Parameterization of the Turbulent Schmidt Number in the Numerical Simulation of Open-Channel Flows

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ABSTRACT: Computational Fluid Dynamics (CFD) is being increasingly used to study a wide variety of complex environmental phenomena. Oftentimes, the accuracy and reliability of CFD modelling and the correct interpretation of CFD results become under scrutiny because of implementation issues. One aspect that must be carefully addressed during the simulation process pertains to the proper selection of the input parameters. If the approach of the model is based on the Reynolds-Averaged Navier–Stokes equations (RANS), the turbulent scalar fluxes are generally estimated by assuming the gradient-diffusion hypothesis, which requires the definition of the turbulent Schmidt number, Sc_T. This parameter is defined as the ratio of momentum diffusivity to mass diffusivity in a turbulent flow. In spite of its widespread use, no universally-accepted values of this parameter have been established. It is sometimes assumed, by analogy between momentum and mass transport, that Sc_T is equal to one (Prandtl analogy); however, different values are suggested in commercial CFD codes and applications, and other empirical values have been used in different studies.This paper presents two case studies where the role of a correct parameterization of the turbulent Schmidt number for a reliable estimation of turbulent transport is assessed. They are: (1) modelling of contaminant dispersion due to transverse turbulent mixing in a shallow water flow, and (2) modelling of sediment-laden, open-channel flows. The comparison between numerical results and the available experimental data shows that the turbulent Schmidt number is a key parameter to obtain satisfactory predictions of both solute mixing and sediment transport in suspension.

KEY WORDS: Sediment and contaminant transport, Computational Fluid Dynamics, Reynolds-Averaged Navier-Stokes equations (RANS), Turbulent schmidt number.

1 INTRODUCTION

The study of turbulent open-channel flows has been developed through field experiments, laboratory (full-scale and small-scale) experiments, analytical and semi-empirical modeling, and numerical simulations with Computational-Fluid-Dynamics (CFD) codes (Blocken and Gualtieri, 2012). The main advantages of CFD are as follows: a) it allows full control over the boundary conditions; b) it provides data in every point of the computational domain at different times (“whole flow-field data”); and c) it does not suffer from potentially incompatible similarity requirements due to scaling issues, because simulations can be performed at full scale. CFD also allows efficient parametric analysis of different configurations for diverse conditions. Oftentimes, the accuracy and reliability of CFD modelling, and the correct interpretation of CFD results, become under scrutiny because of implementation issues. One issue that must be carefully addressed during the simulation process pertains to the proper selection of the input parameters to be applied in the numerical simulations. This is of particular importance if turbulent flows with mass transport are considered. The most widely applied approach for simulating turbulent flows is that based on the concept of Reynolds-averaging, where turbulent fluctuation terms are expressed by means of time-averaged quantities. If the transport of a scalar through a turbulent flow is modeled, that approach results in the well-known advection-diffusion equation:

$$\frac{\partial \overline{C}}{\partial t}+\overline{u}\frac{\partial \overline{C}}{\partial x}+\overline{v}\frac{\partial \overline{C}}{\partial y}+\overline{w}\frac{\partial \overline{C}}{\partial z}=-\frac{\partial\left(\overline{u'C'}\right)}{\partial x}-\frac{\partial\left(\overline{v'C'}\right)}{\partial y}-\frac{\partial\left(\overline{w'C'}\right)}{\partial z} \qquad (1)$$

where molecular diffusion was neglected. In Eq. (1), u, v and w are velocity components in the x, y and z directions, respectively, and C is the solute concentration. The overbar indicates time-averaged quantities, while the prime stands for fluctuating quantities. Eq. (1) is modified by assuming the gradient-diffusion hypothesis (Pope, 2000):

$$\begin{aligned}\overline{u'C'}&=-D_{t\text{-}x}\frac{\partial \overline{C}}{\partial x}\\ \overline{v'C'}&=-D_{t\text{-}y}\frac{\partial \overline{C}}{\partial y}\\ \overline{w'C'}&=-D_{t\text{-}z}\frac{\partial \overline{C}}{\partial z}\end{aligned} \qquad (2)$$

