SCALE PROBLEMS IN 3D SEDIMENT-TRANSPORT MODELLING, AND SUGGESTIONS TO OVERCOME THEM

Problèmes d'échelles dans les modèles 3D de transport des sédiments et suggestions à les résoudre

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ABSTRACT

Sediment transport models are helpful tools to study the dispersion of contaminants attached to fine-grained sediments in the marine environment. Currently used 3D sediment transport models still fail to make good quantitative predictions. Several causes can be attributed to the inadequate description of physical processes which occur at the subgrid scale level. Specific attention is given to the modelling of turbulent mixing, particle turbulence interactions and near-bottom boundary layer processes. A procedure for the development of new subgrid scale closures for engineering models applied to problems at geophysical scales of coastal waters and estuaries, based on two-phase flow theory and data generated by Large Eddy Simulation and low-Reynolds RANS models, is described. This leads to a three-layer approach, comprising a supersaturated near-bed layer, a transition layer (under certain conditions) and the fully developed turbulent water column.

RESUME

Les modèles numériques de transport des sédiments sont très utilisables pour étudier la dispersion des contaminants attachés aux particules fines dans le milieu aquatique. Les modèles 3D utilisées aujourd'hui ne réussissent pas à faire des prédictions quantitatives correctes, ce qu'on peut attribuer à la description inadéquate des processus qui ce manifestes sur les échelles non résolues. Dans cette étude attention est dirigée aux processus près du sol marin, diffusion turbulente et interactions entre turbulence et particules. Une procédure est présentée pour le développement des nouvelles lois de clôture pour les processus nouvelles lois de clôture pour les processus de sous-maille dans les modèles utilisées par des ingénieurs, appliquées aux problèmes à grandes échelles dans les eaux côtières et estuariennes. Cette procédure est basée sur la théorie des écoulements diphasiques et des donnés provenant des modèles LES et RANS à petit nombre de Reynolds. Cela résulte dans une approche à trois couches, comprenant d'une couche super-saturée sur le sol, une couche transitoire (dans certaines conditions) et la colonne d'eaux d'écoulement turbulente pleine développée.

I. INTRODUCTION

Many types of pollutants in the marine environment are attached to sediment particles, in particular the cohesive sediments, which contain a high clay fraction. Therefore, the prediction of the dispersion of sediment particles often can be used to determine the spreading of these contaminants. Usually, the large time and length scales for this dispersion, which are of importance for impact assessment, confict with the small scales of the governing processes. Currently used 3D engineering

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models for large scale sediment transport studies in estuaries and coastal areas sediment transport models prove to be very inaccurate, especially quantitatively. Close examination shows that these models have many limitations. Without a clear understanding of these, it is virtually impossible for "blind" users and customers to make a proper interpretation of the model results. The limitations of the numerical models can be divided into three major classes: physical, mathematical and numerical.

In the present study we limit ourselves to three-dimensional (3D) sediment transport models which resolve the Reynolds-averaged Navier-Stokes (RANS) equations for the hydrodynamics together with a sediment mass balance, and which are applied to problems with a typical duration of maximal a spring-neap cycle. The type of problems we consider then typically have grid sizes of the order of 0.1-10 m in the vertical and 10-1000 m in the horizontal and time steps in the order of 0.1-10 minutes. Many processes, however, occur at smaller scales and therefore cannot be resolved explicitly. These processes have to be described by so-called subgrid scale models, which apply some sort of averaging over the resolved scale. Within the framework of a research project funded by the Flemish Fund for Scientific Research, entitled "*Development of simulation models for two-phase flow on a geophysical scale, with applications to sediment transport in estuaries and coastal zones*", this problem of subgrid scale modelling is studied.

Reynolds-averaging is already an example of time-averaging of the small scale turbulence. Modern 3D sediment transport models use the k-ε turbulence model to describe the vertical eddy viscosity, but for the horizontal turbulent mixing the grid sizes are too large and a much simpler closure is used. Recently, attempts are undertaken to develop 2D Large Eddy Simulation (LES) closures. This new approach has been studied in the present project.

Two major spatial scaling problems need special consideration as they have large consequences on the modelling. They are related to the small scales of particle size and of turbulence. Waves and flocculation are also briefly discussed, but are not studied within the presented project.

