Benchmarking an unstructured grid sediment model in an energetic estuary.

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Abstract

A sediment model coupled to the hydrodynamic model SELFE is validated against a benchmark combining a set of idealized tests and an application to a field-data rich energetic estuary. After sensitivity studies, model results for the idealized tests largely agree with previously reported results from other models in addition to analytical, semi-analytical, or laboratory results. Results of suspended sediment in an open channel test with fixed bottom are sensitive to turbulence closure and treatment for hydrodynamic bottom boundary. Results for the migration of a trench are very sensitive to critical stress and erosion rate, but largely insensitive to turbulence closure. The model is able to qualitatively represent sediment dynamics associated with estuarine turbidity maxima in an idealized estuary. Applied to the Columbia River estuary, the model qualitatively captures sediment dynamics observed by fixed stations and shipborne profiles. Representation of the vertical structure of suspended sediment degrades when stratification is underpredicted. Across all tests, skill metrics of suspended sediments lag those of hydrodynamics even when qualitatively representing dynamics. The benchmark is fully documented in an openly available repository to encourage unambiguous comparisons against other models.

Keywords: sediment model, model validation, sediment dynamics, estuaries, Columbia River

1 Introduction

Sediment dynamics of estuaries control morphodynamic and biogeochemical processes with implications ranging from ecosystem function and health (Ferguson et al., 1996) to navigation (Meade, 1972) among other aspects of system sustainability, management and operation. Driven by tides and buoyancy, estuarine circulation commonly leads to a complex vertical structure of density and currents requiring three-dimensional modeling to represent the inherently depth-varying circulation and sediment processes. As a consequence, sediment modules have been developed for existing three-dimensional circulation models including structured grid models such as Delft3D (Lesser et al., 2004) and ROMS (Warner et al., 2008) and unstructured grid models including FVCOM (Chen et al., 2003), SUNTANS (Fringer et al., 2006), and SELFE (Zhang & Baptista, 2008) and its derivative SCHISM (Zhang et al., 2016). Regardless of the grid structure and specific numerics, sediment modeling systems generally solve the advection-diffusion equation for a user-defined number of suspended sediment classes with distinct approaches for boundary conditions, interactions with bathymetry, and bed load transport.

Validation of sediment models has consisted predominantly of idealized cases with assessments against analytical or laboratory results. Open channel cases without density effects requiring reproduction of a Rouse profile are a common test to evaluate suspended sediment dynamics (Lesser et al., 2004; Pinto et al., 2012; Warner et al., 2008). The trench migration test case of *van Rijn* (1986) is commonly used to evaluate simulation skill for predictive bedload and morphodynamic behavior (Lesser et al., 2004; Pinto et al., 2012; Warner et al., 2008). Idealized estuarine test cases that include density effects have been used to evaluate sediment behavior in controlled conditions, but lack quantitative solutions (Burchard & Baumert, 1998; Warner et al., 2008). Validation tests inclusive of short wave effects include both laboratory experiments (Lesser et al., 2004) and comparisons against field observations (Warner et al., 2008).

Realistic applications of suspended sediment models are frequently used to study processes associated with estuarine turbidity maxima (ETM). *Brenon & Hir* (1999) studied the development of the Seine ETM using a single non-cohesive class with a parameterization derived from literature values. *Burchard et al.* (2003) used a single non-cohesive class characteristic of that system to simulate and study the Elbe ETM using GETM. *Lin et al.* (2003) characterized the ETM and a secondary turbidity maximum in the York River using a single non-cohesive class with other parameterizations derived from sensitivity studies. *de Nijs & Pietrzak* (2012) evaluated the skill of Delft3D to represent the characteristics of multiple ETMs in the stratified Rotterdam Waterway in realistic conditions using a single non-cohesive sediment size class, with the derivation of sediment parameterization details not disclosed. *Ralston et al.* (2012) used four non-cohesive classes with sediment parameterization based on previous studies to describe the effects of bathymetry on sediment transport in the Hudson using ROMS. In another study with multiple classes, *Ralston et al.* (2013) used three non-cohesive classes to study sediment dynamics along intertidal flats in the Skagit Bay using FVCOM with the parameterization derived from available observations and literature values.