where $D_{t\text{-}x}$, $D_{t\text{-}y}$ and $D_{t\text{-}z}$ are the turbulent diffusivities in the x, y and z directions, respectively, of the scalar being transported within the turbulent flow. Hence Eq. (1a) becomes:

$$\frac{\partial \overline{C}}{\partial t}+\overline{u}\frac{\partial \overline{C}}{\partial x}+\overline{v}\frac{\partial \overline{C}}{\partial y}+\overline{w}\frac{\partial \overline{C}}{\partial z}=\frac{\partial}{\partial x}\left(D_{t-x}\frac{\partial \overline{C}}{\partial x}\right)+\frac{\partial}{\partial y}\left(D_{t-y}\frac{\partial \overline{C}}{\partial y}\right)+\frac{\partial}{\partial z}\left(D_{t-z}\frac{\partial \overline{C}}{\partial z}\right) \qquad (3)$$

where the terms on the second hand are related to the turbulent diffusion. The gradient-diffusion hypothesis relates the advective transport of a scalar due to turbulent fluctuations to the spatial gradient of the time-averaged concentration through the turbulent diffusivity. It has been long recognized that this approximation is not always correct; however, it is more than justified for engineering purposes in simple turbulent shear flows (Pope, 2000; page 362). It is also worth mentioning that the above expressions assume that the off-diagonal components of the turbulent diffusion tensor are zero. Different, more complex approaches have been proposed (Rossi and Iaccarino, 2009)

The gradient diffusion hypothesis requires the estimation of the turbulent Schmidt number, Sc_t; this parameter is defined as the ratio of momentum diffusivity to mass diffusivity in a turbulent flow:

$$Sc_{t\text{-}i}=\frac{\nu_{t-i}}{D_{t-i}} \qquad (4a)$$

where $\nu_{t\text{-}i}$ is the eddy kinematic viscosity in the i-direction. Hence, if the turbulent Schmidt number is known, the turbulent diffusivities can be estimated as:

$$D_{t-i}=\frac{\nu_{t-i}}{Sc_{t\text{-}i}} \qquad (4b)$$

The turbulent Schmidt number is the analogous for turbulent flow of the Schmidt number:

$$Sc=\frac{\nu}{D_m} \qquad (5)$$

where ν is the molecular kinematic viscosity of the fluid and D_m is the molecular diffusivity of the scalar within the fluid. Therefore, the turbulent Schmidt number is a property of the turbulent flow, whereas the Schmidt number is a property of the fluid and of the substance being diffused within the fluid. The Schmidt number Sc usually varies in the range 10^0–10^3 depending on temperature for environmental flows water. On the contrary, as Sc_t is a characteristic feature of the turbulent flow, no universal value could be established. By analogy between momentum and mass transport Sc_t is often assumed to be as first approximation equal to unity. However, empirical values different from unity, have been used in different studies.

This paper first presents a review of previous literature studies about the turbulent Schmidt number in the field of Environmental Hydraulics (Cushman-Roisin et al., 2012). Second, two case studies are presented where the role of a correct parameterization of the turbulent Schmidt number for a reliable estimation of turbulent transport is assessed. They are: (1) modelling of contaminant dispersion due to transverse turbulent mixing in a shallow water flow, and (2) modelling of sediment-laden, open-channel flows. With these examples, we intend to compare the Schmidt number of particulate flows (sediment transport) versus that of non-particulate cases (dissolved contaminants).

