\partial\varphi}{\varphi} = -\int_{0}^{z} \frac{w_{s}}{D_{z}}\partial z = \ln[\varphi]_{0}^{z} = \ln(\frac{\varphi(z)}{\varphi(0)}) = -\int_{0}^{z} \frac{w_{s}}{D_{z}}\partial z \rightarrow \frac{\varphi(z)}{\varphi(0)} = \exp\left[-\int_{0}^{z} \frac{w_{s}}{D_{z}}\partial z\right]$$

Then, the equilibrium vertical profile for the suspend sediment concentration is given by the following equation:

$$j(z) = j_{0} \exp\left[-\int_{0}^{z} \frac{W_{s}}{D_{z}(z')} \partial z'\right]$$
 (3)

Where \mathcal{P}_0 is a reference sediment concentration at the bed level z = 0.

Transport of chemical species.

When the pollutant is discharged to the stream, the chemical specie is partitioned in dissolved (aqueous) and sorbed (solid) phases; therefore, the total mass concentration (mass of chemical per bulk volume) Ctot (x,z,t) is:

$$C_{tot} = C + C_s \varphi \tag{4}$$

Where C(x, z, t) is the mass of aqueous phase per volume of water, and Cs (x, z, t) is the mass of the sorbed concentration per mass of solid. The, the mathematical model that represents the chemical transport in the domain 0 < z < h is the following:

$$\frac{\partial C_{tot}}{\partial t} + u \frac{\partial C_{tot}}{\partial x} - w_s \frac{\partial C_s \mathbf{j}}{\partial z} = \frac{\partial}{\partial x} \left(D_x \frac{\partial C_{tot}}{\partial x} \right) + \frac{\partial}{\partial z} \left(D_z \frac{\partial C_{tot}}{\partial z} \right)$$
(5)

The first term represent the local rate of change of the total mass concentration at a given location. The second term is the change (gradient) of C_{tot} in the x direction as result of the advection of the particles from one location to another where the value of chemical mass is different and where u is the advection velocity. The terms on the right side are the horizontal and vertical diffusion of the total mass concentration. At the free surface and the bottom of channel, the vertical net flow will be zero; then the boundary condition is:

$$w_s C_s \mathbf{j} + D_z \frac{\partial C_{tot}}{\partial z} = 0 \text{ at } \mathbf{z} = 0, \mathbf{h}$$
 (6)

Using condition (2), the equation (4) can be written the following way:

$$\frac{\partial C_{tot}}{\partial t} + u \frac{\partial C_{tot}}{\partial x} = \frac{\partial}{\partial x} \left(D_x \frac{\partial C_{tot}}{\partial x} \right) + \frac{\partial}{\partial z} \left(D_z \left(\frac{\partial C}{\partial z} + \mathbf{j} \frac{\partial C_s}{\partial z} \right) \right)$$
(7)

For 0 < z < h, the boundary condition is:

$$D_{z}\left(\frac{\partial C}{\partial z} + j \ \frac{\partial C_{s}}{\partial z}\right) = 0 \qquad z = 0, h \tag{8}$$

It is noted that vertical diffusion has been breakdown in two components: vertical gradient of the aqueous and sorbed phases respectively.

Also, assuming that the sorption rate can is described by a first- order linear kinetics equation:

$$\frac{\partial C_s}{\partial t} = k_f C - k C_s \tag{9}$$

Where the kf and k are the forward and reverse rate constants for the sorption reaction. Dissolved and solid phases will be in chemical equilibrium when the reaction is fast compared with other processes; therefore the ratio of their concentration is given by:

$$\frac{C_s}{C} = \frac{k_f}{k} \equiv K_d \tag{10}$$

Where Kd is the sorption partition coefficient which depends on the properties of both sorbed (solid) and dissolved phases. When the concentration of the dissolved phase tends to be small, Kd is bigger.

Now substituting (10) into (9), the first- order linear kinetics can be expressed as:

$$\frac{\partial C_s}{\partial t} = k(K_d C - C_s) \tag{11}$$

Where, the reverse reaction rate k can be interpreted as a sorption rate constant. Furthermore, eq. (11) means that the rate of change of the sorbate concentration (mass solid phase of chemical sorbed) regard the change of time is linearly proportional to the deviation from local equilibrium.

Decay process.

Decay process of chemical substances in a river, as result of transport phenomenon, is very important in the analysis and chemical reactions of suspend solids. Revelli and Ridolfi (2002) considered this aspect, apart from the effect of sorption –desorption kinetics. Decay for dissolved and sorbed phases with corresponding reaction rates is pointed in this research project. Using power laws, reactions can be modeled of the following way:

$$R = -I C^n, \qquad R_s = -I_s C_s^m \tag{12}$$

Where R and Rs are the reactions for the dissolved and sorbed phases. λ and λ s are constant values of decay rate for the dissolved and solid (sorbed) phases, respectively. In the equation 12, if the power values n and m are equal to zero, the respective reaction will be equal to a constant decay rate which indicate an irreversible degradation of a reactant independent of its concentration. On the other hand, the reactant can be represented as a variation of its concentration regard to the time:

$$\frac{\partial C}{\partial t} = R = -|C^n, \qquad \frac{\partial C_s}{\partial t} = R_s = -|_s C_s^m$$
(13)