The aim of this paper is to validate an unstructured grid sediment model coupled to SELFE through a combination of idealized test cases (barotropic open channel, barotropic trench migration, and baroclinic tidally driven estuary) and a realistic application to an energetic estuary. The idealized tests are drawn from literature, and are designed to assess model skill at representing essential processes: suspended sediment transport, erosion and deposition, bed load transport, and morphological evolution. Model sensitivity to hydrodynamic and sediment parameterizations are described and optimal results are qualitatively compared against previous work and available analytical, semi-analytical, or laboratory results. Field observations from endurance stations and shipborne instrumentation in Columbia River estuary, USA are used to assess model skill in representing observed sediment dynamics in the complex and energetic Columbia River estuary. To facilitate future model inter-comparison and to promote the improvement in skill of sediment models, the tests and data are publically available as a benchmark (Lopez & Baptista, 2016).

2 Methods

2.1 Hydrodynamics model

SELFE (Zhang & Baptista, 2008) solves the Reynolds-averaged Navier-Stokes equations using both hydrostatic and Boussinesq assumptions. The governing equations are solved in a semi-implicit finite element (P_1-P_{NC}) framework using a combination of numerical methods. The advection of momentum is solved with a semi-Lagrangian method following *Casulli & Cheng* (1992). Scalar transport is solved using either upwind or total variation diminishing (TVD) Eulerian finite volume methods. Beyond the intrinsic differences between upwind and TVD, in SELFE the upwind scheme includes an implicit calculation of vertical flux, whereas TVD utilizes an explicit calculation resulting in a much slower time to solution. Comparisons of upwind and TVD transport schemes reveal minor differences in model skill of temperature and salinity in the Columbia River estuary. Because of the minor differences in skill and large differences in computational cost, we chose to use the much faster upwind scheme. Governing equations are closed by the general length scale (GLS) equations (Umlauf & Burchard, 2005) implemented in either a native SELFE implementation or by on-line coupling the GOTM library. The domain is discretized using a triangular, unstructured mesh in the horizontal similar to a hybrid CD grid and a hybrid Z- and S-level approach in the vertical.

In this paper we discuss the implications of two distinct treatments for the solution of the momentum equation at the bottom boundary on represented sediment dynamics. As is common in coastal hydrodynamic models, SELFE uses a bottom boundary condition where the internal Reynolds stress is balanced with the stress from bottom friction

$$\boldsymbol{\nu}\frac{\partial \boldsymbol{u}}{\partial \boldsymbol{z}} = \boldsymbol{\tau_b} \qquad 1)$$

where ν is the vertical eddy viscosity, u is the velocity, z is the vertical coordinate, and τ_b is the bottom stress. Assuming a turbulent boundary layer, a logarithmic velocity profile in the bottom boundary layer, and using turbulence closure theory to find the eddy viscosity results in a constant Reynolds stress in the bottom boundary layer:

$$\nu \frac{\partial u}{\partial z} = \frac{\kappa_0}{ln(\delta_b/z_o)} \sqrt{C_D} |u_b| u_b \qquad 2)$$

where C_d is the drag coefficient, z_0 is the bottom roughness, κ_0 is the von Karman, δ_b is the thickness of the computational cell, and $\boldsymbol{u_b}$ is the bottom velocity (Zhang & Baptista, 2008). Specifically, $\boldsymbol{u_b}$ is taken to be the velocity at the top of the bottommost computational cell. Traditionally in SELFE, the discretized momentum equation was solved from the free surface to the top of the bottommost computational cell with the bottom node assigned a velocity of 0 to be consistent with a log layer adhering to the law of the wall. A new implementation, starting with version 4.0 of SELFE, solves the momentum equation from the surface to the bottom node to be consistent with the finite element formulation resulting in a non-zero velocity at the bottom node and an improved representation of the bottom boundary layer. The two implementations produce distinct estimates of $\boldsymbol{u_b}$ used in Equation 2 resulting in distinct representations of bottom stress and shear. The implications of the new bottom boundary treatment of momentum for sediment modelling are discussed in idealized test cases. For convenience in differentiation, we refer to the traditional implementation as "no-slip" and the newer treatment as "slip" recognizing that formally both treatments are partial slip conditions.