2 REVIEW OF THE LITERATURE ON THE PARAMETERIZATION OF THE TURBULENT SCHMIDT NUMBER

Several studies about the turbulent Schmidt have been recently published in various contexts. Some of them have addressed the simulation of flow and tracer transport (Arnold et al., 1989; Djordjevic, 1993; Lin and Shiono, 1995; Simões and Wang, 1997); others have addressed the analysis of inclined negatively buoyant discharges (Oliver et al., 2008) and sediment-laden flows (Graf and Cellino, 2002; Amoudry et al., 2005; Muste et al., 2005; Toorman, 2008; Absi, 2010).

Arnold et al. (1989) made extensive measurements in compound channel flow, and were able to determine experimentally the values of Sc_t . They found that Sc_t varied in the range 0.1-1.0, with the vast majority of the values situated between 0.5 and 0.9. Djordjevic (1993) presented a mathematical model of transport processes in open-channel flow and the experimental verification of the model in a rectangular and in a compound channel. He experimentally determined a value of the eddy viscosity equal to the transverse mixing coefficient, implying that Sc_t was close to unity for both section shapes. Lin and Shiono (1995) solved numerically the 3D Reynolds-Averaged Navier-Stokes equations in conjunction with the linear and nonlinear k–ε models to predict flow fields and turbulent parameters in a compound open channel and estimated Sc_t =0.72. Simões and Wang (2007) developed a numerical model to simulate time-dependent turbulent flows in open channels, including the transport of dissolved materials. The turbulence closure was provided by two algebraic eddy viscosity models. In the simulation, they used an anisotropic eddy diffusivity tensor with a Sc_t of 0.5 for the horizontal mixing and 1.0 for the vertical mixing coefficient to obtain the best agreement with the experimental data. Oliver et al. (2008) applied the standard k–ε model to study positively buoyant vertical discharges and then applying it to inclined negatively buoyant discharges. The numerical results were compared with experimental data. The k–ε model was first implemented using standard parameter settings and Sc_t equal to 0.9. To improve the agreement with the experimental data, the turbulent Schmidt number was calibrated to 0.6.

Several studies discussed the case of sediment transport. Graf and Cellino (2002) carried out experimental tests to determine a depth-averaged value of Sc_t by evaluating momentum and sediment diffusivity (Eqs 1) from laboratory experimental measurements of instantaneous velocity and concentration profiles. Considering also previous literature data, they concluded that for the suspension flows over bed without bed forms $Sc_t > 1$, while for the ones over bed with bed forms as in natural waterways $Sc_t < 1$. Adopting a constant value of Sc_t and van Rijn pick-up function, Hsu and Liu (2004) calibrated the turbulent Schmidt number using the experimental results of Ribberink and Al-Salem (1995) and obtained Sc_t=0.7. Amoudry et al. (2005) investigated the role of Sc_t for a dilute two-phase sediment transport model with a k-ε fluid turbulence closure. They first used a constant value of Sc_t and found that the best fit with the experimental data was obtained with Sc_t=0.7 close to the bed and Sc_t=0.52 far from it. They concluded that describing the Schmidt number as a constant value might not be appropriate and to improve their prediction decided to use a Sc_t that depends on concentration, which generally gives the expected dependence on the elevation from the bed. Muste et al. (2005) applied PIV-PTV measurements to study the interactions between suspended particles and flow turbulent structures. They compared the traditional mixed-flow approach to sediment-laden flows that treats these flows essentially as flow of a single fluid with a two-phase flow perspective. The calculated Sc_t values were much larger than 1.0, namely from 1.4 to 2.11, for experiments with natural sand, and much smaller than 1, namely from 0.22 to 0.52, for the experiments with neutrally buoyant sediment formed of crushed nylon. Toorman (2008) derived Eulerian equations for the vertical flux and momentum of suspended particles in dilute, sediment-laden, open-channel flow in equilibrium using the two-fluid approach. Reynolds averaging was applied in order to allow validation of individual terms with experimental data. Using the experimental data from Cellino (1998), he concluded that the turbulent Schmidt number for suspension-free conditions is in the range from 0.5 to 0.8. Absi (2010) first argued that field and laboratory measurements of suspended sediments over wave ripples showed a contrast between an upward convex concentration profiles, time-averaged in semi-log plots, for fine sand and an upward concave profiles for coarse sand. Second, the application of a 1D vertical gradient diffusion model with Sc_t=1.0 resulted in a good prediction of the concentration profile for fine sediments but it fails for coarse sand. Hence, he proposed to consider Sc_t as function of the distance from the bed and of an additional parameter, which is function of the settling velocity.