II. ONE-FLUID MODELLING APPROACH

The size of the individual particles is of course much smaller than the grid size. In theory it would be possible to solve the movement of individual particles using Lagrangian particle tracking (Crow *et al.*, 1996). However, a quick calculation shows that a concentration of 1 g/l of 200 μm sand grains corresponds to a number density of 10^9 particles per liter. Even for LES simulations, with Lagrangian particle tracking, applied to small laboratory scale experiments, this number is becoming too high. Furthermore, this approach would require a good description of the fluid-particle interaction. Even though the theoretical equations are known (Maxey & Riley, 1983), they are difficult to apply and to calibrate, even for idealized spherical particles of uniform size. This is also one reason for not solving sediment transport by the full two-phase flow equations.

Sediment transport models apply another approach, which can be named the "one-fluid" approach. In essence, it shows close similarity to the well-known two-fluid approach applied in two-phase flow modelling of dispersions (Crow *et al.*, 1996). Historically, the equations solved by sediment transport models are those for the fluid phase alone, with some empirical corrections for particle-fluid interactions. This traditional approach works satisfactory as long as the sediment concentrations remain very small. However, near the bed this assumption no longer holds.

At present, there is no usable model available to describe the high-concentration particle-turbulence interactions near the bed. For this reason a new one-fluid formulation is under development, which rebuilds the suspension conservation equations (for volume, mass, momentum and turbulent kinetic energy) by weighted averaging of the conservation equations for the two phases. Depending on the choice of averaging, this leads to extra terms in the basic conservation equations for the fluid phase, which account for the particle-fluid interactions. The definition of closures for these extra terms is still under investigation, in particular for the turbulent kinetic energy (TKE) equation. For comparison: Abou-Arab & Rocco (1990) obtained 30 extra terms for the TKE equation of the fluid phase in a two-phase flow formulation. Many of these extra term consist of higher order correlations between fluctuations of fluid and particle velocities *and* concentration. No matter how these additional terms are treated, it is evident that eventually it has to led to a TKE equation with an additional dissipation term (Frey & Simonin, 2000; quoted in Villaret *et al.*, 2000).

III. TURBULENCE

Turbulence is generated due to microscopic hydrodynamic instabilities in shear flow, resulting in the creation of eddies, which grow (from sizes much smaller up to length scales larger than the grid size) and eventually dissipate. Therefore, turbulence is mainly produced where water shears a solid surface and another water body which streams at a very different speed.

The first type occurs along solid walls, i.e. shores and bottoms in the case of the marine environment. The second type is found along sharp density interfaces or lutoclines (e.g. a sediment-laden river plunging into the ocean), cavity-like flow (i.e. a stream along a body of stagnant water, e.g. a river generating an eddy in a harbour basin) or flow over a strongly varying bottom topography (e.g. the shear layers between a river and the adjacent shallow flood plains in compound channel flows). A majority of the examples of the second type of turbulence generation happen in primarily in the horizon plane, and can generate eddies significantly larger than the water depth. When the latter criterion is met, this is designated as quasi-2D (horizontal) turbulence (Nadaoka & Yagi 1998; Awad, 2005).

III.1. Wall-bounded turbulence

Turbulence is generated in the boundary of shear flow along a wall. The “baby” eddies are generated in the viscous sublayer and are of the size of the Kolmogorov length scale ($\nu^{3/4}/\varepsilon^{1/4}$, where ν is the kinematic viscosity of the fluid and ε the turbulent energy dissipation rate) and grow proportionally to the distance from the wall. The thickness of the viscous sublayer is of the order of $10\nu/u_*$ (with $u_* = (\tau_0/\rho)^{1/2}$, the shear velocity and τ_0 the wall shear stress), which corresponds to sizes of the order of mm or less. On top of that layer one finds the transition layer which is one order of magnitude thicker. Considering the typical vertical grid size for estuarine problems, which is of the order of meters (seldom decimetres), it is evident that the wall layer (the sum of the two latter layers) cannot be resolved by the numerical model. Nevertheless, within the wall layer the turbulence production is maximal.

In the current practice of state-of-the-art 3D sediment transport models, the bed generated turbulence is modelled by the standard k-ε turbulence model (Rodi, 1980), at least for the vertical turbulent mixing. This turbulence model is only valid for fully-developed turbulent flow, i.e. outside the inner wall layer. Therefore, the wall layer is not resolved, but instead wall functions, based on local equilibrium between production and dissipation in combination with the Prandtl mixing length theory, are used to define boundary conditions at the (near-) bottom nodes of the mesh (e.g., Benim & Zinser, 1985).