2.2 Sediment model

The sediment model evaluated here is derived from the Community Sediment Transport Model (CSTM) (Warner et al., 2008). The non-cohesive classes, bed property changes, and bed morphology from the CSTM model were ported by *Pinto et al.* (2012) to work with the unstructured grids and methods used in SELFE. The model used here is algorithmically similar to *Pinto et al.* (2012), but was substantially refactored to align more closely with the original CSTM implementation. Minor implementation changes to improve stability including limiting slopes and increasing checks for numerically undefined numbers were required for the model to work in the Columbia River domain.

The sediment model solves for the time evolution of suspended sediments in three-dimensions and morphological changes. Specifically, the model calculates the vertical settling, bed load transport, and interactions with the bed through erosion and deposition for a user-defined number of non-cohesive classes. Suspended sediment concentrations are calculated by solving the advection-diffusion equation with additional terms for settling velocity and horizontal velocity

$$\frac{\partial C_n}{\partial t} + u\frac{\partial C_n}{\partial x} + v\frac{\partial C_n}{\partial y} + w\frac{\partial C_n}{\partial z} = \frac{\partial}{\partial z}\left(\kappa\frac{\partial C_n}{\partial z}\right) + w_{s,n}\frac{\partial C_n}{\partial z} + F_h \quad 3)$$

where C_n is the sediment concentration of class n, (u, v, w) are the directional velocity components, κ is the eddy diffusivity, $w_{s,n}$ is the settling velocity of class n, and F_h is the horizontal diffusion. Equation 3) is solved using either the upwind or TVD transport schemes in SELFE (Zhang & Baptista, 2008). The vertical movement of sediment is handled using a hybrid WENO-PPM semi-Lagrangian method (Warner et al., 2008). Multiple bed layers are supported and erosional flux is calculated using the method outlined by *Harris & Wiberg* (2001). Specifically, the depositional flux, D_n, is calculated using

$$D_n = w_{s,n} \cdot C_b \quad 4)$$

where $w_{s,n}$ is the settling velocity for sediment class n and C_b is the total sediment concentration in the bottom cell. The erosional flux for sediment class n, E_n, is defined as

$$E_n = \begin{cases} E_{0,n}(1-p)f_p\left(\frac{\tau_{sf}}{\tau_{cr,n}} - 1\right), & if\ \tau_{sf} > \tau_{cr,n} \\ 0, & otherwise \end{cases} \quad 5)$$

where $E_{0,n}$ is the bed erodibility constant, p is the porosity of the top layer of the sediment, f_p is the volumetric fraction, τ_{sf} is the bed shear stress, $\tau_{cr,n}$ is the critical shear stress, $d_{50,n}$ is the median sediment diameter, $\rho_{s,n}$ is the density of the sediment, and ρ_w is the density of the water. Bed load calculations use the formulation of either *Meyer-Peter & Müller* (1948) or *van Rijn* (2007). Updates to bathymetry resulting from erosion, deposition, and bed load, the Exner equation, are calculated using the SAND2D bottom update module (Fortunato & Oliveira, 2004). This module uses a finite volume method where the sediment flux is conserved over the cells neighboring a node center using a forward Euler time-stepping scheme. The sediment module is also two-way coupled to the hydrodynamics of SELFE through the equation of state

$$\boldsymbol{\rho} = \boldsymbol{\rho_o} + \sum_{n=1}^{N} \frac{\boldsymbol{C_n}}{\boldsymbol{\rho_{s,n}}} (\boldsymbol{\rho_{s,n}} - \boldsymbol{\rho_w}) \qquad 6)$$

where the new density ρ includes densities of water and each sediment class weighted by their respective concentrations.

2.3 Model skill

As is common practice in applied sediment modeling, an important part of the skill assessment in this paper is qualitative. However, we also explore quantitative metrics that are commonly used in circulation modeling: root mean square error (RMSE), Willmott Score (WS), Murphy Score (MS), correlation coefficient (Corr), and bias.

The root mean square error (RMSE) is defined as,

$$\boldsymbol{RMSE} = \sqrt{\langle(\boldsymbol{m} - \boldsymbol{o})^2\rangle} \qquad 7)$$

where $m = {m_i}_{i=1}^{n}$ are the modeled time series, $o = {o_i}_{i=1}^{n}$ are the observed times series, and $\langle\cdot\rangle$ indicates the average over the series. The primary advantage of using RMSE results from the intuitive interpretation because the metric and measured values sharing the same units. A disadvantage of using RMSE is the large weight outliers impart on the metric and that it does not provide a means to compare variables measured in different units.