3 CASE STUDIES

3.1 Contaminant dispersion due to transverse turbulent mixing in a shallow water flow

We first discuss the case of transverse turbulent mixing of a steady-state point source of a tracer in a two-dimensional rectangular geometry, which is expected to reproduce a shallow flow (Fig.1).

Although transverse mixing is a significant process in river engineering when dealing with the discharge of pollutants from point sources or the mixing of tributary inflows, no theoretical basis exists for the prediction of its rate, which is indeed based upon the results of experimental works carried on in laboratory channels or in streams and rivers. This case was presented in details in Gualtieri (2010). to whom the interested reader is deferred. The geometry was that of Lau and Krishnappan (1977), who collected turbulent mixing data for a shallow flow. In the numerical study to solve the flow field an approach based on the Reynolds Averaged Navier-Stokes (RANS) equations was applied, where the closure problem was solved by using turbulent viscosity concept. Particularly, the classical two-equations k-ε model was used. The transport of a tracer was simulated by using Eq. (1b), as adapted for a 2D geometry, steady-state conditions and isotropic turbulence. The turbulent Schmidt number was assumed to be equal to the unity. These equations were solved using Multiphysics 3.4™ modeling package, which is a commercial multiphysics modeling environment (Multiphysics, 2008).

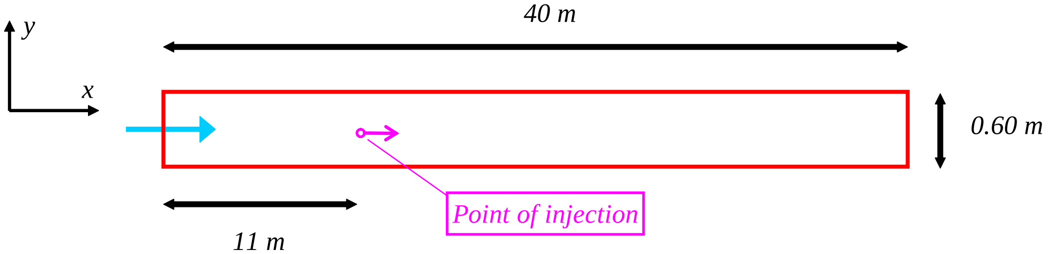

Fig 1 – Sketch of the simulated 2D geometry.

After a preliminary mesh convergence study, both the time-averaged flow and the concentration field were obtained. Two methods were first applied to the model results in terms of time-averaged concentration to evaluate the turbulent transverse mixing coefficient $D_{t\text{-}y}$ for several cross-section downstream of the point of injection. They were the methods of moments (Rutherford, 1994) and a method based on the transverse profile of turbulent kinematic viscosity ν_t, which provides a local value of the turbulent diffusivity. A value of $D_{t\text{-}y}$ for the whole geometry was obtained considering that in a Fickian process, $D_{t\text{-}y}$ and the transverse variance σ_y^2 are related as (Rutherford, 1994):

$$\sigma_y^2 = 2\, D_{t\text{-}y}\, t \qquad (6)$$

Hence, the data of spatial variance of the tracer transverse profile were plotted against the travel time of the plume t, as suggested by Rummel et al. (2005). In this plot, the transverse mixing coefficient $D_{t\text{-}y}$ was taken as the fitting parameter and the line was forced to go through zero. However, numerical value was of about 30% above the maximum experimental data in Gualtieri (2010). This value is listed in Table 1 as Run 3. Overall, the comparison with the experimental data collected by Lau and Krishnappan for a shallow flow in the same 2D geometry confirmed that k-ε model due to the assumption of isotropic turbulence tended to overestimate the rate of transverse turbulent mixing since this model produces large turbulent viscosity and, consequently, with Sc_t=1.0, high turbulent diffusivities.