III.2. Particle-turbulence interaction

However, in the presence of sediment particles, the turbulence production is strongly modified. From stratified flow studies it is known for a long time that turbulence is damped by density gradients. This type of particle-turbulence interaction is called two-way coupling, since the fluid turbulence is affected, which in turn modifies the turbulent mixing. Up till now, sediment transport models have implemented empirical relationships of damping factors as a function of a Richardson number (usually the gradient Richardson number), following the long tradition in atmospheric science (Turner, 1973). Recent studies have revealed that this is unsatisfactory, both from an experimental as from a theoretical perspective (Toorman, 2000; Toorman, 2002). A new analysis of the vertical momentum balance has allowed the derivation of a theoretical closure for the turbulent Schmidt number, the ratio of eddy viscosity to eddy diffusivity, in the fully-developed turbulent outer layer of sediment-laden shear flow, which reveals that the controlling parameter actually is the ratio of settling velocity to the r.m.s. turbulent fluctuation of the vertical velocity (Toorman, 2007). This study furthermore reveals that the sediment flux balance actually consists of three contributions, i.e.: turbulent lift, gravity and turbophoresis (a particle flux in the opposite direction of the gradient of the vertical turbulence intensity).

The inner (or wall) layer in the case of sediment-laden turbulent shear flow can thicken considerably by the presence of sediment particles. Experimental evidence, combined with a new analysis of the suspension capacity condition (Toorman, 2002), suggests that this layer is actually super-saturated (i.e., suspending a load higher than the local suspension capacity), which is explained in terms of four-way coupling particle-fluid interactions, i.e., particles collide with each other due to the high densities and affect both the particle and the fluid turbulent fluctuations. The concentration limit for four-way coupling is estimated by Elghobashi (1994) at 0.1%. This roughly corresponds to concentrations of the order of g/l for sand particles, and even lower for aggregated cohesive sediment particles. The flow conditions in this layer correspond to sheet flow (at high enough shear velocities) or bed load.

Contradicting conclusions can in found in the literature with regard to the overall effect of particles in turbulent flow. The majority claim turbulence damping with drag reduction, while other find (apparent) enhancement of turbulence with increase in apparent bottom friction. Particle size and density certainly matter here. Gore & Crowe (1989) concluded from the analysis of various experimental data, that whether turbulence is damped or enhanced by the presence of particles, depends on the particle size relative to the length scale of the most energetic eddy. Small particles cause damping, while large particle cause turbulence production (at least far enough from walls).

A usable mathematical description for the sediment-laden wall layer is at present one of the major missing elements in improving sediment transport models. Besides the scale problem of the small subgrid scale thickness, also a suitable physical description is missing. In practice, this comes down to finding a formulation for the additional so-called grain shear stress, generated by particle collisions, which contributes to suspending particles. It is found that Bagnold’s theory (1954) for hyperconcentrated flow (and later improvements) highly underestimates this grain shear stress, which is attributed to the fact that this theory is only valid for even higher concentrations where the voids between the particles are too small for turbulent eddies to develop (Toorman, 2007). This is in agreement with the proposal of Frey & Simonin (2000; quoted in Villaret *et al.*, 2000) that an extra eddy viscosity should be introduced, which respresents small scale turbulence produced in the wake of particles. Alternatively, Villaret *et al.* (2000) have tested a grain stress closure derived from kinetic gas theory, generally resulting in an overprediction of concentrations and transport rates. Turbophoresis has an important contribution within this layer and can be well predicted by LES, at least for low concentrations (Widera *et al.*, 2007).

III.3. Bottom roughness

But there remains another problem: the bottom of the bed grid cell is described in the model as a flat plate, while the real bottom usually will be uneven, with various features at different scales (from particle scale up to topographic variations). This complicates the definition of the bottom and its representative roughness.

The bottom roughness usually is determined as a best fitting constant which produces the best agreement between simulated and observed water levels. However, usually the corresponding fluxes are not correct. In a few exceptional cases one accounts for spatial variation of roughness, directly related to the spatial variation in particles size classes. But the traditional roughness closures are based on empirical steady flat plate roughness laws. Physically, the representative roughness in each grid cell should account for the subgrid scale roughness scales, which include grain roughness, (time-dependent) form roughness and subgrid topographic variations, and its modulation by particle-turbulence interaction in the mobile near-bed layer, which thickness usually also is of subgrid scale size.

In the present research project, the latter problem is addressed by using different models with various degrees of vertical grid size scales, going from 3D LES (Widera *et al.*, 2007), over fine-meshed two-layer low-Reynolds (2L) RANS (Heredia, 2006) to coarse-meshed high-Reynolds RANS models. The micro-scale LES models produce numerical data at a scale where physical measurements cannot be applied. The 2L models are used as intermediate models to make the first step of upscaling and to develop a low-*Re* strategy for coarse mesh RANS, where the final step of upscaling will be applied. Eventually, the final model will actually become a three-layer RANS model, with one layer describing the mobile near-bed layer, a possible intermediate low-*Re* layer in the case that low-*Re* effects extend into the next coarse layers (which possibly may occur around slack water), and a traditional high-*Re* layer.

