Model Modelling: How to Think Inside the Box

Brynna Downey, Philippe Delandmeter

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Abstract

Herein lies an exercise to determine the efficacy of box models to describe complicated physical phenomena. Mass transport from the mouth of the Burdekin River to the Great Barrier Reef lagoon was simulated using the unstructured-mesh SLIM 3D hydrodynamic model. Results were isolated to the time period of January 1st to March 1st, 2007. Data of wind strength and direction, of water flux, and of sediment concentration had been collected for this time period and were used in the modelling process. A box model was then constructed to recreate as accurately as possible the results from the SLIM 3D model runs. Limitations of the box model were expected and observed appearing most prominently in the box model's inability to resolve small-scale features. However, the desire to have a simple yet comprehensive model was satisfied as the box model was able to resolve the large-scale features, allowing the most important physical processes to be illuminated.

Introduction

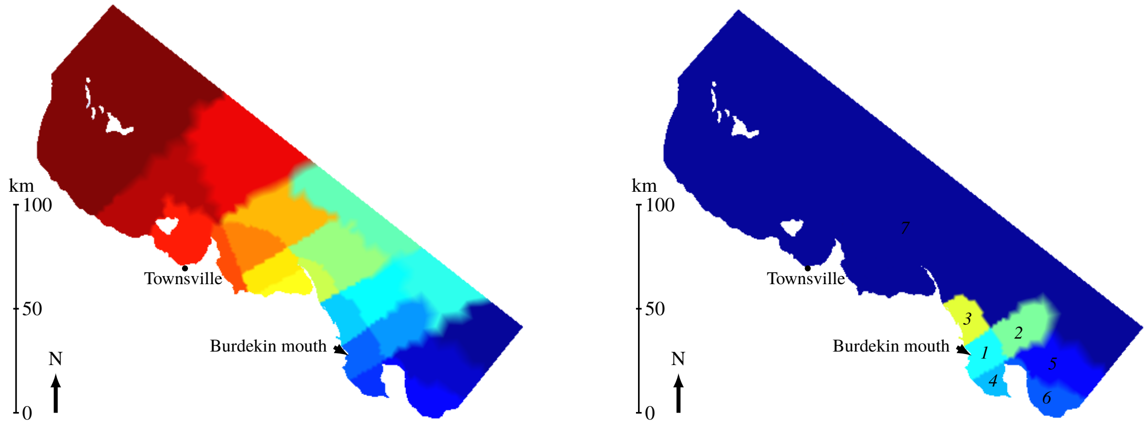
In contrast to the growing field of sophisticated simulations with large computation times and fully-fledged hydrodynamic equations, we present a box model meant to simulate particulate mass transport except in less time and with simpler flux expressions. The development of this box model is an experiment in numerical modelling to see whether the simplicity of the box model can fare as well as these sophisticated simulations. The success of the box model is determined by how closely it can replicate the results of SLIM 3D [1] as it is used in Delandmeter et al. (2015). It was not expected that the results would perfectly match those of SLIM 3D nor would it have been a surprise had nothing come to fruition. Since there is no established rubric for building box models, the methods with which this box model was developed are discussed, and the results are presented.

Methods

Domain division

The birth of the box model began with dividing the domain of interest into sub-domains with the intention that each sub-domain would be modelled by a uniform box. While there is no convention for the number, size, and boundary placement of these boxes, it is important to have a method to the madness that is making these seemingly arbitrary choices. In this example, regions of high

[1] Second-generation Louvain-la-Neuve Ice-ocean Model (www.climate.be/slim)



(a) All twenty-one zones

(b) Top six zones by mass

Figure 1: Area affected by Burdekin River with zones separated by color

mass accumulation previously observed via SLIM 3D and regions bordering land were divided more finely so as to see the direction of fine sediment movement and to observe what happens close to the nearby town, Townsville. Regions were further divided based on bathymetry with the cutoffs being less than 22 m, between 22 m and 40 m, and greater than 40 m. These values were chosen based on Delandmeter et al. (2015), and they represent the inner shelf, the middle shelf, and outer shelf respectively of the coastal waters. This whole process led to dividing the coast affected by the Burdekin River into twenty-one different zones as shown in figure 1 (a). For every zone, two boxes were created, one spanning the volume of water between the seafloor and the surface to model suspended mass and the other spanning the seafloor to model deposited mass. Having a box model with forty-two boxes defeats the purpose of having a simple model, and so the box model used the six zones with the most mass. These six zones were identified via running the SLIM 3D model, and the remaining zones were combined to form a seventh remainder zone. Figure 1 (b) shows the seven zones. The purpose then became to create a box model with seven zones i.e. fourteen boxes. The box model was built one zone at a time in order to increase the complexity gradually until a model of seven zones was obtained.