Later on, further numerical simulations were carried out to investigate how the parameterization of Sc_t affects the numerical results, which is the focus of the present paper (Table 1). As expected, values of Sc_t lower than 1 resulted in stronger lateral spreading of the tracer with a larger transverse variance and, according to Eq.(6), in larger $D_{t\text{-}y}$. On the contrary, if it was assumed that Sc_t>1.0, the turbulent transverse mixing coefficient tended to a lower values. For Sc_t=1.3, $D_{t\text{-}y}$ was very close to the experimental value.

Overall, the above results confirmed that the turbulent Schmidt number is a very important parameter in the numerical modelling of environmental flows.

Table 1 Numerical simulations carried out

Run	Sc_t	$D_{t\text{-}y}$ – m²/s	Reference
Exp.	---	1.41×10^{-4}	Lau and Krishnappan (1977)
1	0.8	2.10×10^{-4}	Present study
2	0.9	1.95×10^{-4}	Present study
3	1.0	1.88×10^{-4}	Gualtieri (2010)
4	1.2	1.51×10^{-4}	Present study
5	1.3	1.42×10^{-4}	Present study

3.2 Sediment transport in suspension

In this sub-Section, we analyze the particulate flow of solids in open channels. We focus on a one-dimensional model at the wall-normal direction.

Bombardelli and Jha (2009) and Jha and Bombardelli (2010; 2011) developed a hierarchy of models based on the two-phase flow theory. This theory solves for mass and momentum equations of both the carrier (water) and disperse phases (sediment). Since the traditional Rouse's model (see Vanoni, 1975; Parker, 2004) is unable to explain quantitatively many of the laboratory and field datasets (even for dilute cases), Bombardelli and Jha investigated the potential of the two-phase flow theory to contribute to a better understanding and prediction of the contributions to the mass and momentum equations. Further, they were interested in obtaining models able to simulate both dilute and non-dilute conditions. (We indicate by "non-dilute," those conditions in which the concentration of sediment is larger than, say, 2-4% in the entire water depth; see Jha and Bombardelli (2010).) Usually, non-dilute conditions have been addressed in the literature following the balance by Hunt, who employed a non-linear term for the action of gravity. This means that two different approaches were used for in the past, i.e., Rousean and Hunt distributions, for two diverse behavior ranges of sediment; in this framework, both cases appear as special conditions of a more general model.

Bombardelli and Jha (2009) defined three levels of complexity for the models, as follows: a) the simplest level in which the quasi-horizontal velocity of the disperse phase (sediment) is considered to be equal to the quasi-horizontal velocity of water, while the wall-normal velocity of the disperse phase is given by the fall velocity of sediment. Thus, no momentum equation is needed for the disperse phase in this approach, which we call the Pseudo-Single Phase-Flow Model (PSPFM); b) the most comprehensive way includes a full discrimination of the velocities of water and sediment, and separate mass conservation for both phases, which we call Complete Two-Phase Model (CTFM). This last model allows in particular to address the velocity lag observed experimentally by, for example, Muste et al. (2005). Finally, an intermediate case was developed, in order to address the possibility of avoiding the complexity of the CTFM (which we call a Partial Two-Fluid Model, PTFM). The CTFM possesses an ensemble average and a second average over turbulence. The eqs for the CTFM are as follows (Bombardelli and Jha, 2009; Jha and Bombardelli, 2010):

Mass balance:

$$\frac{\partial\left(\alpha_k\ \overline{\rho_k}\right)}{\partial t} + \frac{\partial}{\partial x_j}\left(\alpha_k\ \overline{\rho_k}\ \overline{U_{j,k}}\right) = \frac{\partial}{\partial x_j}\left(\rho_k\ \overline{\alpha_k^{'}\ u_{j,k}^{'}}\right) + \Gamma_k \qquad (7)$$