For m = n = 0, the solution will be:

$$\frac{\partial C}{\partial t} = -\lambda C^0 = -\lambda \rightarrow C = \int (-\lambda)\partial t = C_0 - \lambda t \text{ and } C_s = C_{s0} - \lambda_s t \quad (14)$$

Where C0 is the initial concentration at t = 0. Equation above represents a zero-order reaction. Introducing (13) in (7), we have the following equation (Revelli & Ridolfi, 2002):

$$\frac{\partial C_{tot}}{\partial t} + u \frac{\partial C_{tot}}{\partial x} = \frac{\partial}{\partial x} \left(D_x \frac{\partial C_{tot}}{\partial x} \right) + \frac{\partial}{\partial z} \left(D_z \left(\frac{\partial C}{\partial z} + \varphi \frac{\partial C_s}{\partial z} \right) \right) - \left(\lambda C^n + \varphi \lambda_s C_s^m \right)$$
(15)

Equation (15) is a two dimensional mathematical model for the transport and fate of the pollutant in which decay processes for the dissolved and solid phase are considered. On the other hand, the concentration of the solid phase (Cs) is governed by the kinetics of the sorption exchange with the dissolved phase and the decay reaction in the solid phase.

In the domain 0 < z < H, considering decay process, the behavior of the sorbate concentration may be described through of mathematical model:

$$\frac{\partial C_s}{\partial t} = k(K_d C - C_s) - \lambda_s C_s^m \tag{16}$$

Equation above indicates that rate of change of the sorbate concentration is linear proportional to deviation of the equilibrium subtracted by its process of decay.

The boundary conditions for (15) are the same of those pointed in the expression (8) which considers zero flux for the free surface and the bed of the channel or river.

The mathematical model (15), the sediment profile equation, and the boundary conditions pointed respectively, are the expressions that describe *the interaction between the advection-diffusion-decay process and the suspend load*.

Using the homogenization method to derivate the effective mass transport equations for Taylor dispersion, two very important mathematical expressions are established. This technique is a multi-scale procedure that allows derivate the coefficient of dispersion at long time for any Taylor dispersion problems (Ng, 2003). Spatial scales need to be applied: Ratio of the longitudinal dispersion coefficient to Eddy diffusivity, ration of longitudinal to vertical length scale, ration advection to vertical diffusion rates, ratio of desorption to vertical diffusion rates, ratio of dissolved phase to the advection, and three times scales, T_0 , T_1 , and T_2 are important in the process, which correspond to the times scales for the vertical diffusion of flow, longitudinal advection and longitudinal dispersion.

Discussion

A set of mathematical equations to analyze the effect and the sorptive exchange on the transport of chemical in a sediment open channel flow are studied. Likewise, a method scale of homogenization is used to derivate the effective transport equation in 1D for chemical species where the sorptive phase (solid) exchange is produced between the water depth and a steady uniform distribution of suspend solids (Ng, 2000; Ng & Yip, 2001; Revelli & Ridolfi, 2002). Using the homogenization method to derivate the effective mass transport equations for Taylor dispersion (Ng, 2000; Ng & Yip, 2001), two important mathematical expressions are established. The effective transport equation for the sediment concentration in 1D is written as follow:

$$\frac{\partial \varphi_b}{\partial t} + u_s \frac{\partial \varphi_b}{\partial x} = D_s \frac{\partial}{\partial x} \left(\frac{\partial \varphi_b}{\partial x} \right)$$
(17)

Where $\varphi(x,t)$ is the sediment concentration and it will be zero at the bed level (z=0), first and second terms of the left side of this equation were defined in previous sections, being us the effective advection velocity for the sediment (Ng & Yip, 2002) and defined as: $u_s = \overline{fu}/\overline{f}$ which is a depth average speed, weighted by the sediment distribution factor f which results from a equilibrium between the sedimentation and the turbulent mixing and can be derived from expression (2) with the respective boundary conditions. On the right side, the only one term is the horizontal diffusion where Ds is the diffusivity coefficient which is set up as $D_s = \overline{fD_x}/\overline{f} + D_T$. The first term of this expression is depth-averaged eddy diffusivity in the horizontal direction and weighted by the sediment factor f, the second one is the Taylor dispersion coefficient. The effective transport equation for chemical pollutants is:

$$\frac{\partial C_o}{\partial t} + (u_c + u_c)\frac{\partial C_o}{\partial x} = \frac{\partial}{\partial x} \left(D_c \frac{\partial C_o}{\partial x} \right)$$
(18)