Equations

A system of fourteen linear differential equations describing mass transport among the boxes was constructed. The unknowns to solve for are defined here:

variable	definition
S_i	Suspended mass in zone i (kg)
D_i	Deposited mass in zone i (kg)
φ_{ij}	Flux from zone i to zone j $(\frac{kg}{s})$

The equations to solve for are defined below. Note that i spans $1, 2, ..., 7$ to account for each zone, whereas j spans $1, 2, ..., 8$ to account for each zone and everything outside the domain of the lagoon. Only for specific zone pairings where dispersive flux naturally goes from zone i to zone j is $\varphi_{ij} \neq 0$. Because of this, φ_{ji} is defined as $-\varphi_{ij}$. Even though zones 6 and 7 border the edge of the domain in addition to zone 5, no substantial flux was found to leave the domain here, and so $\varphi_{68} = \varphi_{78} = 0$.

$$\frac{dS_i}{dt} = -\delta_i\alpha_i S_i\left(\frac{w_0+W_i-\|\vec{w}\|}{w_0}\right)^{\frac{1}{4}} + \epsilon_i\beta_i D_i\left(\frac{\|\vec{w}\|}{w_0}\right)^3 \frac{\|\vec{w}\|-(w_0+W_i)}{w_0} + \sum_{j=1}^{8}\varphi(i,j) \quad (1)$$

$$\frac{dD_i}{dt} = \delta_i\alpha_i S_i\left(\frac{w_0+W_i-\|\vec{w}\|}{w_0}\right)^{\frac{1}{4}} - \epsilon_i\beta_i D_i\left(\frac{\|\vec{w}\|}{w_0}\right)^3 \frac{\|\vec{w}\|-(w_0+W_i)}{w_0} \quad (2)$$

$$\varphi = \begin{bmatrix} 0 & \varphi_{12} & \varphi_{13} & \varphi_{14} & 0 & \varphi_{16} & 0 & F \\ -\varphi_{12} & 0 & 0 & 0 & \varphi_{25} & 0 & \varphi_{27} & 0 \\ -\varphi_{13} & 0 & 0 & 0 & 0 & 0 & \varphi_{37} & 0 \\ -\varphi_{14} & 0 & 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & -\varphi_{25} & 0 & 0 & 0 & \varphi_{56} & \varphi_{57} & \varphi_{58} \\ -\varphi_{16} & 0 & 0 & 0 & -\varphi_{56} & 0 & 0 & \varphi_{68} \\ 0 & -\varphi_{27} & -\varphi_{37} & 0 & -\varphi_{57} & 0 & 0 & \varphi_{78} \end{bmatrix} \quad (3)$$

$$\varphi_{ij} = S_i min(\lambda_{ij}\vec{w}\cdot\hat{n}_{ji} - k_{ij}, -k_{ij}) + S_j max(\lambda_{ji}\vec{w}\cdot\hat{n}_{ji}, 0) \quad (4)$$

The three domain variables and six parameters are as follows with $\hat{n}_{ji} = -\hat{n}_{ij}$, λ_{ij} independent of λ_{ji}, and k_{ij} only defined when φ_{ij} is defined:

variable	definition
F	Flux entering lagoon from Burdekin River ($\frac{kg}{s}$)
$\vec{w}$	Averaged wind velocity taken at all time ($\frac{m}{s}$)
$\hat{n}_{ji}$	Unit vector from zone j to zone i perpendicular to boundary
α_i	Deposition parameter for zone i ($\frac{1}{s}$)
β_i	Re-suspension parameter for zone i ($\frac{1}{s}$)
w_0	Wind threshold ($\frac{m}{s}$)
W_i	Wind threshold variation for zone i ($\frac{m}{s}$)
λ_{ij}	Parameter for wind from zone i to zone j ($\frac{1}{m}$)
k_{ij}	Parameter for flux between zones i and j ($\frac{1}{s}$)
δ_i	$= 1$ if $\|\vec{w}\| < (w_0+W_i)$, else 0
ϵ_i	$= 1$ if $\|\vec{w}\| > (w_0+W_i)$, else 0

Between adjacent suspended mass boxes, flux occurs due to natural dispersion and due to wind forcings. The dispersive flux is proportional to the mass concentration of the box from which the mass leaves and to a flux constant that is unique to each set of neighboring boxes. The degree to which wind affects movement depends linearly on the wind strength and direction. The dot product of the wind direction and the line perpendicular to the boundary between adjacent boxes is taken to ensure that mass will flow in the correct direction. Parameters are multiplied by each wind expression to account for any physical effects that might otherwise cause more or less flux. Between the suspended and deposited boxes in each zone, whether sediment deposition or re-suspension occurs depends on the wind strength. If the wind strength is below a threshold level, then sediment from the suspended box will settle down to the deposited box, and if the wind strength is above this threshold, then sediment in the deposited box will become agitated and rise up via dispersion into the suspended box. It should be noted that there is no expression for flux from the deposited box of one zone to that of another since this quantity was found to be negligible by running SLIM 3D.