Momentum balance:

$$\frac{\partial\left(\alpha_k\ \overline{\rho_k}\ \overline{U_{i,k}}\right)}{\partial t} + \frac{\partial}{\partial x_j}\left(\alpha_k\ \overline{\rho_k}\ \overline{U_{i,k}}\ \overline{U_{j,k}}\right) = -\alpha_k\ \frac{\partial \overline{P_k}}{\partial x_i} + \frac{\partial}{\partial x_j}\left[\alpha_k\left(\overline{T_{ij,k}} + T_{ij,k}^{\mathrm{Re}}\right)\right] + \alpha_k\ \rho_k\ g_i \pm M_i \qquad (8)$$

where α indicates the volume fraction of the phase k; ρ, U, and u' represent the density, averaged velocity and velocity fluctuation of phase k; P is the pressure; i and j vary from 1 to 3 (spatial dimensions); Γ is the mass transfer between phases; g is the acceleration of gravity; M is the interaction forces between phases; T is the shear stress tensor. In turn, the superscript RE refers to the remaining tensor of the averaging processes and the overbars indicate the averaging on turbulence. In the wall-normal direction, these eqs give:

Carrier phase (water):

$$\frac{\partial W_c}{\partial z} = 0 \qquad (9a)$$

$$\frac{\partial\left[\left(1-\alpha_d\right)\rho_c\ U_c\right]}{\partial t} = -\frac{\partial}{\partial z}\left\{\left(1-\alpha_d\right)\rho_c\ \overline{u_c^{'}\ w_c^{'}}\right\} + \left(1-\alpha_d\right)\rho_c\ g\ S - F_{D,x} \qquad (9b)$$

$$W_c = 0 \qquad (9c)$$

Disperse phase (sediment):

$$\frac{\partial\left(\alpha_d\ \rho_d\right)}{\partial t} + \frac{\partial\left(\alpha_d\ \rho_d\ W_d\right)}{\partial z} = -\frac{\partial}{\partial z}\left[\rho_d\ \overline{w_d^{'}\ \alpha_d^{'}}\right]$$

$$(9d)\ \frac{\partial\left(\alpha_d\ \rho_d\ U_d\right)}{\partial t} + \frac{\partial\left(\alpha_d\ \rho_d\ U_d\ W_d\right)}{\partial z} = -\frac{\partial}{\partial z}\left[\alpha_d\ \rho_d\ \overline{u_d^{'}\ w_d^{'}}\right] + \alpha_d\ \rho_d\ g\ S + F_{D,x} \qquad (9d)$$

$$\frac{\partial\left(\alpha_d\ \rho_d\ W_d\right)}{\partial t} + \frac{\partial\left(\alpha_d\ \rho_d\ W_d\ W_d\right)}{\partial z} = -\alpha_d\ \frac{\partial P_c}{\partial z} - \frac{\partial}{\partial z}\left[\alpha_d\ \rho_d\ \overline{w_d^{'}\ w_d^{'}}\right] - \alpha_d\ \rho_d\ g\ \cos\theta + F_{D,z} \qquad (9e)$$

where the overbars have been eliminated. With different closures for the unknowns, the distributions of water horizontal velocity (U_c), sediment horizontal velocity (U_d), sediment concentration (α_d) and vertical sediment velocity (W_d) can be obtained. In the above eqs, the terms in overbars have been closed via the use of the gradient-diffusion hypothesis. The numerical integration of the equations has been developed by using the finite-volumes method. It is worth emphasizing that in the CTFM the vertical velocity of the sediment is calculated, and that the computed value can in principle be different than the value of the settling velocity (w_s) obtained from available formulas.

As a result, Fig. 2 shows the values of the turbulent Schmidt number obtained by adjustment of the numerical solutions to match data from Lyn (1988), Muste and Patel (1997) and Muste et al. (2005).