Where uc is the effective advection velocity for the solute concentration which is given by $u_c(x,t) = \overline{Ru}/\overline{R}$ which is a velocity weighted by the retardation factor R for the chemical partitioning. This factor is given by $R = 1 + K_d \varphi_o$. Where the sorption partition coefficient can be computed by (9). Co is the solute concentration and Dc is the effective dispersion coefficient which is a depth average longitudinal eddy diffusivity weighted by the retardation factor R (Ng 2000). The one-dimensional depth-averaged transport equation for chemical pollutant which includes decay processes is established as follow:

$$\frac{\partial C_0}{\partial t} + u_e \frac{\partial C_0}{\partial x} + u^* \frac{\partial C_0^n}{\partial x} + u^{**} \frac{\partial C_0^m}{\partial x} = D^* \frac{\partial^2 C_0}{\partial x^2} - (\lambda^* C_0^n + \lambda^{**} C_0^m + \lambda' C_0^{2n-1} + \lambda'' C_0^{2m-1} + \lambda C_0^{m+n+1})$$
(19)

Where ue is the effective advective velocity for the concentration of the chemical defined by $u_e = \overline{Ru}/\overline{R}$. As it is noted, this velocity is proportional to the average velocity weighted by the retardation factor R and inversely proportional to the same average factor. $\lambda^* = \lambda/\overline{R}$ and $\lambda^{**} = \lambda_s K_d^m \overline{\varphi}/\overline{R}$ being λ^* and λ^{**} the effective no linear decay coefficient, u* and u** are the effective coefficients for two pseudo advective no linear terms (Revelli & Ridolfi, 2002). D* is the effective coefficient for dispersion in the horizontal direction which can be estimated with the velocity and effective velocity, retardation factor R, sorption partition coefficient Kd and the concentration of the sediments. λ', λ'' , and λ''' are the coefficients, Kd, R, and variance of the concentration of sediment.

Now, let me to illustrate the importance of the bulk solid-water distribution ratio $K_d \varphi_0$ in regulating the influence of the suspend load on the chemical dynamics. For this end, the effective velocity us give by equation below:

$$\hat{u}_{e} = f_{b} + \frac{5.26}{3kR} + \frac{5.26K_{d}\varphi}{kR} \left[\frac{(2-\alpha^{2})e^{-\alpha} - 2(1-\alpha)}{2\alpha^{3}} \right]$$
(20)

Where α is a suspension number proportional to the depth of channel weighted by the settling velocity and inversely proportional to the vertical eddy diffusion. The term fb is the slip velocity relative to shear velocity (Ng 2000) and can be computed through equation:

$$f_b = \frac{1}{k} \ln \frac{h}{E_s} + 8.5 - \frac{2.63}{k}$$
(21)

Also the depth average velocity is given by:

$$\overline{u} = f_b + \frac{5.26}{3k}$$
 (22)

Where k is the Karman constant equal to 0.4, h/Es =1000, for $\alpha = 0.1, 1, 5, \text{ and } 10, \text{ and } 0 < K_d \varphi_0 < 5$. Figure 2 shows that the effective advection velocity decreases when $K_d \varphi_0$ increases whose effect is more notable for higher suspension number. Also, when $K_d \varphi_0$ trends to zero the sediment transport loses influence and the transport of the dissolved phase is given.



Figure 2. Effective advection velocity as function of the bulk solid-water distribution and suspension number α .

Source: Adapted from Ng, C.O. (2000)

On other hand to study of the effect of decay process, the linear decay is addressed using the following equation:

$$\lambda_e = \lambda^* + \lambda^{**} = \frac{e^{\alpha}\alpha + (e^{\alpha} - 1)\beta K_d \varphi_0}{e^{\alpha}\alpha + (\alpha^{\alpha} - 1)K_d \varphi_0} \lambda$$
(23)

Where λ_e is the effective coefficient of reaction, and β is defined as the ratio between the rate decay of the sorbed and dissolved phase. Figure 3 shows the effects of these parameters. It is noted that the ration of the decay constant decrease with small β values. Also it decrease when the suspension number α increment.



Figure 3. Linear Decay. Influence of the bulk solid-water distribution ratio, β , and the ratio between decay constants on the effective decay, for α =0.1 and for α =10. Source: Adapted from Revelli & Didolfi (2002)

Conclusions

Interaction between the suspend solids and chemical pollutant in open channel flow has been studied, using three major papers. Mathematical equations that govern the transport of suspend solids and chemical species, and boundary conditions were described. These models take account the advection, turbulent diffusion, and the exchange kinetics between the sorbed and dissolved phases. Additionally to this, decay processes for the same phases were included in equation (15), for instance, which describe the interaction between the advection-difussion-decay processes and the suspend sediment. Likewise, longitudinal and vertical scales for the dispersion, vertical diffusion and longitudinal advection are pointed for the perturbation analysis, and time scales for the diffusion across the flow, and longitudinal dispersion and advection.

It is shown that exchange kinetics given between the dissolved and solid phase can influence on the advection and dispersion of chemical substances in an open channel flow. The Mathematical model in (19) shows the influence of the suspended sediments and decay process on the alteration of the mechanism of transport. Additionally, the influence of the bulk solid-water distribution ratio $K_d \varphi_0$ on the advective velocity and on the ration of the rate decay between the effective coefficient of reaction and the coefficient constant coefficient decay for the dissolved phase has been addressed. It is noted that when $K_d \varphi_0$ increases the effective velocity decreases and it increases when $K_d \varphi_0$ tends to zero.

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