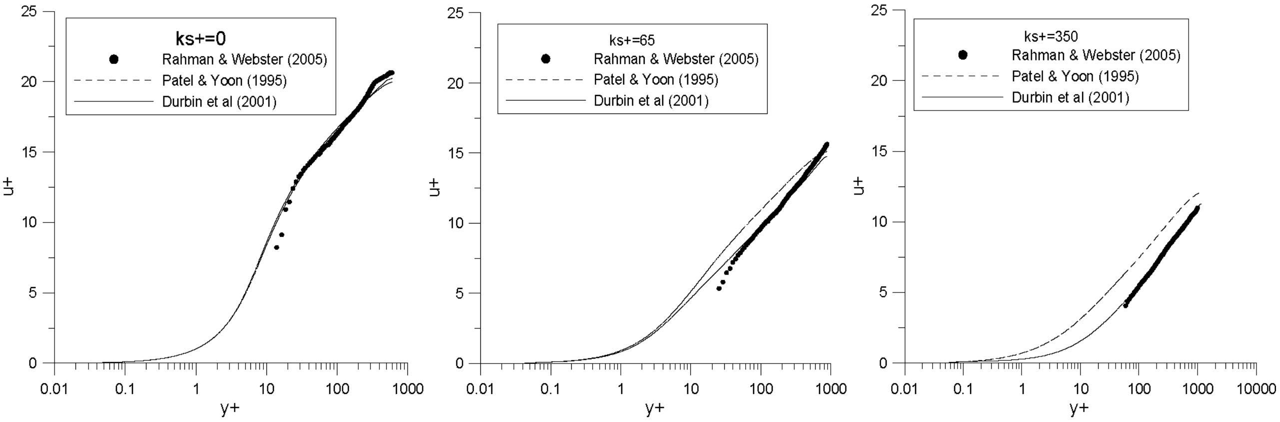

Figure 1. *Observed and predicted velocity profiles for the clear water experiments of Rahman & Webster (2005) for a smooth wall ($k_s^+ = 0$, left) and rough walls with $k_s^+ = 65$ (center) and 350 (right). 2L low-Re RANS model (Heredia, 2006).*

Figure 1 shows results from two formulations of a 2L low-*Re* RANS model adapted for rough boundaries. The model can be applied over the full range of roughness heights, from smooth up to fully rough hydraulic conditions (Heredia, 2006). In a following step, this model will be extended to account for suspended particles.

III.4. Three-layer approach

In order to allow inclusion of the near-bottom processes as well as transitional flow conditions into large scale 3D models, a three-layer approach is proposed. This is in fact a hybridization of the standard high-Reynolds model and the two-layer low-Reynolds model, both implemented in FENST-2D, the research code of the K.U.Leuven Hydraulics Laboratory. The near-bottom effects in the lowest few centimetres are described by a single layer where the eddy viscosity is computed based on the mixing-length concept. Above this layer, the two-layer low-Reynolds model is applied on a coarse vertical grid. In this way the fine grid requirements at the bottom are removed, but still allows low-Reynolds effects (transitional flow), which may occur around slack water, to be

simulated. The near-bed layer thus comprises bed load transport, sheet flow and fluid mud flow conditions.
The major problem then is concentrated into the description of the near-bottom processes in a single layer and providing the proper continuity of all variables (velocity, turbulent kinetic energy and its dissipation rate) at the interface with the layer above. In the original high-*Re* 2L model, conditions were imposed at the interface, based on wall functions. Now these conditions must be adapted to account for roughness and suspended sediment, which change turbulence production and consumption for maintaining particles in suspension. These modifications are actually comprised into the empirical modulation functions, corrections factors for the eddy viscosity and the eddy diffusivity (Toorman, 2000). In a following step of the project, new turbulence modulation functions will be derived, theoretically, based on one-fluid theory and on a layer integrated energy balance, and empirically, based on experimental sheet flow data and numerically generated data.