In contrast, the Willmott score (WS) allows comparison between variables because it is non-dimensional (Willmott, 1981). The WS is defined as

$$\boldsymbol{WS} = \boldsymbol{1} - \frac{\langle(\boldsymbol{m} - \boldsymbol{o})^2\rangle}{\langle(|\boldsymbol{m} - \langle\boldsymbol{o}\rangle| + |\boldsymbol{o} - \langle\boldsymbol{o}\rangle)^2\rangle} \qquad 8)$$

A frequent criticism of the WS is the yielding of high skill scores for unrelated time series (Ralston et al., 2010).

An alternative skill metric that is not as susceptible to outliers, is non-dimensional, and allows for comparisons between units is the Murphy Score (MS),

$$\boldsymbol{MS = 1 - \frac{\langle (m - o)^2 \rangle}{\langle (m_r - o)^2 \rangle}} \quad 9)$$

where m_r is the reference model that is compared against. A Murphy Score of 1 indicates a perfect model, 0 (zero) indicates that the model is equivalent to the reference model, and a negative score indicates skill worse than the reference. In this study we typically use the mean of the observations as the reference model. However, for the trench migration test in Section 3.2 the reference model is the initial depth, and, following common nomenclature in the morphological literature (Sutherland et al., 2004), we refer in that case to the Murphy Score as the Brier Skill Score (BSS).

Finally, we also consider both correlation coefficient and bias for comprehensive purposes. The correlation coefficient, $Corr$, is a measure of linear correlation between two signals defined as

$$\boldsymbol{Corr = \frac{\mathrm{COV}(m, o)}{\sigma_m \sigma_o}} \quad 10)$$

where $\mathrm{COV}(m, o)$ is the covariance of model results m and observations o and their respective standard deviations are denoted by σ_m and σ_o. The bias, is simply the mean difference between the model results and observations.

3 Idealized Tests

3.1 Transport: Steady open channel

This test evaluates the simulated transport of suspended sediment in an unstratified open channel and has been studied previously in *Warner et al.* (2008) and *Pinto et al.* (2012). The domain is a long open channel (L = 10,000 m, W = 1,000 m, H = 10 m) with a constant slope of 4 x 10^{-5} m m^{-1}. The boundary conditions consist of a fixed depth of 10 m imposed at the downstream end and a logarithmic velocity profile applied at the upstream boundary with a depth-averaged velocity of 1 m s^{-1}. The horizontal grid consists of 2,000 elements and 1,111 nodes, and 21 S-levels ($\theta_b = 1$ and $\theta_f = 3$) were used in the vertical. Both the SELFE and GOTM implementations of the GLS equations were tested to evaluate the effects of turbulence closure on the solution. Specifically, from the native SELFE GLS implementation we use *k-kl*, *k-ε*, and *k-ω* with the Kantha-Clayson stability function and *k-ε* and *k-ω* with the Canuto-A stability function from the GOTM library (Table 1). Strict direct comparisons between SELFE and GOTM implementations of the GLS equations are not possible for any specific closure model. The SELFE implementation does not have an option for the Canuto-A stability function, and GOTM would not converge to a solution when using Kantha-Clayson. Nevertheless, the selected turbulence closure models demonstrate important differences between the GLS implementation in GOTM and SELFE.

We compare the effects of the selection of the turbulence closure model and bottom boundary treatment on eddy diffusivity, turbulent kinetic energy (TKE), suspended sediment concentrations (SSC) and velocity profiles against semi-analytical and analytical solutions. (J. Paul Rinehimer, personal communication; See Appendix). The analytical solution assumes a Prandlt number of 0.8, a logarithmic velocity profile, a no-slip bottom boundary treatment, a Rouse SSC profile, and setting the free parameter z_0 to 0.0053 m to match the numerical experiments. The numerical semi-analytical solution is obtained from the numerical model by imposing a parabolic eddy viscosity, K_M, and eddy diffusivity, K_H, instead of using a GLS turbulence closure model. The semi-analytical eddy viscosity and eddy diffusivity apply the same assumptions used in the calculations of the analytical solution.