Results are expressed in terms of the ratio of the sediment vertical velocity and the shear velocity. In the case of the CTFM, both variables are obtained within the numerical solution, while in the PTFM, only the shear velocity is calculated. It is observed that a good agreement between numerical predictions and observations has been obtained. Differences stem from the fact that the calculated vertical velocity of sediment is not exactly that obtained from usual literature regressions (employed in the PTFM), and that the calculated shear velocity also differs from that reported in the experiments by a relatively small amount.

The above models were used to study non-dilute mixtures by Jha and Bombardelli (2010). They found that the Schmidt number for non-dilute conditions is larger than one, which could be attributed to the smaller distance among particles, in a similar way of what happens with the diffusion of gases.

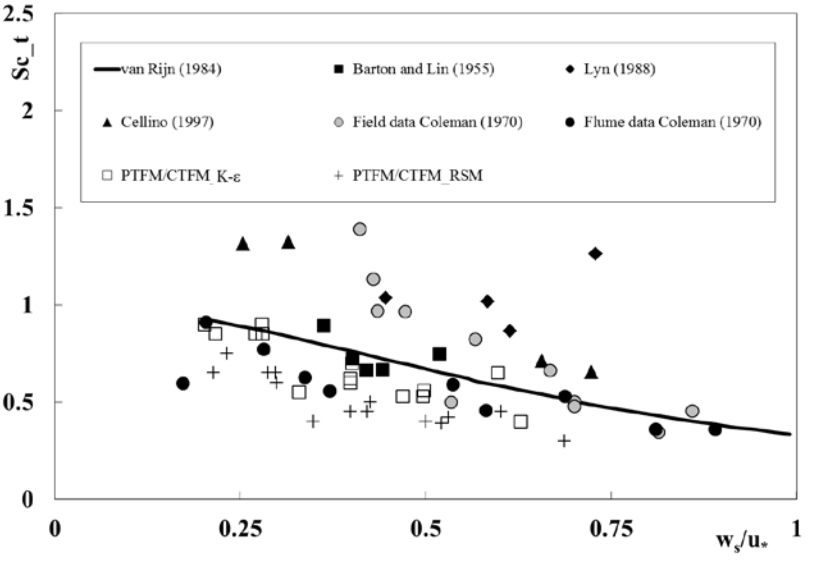

Fig 2 – Comparison of numerical results (open symbols) with experiments (filled symbols) contributed by different authors for the turbulent Schmidt number in a particle-laden, open-channel flow. Adapted from Jha and Bombardelli (2009).

CONCLUSIONS

The most widely applied approach for simulating turbulent flows is that based on the concept of Reynolds-averaging. If the transport of a scalar is simulated under this concept, the value of the turbulent Schmidt number Sc_t must be defined. As no universally-accepted values of this parameter have been established, there is still controversy about the proper parameterization of Sc_t for the various environmental flows.

In the present paper two case studies were presented to assess against experimental data the role of Sc_t in obtaining reliable numerical predictions. First, in both cases, turbulent transverse mixing of a tracer in a shallow water flow and sediment-laden, open-channel flow, the turbulent Schmidt number showed to be a key parameter. Second, in sediment-laden open channel flows Sc_t seems to strongly depend from the ratio of settling velocity to the shear velocity. Third, the above analysis demonstrated that in both the cases of tracer/non dilute mixtures transport values of the turbulent Schmidt number Sc_t larger than one resulted in a better agreement with the experimental data. This result confirmed previous findings by Graf and Cellino (2002) for the flow over bed without bed forms and by Muste et al. (2005) for natural sand. Furthermore, for non-dilute mixtures that finding could be attributed to the smaller distance among tracer/sediment particles, in a similar way of what happens with the diffusion of gases. Nevertheless further research will be needed to achieve a more comprehensive criterion for the parameterization of the turbulent Schmidt number.

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