III.5. Horizontal mixing (Quasi-2D turbulence)

Horizontal grid sizes for coastal sediment transport simulations are usually one to three orders of magnitude larger than the vertical grid size (i.e., of the order of 10^2-10^4 m). The turbulence models used for the vertical mixing cannot be applied for the horizontal turbulent dispersion. Traditional models mostly work with a constant eddy viscosity of the order of 1-100 m^2/s. As long as large scale vortices do not play a role, this rude approach seems to work satisfactory. However, in recent years, more and more interest is growing towards more complicated models, in particular horizontal 2D LES or HLES for short (Nadaoka & Yagi 1998; Uittenbogaard, 2003). HLES can deal with turbulence generated in horizontal shear layers, which may result in horizontal eddies typically larger than the water depth. A major shortcoming in these models is the lack of coupling with the 3D turbulence generated by bottom friction. For this purpose a new double scale HLES model has been developed and is currently being tested. The representation of the backscatter of turbulent kinetic energy is a key element for the accuracy of the 2D subgrid scale model

IV. WAVE EFFECTS

Waves play an important role in sediment transport, especially in shallow coastal waters. They generate additional bed shear stresses and can cause fluidization of sediment bottoms, by which contaminants may be remobilized. But waves also cannot be resolved explicitly, as wave lengths are much smaller than horizontal grid sizes, and often wave periods are smaller than the time step. The free surface treatment can only deal with tidal effects. Therefore, waves have to be modelled also by some sort of subgrid scale model. In practice, wave properties are then predicted using spectral models, which compute the energy transformation of wave fields, from which wave generated stresses can be computed.

V. PARTICLE FALL VELOCITY

The particle terminal fall velocity or settling velocity in quiescent water is one of the most important parameters in the sediment transport equation. Its value is determined by size and density of the particle. But particle size distributions are non-uniform and for cohesive sediments flocculation makes everything even more complicated. In general, particle sizes and, in the case of cohesive sediment, also densities vary in space and time. This is an important source of uncertainty for the model results.

The one-fluid formulation requires all the particles in one (large!) grid cell to represented by a certain value of settling velocity, which results in the same flux as the heterogeneous mixture of effectively present particles. The effect of concentration on the settling velocity can relatively well be described by an empirical hindered settling correction factor (e.g., Toorman, 1999). For cohesive sediment particles, which are most prone to attach contaminants, one has to account for the aggregation and break-up of the flocs, which form as a result of electrostatic forces and organic slimes.

The earliest empirical models produce a value for the settling velocity as a function of the r.m.s. turbulence shear stress and concentration (e.g. Van Leussen, 1994), assuming immediate response to changing conditions. The time scales of the dynamics of aggregation and break-up have not been considered. This can be done with flocculation models based on structural kinetics (e.g. Winterwerp, 1998). The first version assumed a certain constant fractal dimension. But it soon has been realised that also the floc structure and density varies. Recent research is trying to incorporate population balance equations to describe flocculation processes (Nopens *et al.*, 2005). However, for practical application to large scale sediment transport studies, this approach becomes too demanding. One should not forget that with increasing model complexity, the number of model parameters to be calibrated increases, which increases the uncertainty on the model results. A new heuristic proposal has recently been formulated (Winterwerp *et al.*, 2006). Much work remains to be done in this field in order to provide a simple, but accurate fall velocity predictor.

VI. CONCLUSIONS

Sediment transport models are important tools for the assessment of the dispersion of contaminants attached to (primarily) fine-graind sediment particles and aggregates. Currently used 3D sediment transport models are inadequate for the prediction of sediment fluxes, because several physical processes are not described adequately. The major short-coming is the poor description of particle-turbulence interaction. This topic is the major subject of a FWO funded project and is discussed in depth in this paper. Particle-turbulence interactions result in modification of the turbulence properties of the suspending fluid and subsequently alter the bed shear stress. Numerical experiments have shown drag reduction up to a factor 3, in agreement with lab and field data (Toorman, 2002). When the bottom shear stress is not as the model predicts, sediment fluxes (erosion, deposition, sediment budget) will also be wrong. Indeed, presently sediment transport models only succeed in predicting trends, not quantities. Particle exchange with the bottom falls beyond the scope of this paper, even though it is important with regard to (re)mobilization of contaminants from within the bed. But this requires a discussion of the description of bed properties, which is a topic on its own.

A three-layer modelling approach is proposed to allow the modelling of high-concentration effects near the bottom with low-Reynolds number flow on a coarse mesh. Results from a two-layer low-Reynolds model and Large Eddy Simulations are used to help developing proper closures. On the other hand, a one-fluid formulation is proposed to construct the complete suspension conservation equations, valid at high concentrations. A new closure has been found for the turbulent sediment flux, allowing a physically more correct description of the turbulent Schmidt number. Further progress is expected within the near future.

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