Figure 1 shows the results using the “no-slip” bottom boundary described in Section 2.1. All turbulence closures capture the analytical solution of velocity well, but underestimate near-bed velocities (Panel A). The SELFE implemented closures tend to underestimate velocity. The semi-analytical solution uniquely overestimates velocity throughout the water column compared to the analytical solution. The eddy diffusivity (Panel C) is underestimated for all closures, consistent with the findings of *Warner et al.* (2008) and *Pinto et al.* (2012). The native SELFE implementation of the GLS produces eddy diffusivity profiles distinctively skewed near the surface (k-ε and k-ω) and bottom (k-ε), whereas the GOTM closures produce smoother, non-symmetric profiles. Profiles for TKE (Panel D) feature large spikes one level above the bottom for all closures, but are amplified for SELFE implemented closures. SSC profiles (Panel B) are underestimated compared to the analytical and semi-analytical solutions, as found in previous studies (Pinto et al., 2012; Warner et al., 2008). SSC profiles result from a balance of the sediment settling velocity and the upward velocity from the eddy diffusivity implicating the underprediction of erosion and eddy diffusivity in the resulting in the underestimate of SSC.

For contrast, Figure 2 shows results using the “slip” bottom boundary treatment. As was the case with the “no-slip” treatment, velocity profiles are well represented by all closures (Panel A), with the semi-analytical solution producing distinctive overestimations. However, all closures overestimate near-bottom velocities and most underestimate surface velocities when used with the “slip” bottom boundary. All closures again underestimate eddy diffusivity (Panel C), leading in aggregate to lower values than in the “no-slip” case. The convex shape near-the surface in the SELFE closures are still present, but are less severe and the near bed spikes are absent. Also, all profiles are now more symmetrical and thus, in that sense, closer to the analytical solution. The k-ε closures produce the largest diffusivities, with the SELFE native implementation leading to the largest maximum value, but the GOTM implementation most closely aligns with the analytical solution. For TKE (Panel D), the artificial near-bottom spikes are eliminated for GOTM closures and substantially reduced for SELFE implementations. Estimates of SSC (Panel B) are lower than those predicted in the “no-slip” case, which is attributed to the elimination or reduction of artificial near-bed TKE spikes.

Comparisons of bottom shear stress (used to calculate erosion), erosion rate, eddy diffusivity, and SSC are shown in Table 2. These results show that skill of SSC requires accurate predictions of eddy diffusivity and is less sensitive to deviations in bottom shear stress. The SELFE GLS implementations produce higher values of eddy diffusivity and, therefore, SSC, but at the cost of producing physically questionable profiles of eddy diffusivity and TKE. In contrast, the GOTM implementation predicts lower values of eddy diffusivity with smooth profiles that better match the shape of the semi-analytical and analytical solution. Given these tradeoffs, we believe that the combined used of the "slip" bottom boundary and GOTM for turbulence closure is the superior choice. We also note that this test highlights the inherent sensitivity of sediment models to model parameterization and numerical implementation, even in highly constrained tests.

3.2 Bed dynamics: Trench migration

This test is used to validate the implementation of suspended sediment, bed load, and morphology algorithms and is based on the flume experiments described in (van Rijn, 1993). The domain is an open channel (L = 30 m, W = 5 m) with a constant slope of 4.0 x 10^{-4} m m^{-1} featuring a trench cut into the bed. The bed and suspended sediments are comprised of a single non-cohesive class D_{50} = 0.16 mm with the settling velocity derived from the Stokes settling velocity and imposed as a constant value (w_s = 11 mm s^{-1}). The upstream hydrodynamic boundary condition consists of a constant velocity and depth (h_0 = 0.39 m, u_0 = 0.51 m s^{-1}) and suspended sediments are supplied upstream at a constant concentration of 0.14 kg m^{-3} to ameliorate erosion. The model hydrodynamics and suspended sediment are spun up with a fixed bed until the currents and SSC reach a steady state after ~25 minutes. The morphological algorithms are then enabled and the simulation proceeds for 15 h more. A global time step of 0.375 s, corresponding to a CFL (Courant-Friedrichs-Lewy) number of 1.5, was used based on sensitivity analysis (not shown) and is 7.5 times longer than the used in *Pinto et al.* (2012). The parameters were derived from sensitivity analysis to match observations of velocity and suspended sediment as described in *van Rijn* (1986) and to alleviate bed erosion upstream of the trench. We ultimately retained an erosion rate of 0.7 x 10^{-2} kg m^{-2} s^{-1}, compared to the rate of 1.6 x 10^{-2} kg m^{-2} s^{-1} used in *Pinto et al.* (2012), which produced excessive erosion and trench migration in our simulations. A summary of the model parameters is provided in Table 3.

Comparisons of profiles of suspended sediment and velocity between estimates of laboratory observations (markers, *van Rijn* (1986)) and model results (lines) are shown in Figure 3. Model profiles of velocity match observations most closely outside of the trench where a clear logarithmic profile is found in both the observations and model results. Stations within the trench show both slight overprediction and underprediction of velocity within a single profile, but are close to observations in magnitude. Profiles of SSC align with observations but have worse skill than the velocity profiles. In particular, the modeled SSC profiles underestimate concentrations near the bed. The underprediction of SSC is likely due to do a combination of underpredicted erosion and eddy diffusivity, as seen in the open channel case. Increasing the erosion rate yields increased SSC but produces excessive erosion and trench migration. The velocity and SSC skill appears to lag those produced by ROMS (Warner et al., 2008) and Delft3D (Lesser et al., 2004), but are similar to the results in Pinto et al. (2012). The trench migration is very similar to observations and aligns with the previously published results of *Pinto et al.* (2012) and *Warner et al.* (2008) despite using different parameters for erosion rate and critical stress. Skill scores for the trench migration case are shown in Table 4. The difference in the predicted final position of the trench results from underprediction of SSC and likely from underprediction of bedload transport.

Calibration simulations (not shown) confirm that the model is very sensitive to erosion rate parameterizations and must be carefully tuned to ensure that the SSC profiles align with observations. As in the open channel case in Section 3.1, this highlights the inherent uncertainty in sediment models in even highly constrained cases. However, the trench and open channel cases differ in some important respects. In particular, the calculated TKE in the upstream section of the trench does not exhibit the near-bed spike as seen in the open channel case, regardless of whether GOTM or SELFE are used for turbulence closure. Additionally, the GOTM eddy diffusivity deviates from a smooth profile near the surface, whereas the SELFE profile is very similar to that found in the open channel case (Figure 4). This likely results from the much higher vertical resolution used in this shallow test case

(30 vertical levels in 0.4 m) compared to the open channel case (21 vertical levels in 10 m) which is more representative of the resolution used in realistic scenarios.

Another difference is that, unlike in the open channel case (Section 3.1), trench migration results are largely insensitive to the selection of turbulence closure, but quite sensitive to the bottom boundary treatment (results not shown). This is because of the dominance of bed dynamics in the trench case whereas the open channel case lacks morphological evolution. Because the erosional flux is determined by near-bed velocities, changes in the treatment of the bottom boundary layer produce proportional changes in the bed evolution. This suggests that accurate simulation of near-bed velocities and bed properties are more important than turbulence closure in systems dominated by bed interactions.

3.3 ETM dynamics: Idealized estuary

This test is used to assess the ability of the sediment model to represent processes associated with the generation of an estuarine turbidity maximum (ETM). The test is derived from *Burchard & Baumert* (1998) and *Warner et al.* (2007), who used variations of it to assess the importance of ETM related processes and to describe those processes over tidal time scales. The domain is effectively a two-dimensional open channel 100 km in length and 200 m in width. The domain features a constant sloping bottom starting with a 5 m depth at the upstream boundary and ending with a 10 m depth at the downstream boundary. The ocean boundary is forced with a semi-diurnal displacement of the free surface with an amplitude of 0.4 m and a period of 12 hours and the constant imposition of salinity at 30 psu and temperature at 10 C. The upstream boundary is forced with a constant flux of 80 $m^3\ s^{-1}$, salinity of 0 psu, and temperature of 10 C. The hydrodynamics are allowed to spin-up for 14 days whereupon the initial conditions have been eliminated from the domain and a regular pattern of gravitational circulation has been established. We note that the solution to the problem is highly sensitive to the density forcing at the downstream boundary. Sensitivity tests (not shown) suggest that slight perturbations in the forcing results in both different spin-up period lengths and characteristics of the gravitational circulation patterns including salinity and SSC distribution.