Matlab was used to solve the system of differential equations, and a least squares optimization function fine-tuned the parameters that needed to be experimentally determined namely the parameters for dispersive flux, wind, deposition, and re-suspension. By comparing the box model to the SLIM 3D model, we were able to calibrate our parameters to see how close we could get to replicating the SLIM 3D results.

Results

The results of the box model matched very closely with the results of the SLIM 3D model as seen in figures 2-8. How closely the box model matched to SLIM 3D depended greatly on the values of the parameters in the model as was expected. The mass difference between the box model and SLIM 3D is shown as a dashed line in each figure. Zones 5 and 7 show the most erratic error and might thus benefit from further compartmentalization to isolate the main problems be they problems with the box model equations or with the way the domain was divided up. At around 50 days, the box model is unable to resolve the mass peaks in zones 3 and 7, indicating that there are some physical processes that cannot be simplified to the extent done here.

Some zones were only able to replicate the SLIM 3D results by having a different wind threshold for sediment deposit and re-suspension hence the added wind threshold variation parameter. Wind expressions played a major role in forming peaks of mass that were observed in SLIM 3D, identifying the strength and direction of the wind as the main contributor to mass transport in the Great Barrier Reef lagoon.

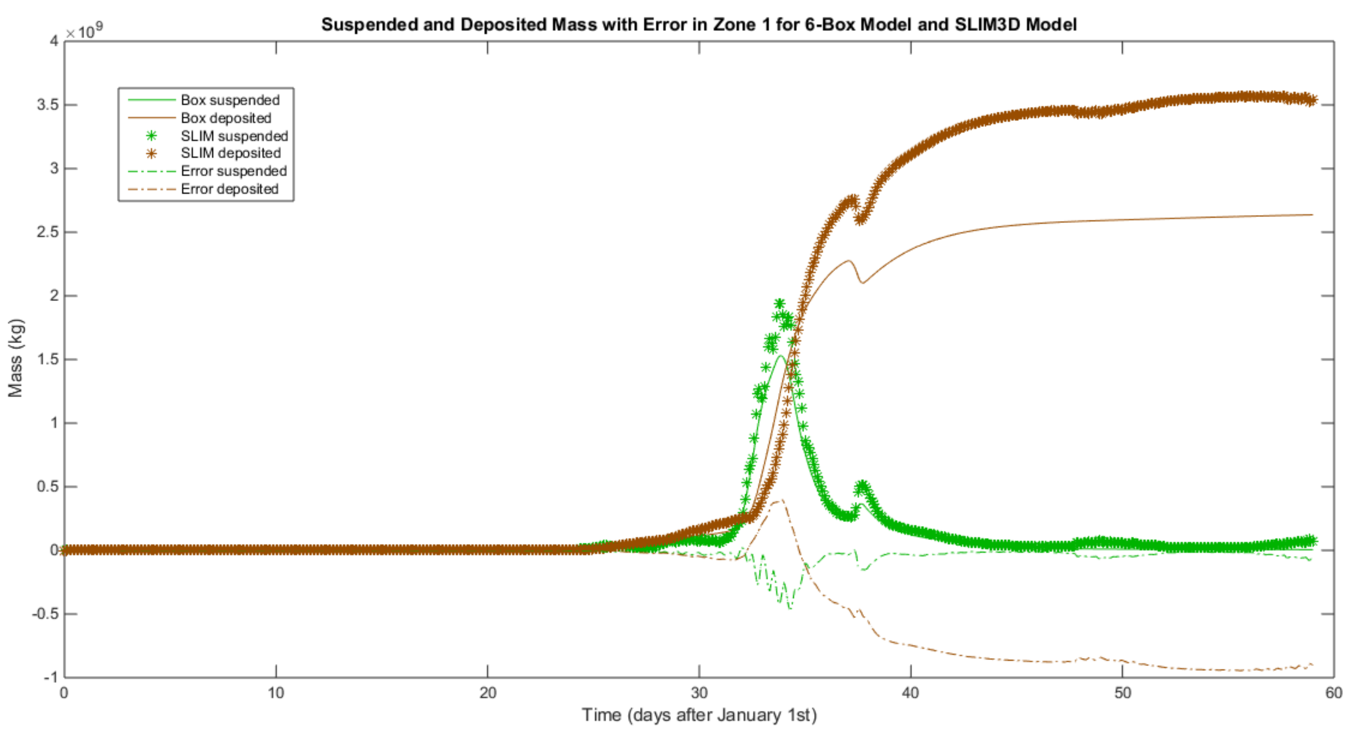


Figure 2: Plot comparing the suspended and deposited mass in zone 1 of the 14-box model to that of the SLIM 3D model. Positive error markings indicate too much mass predicted by box model.

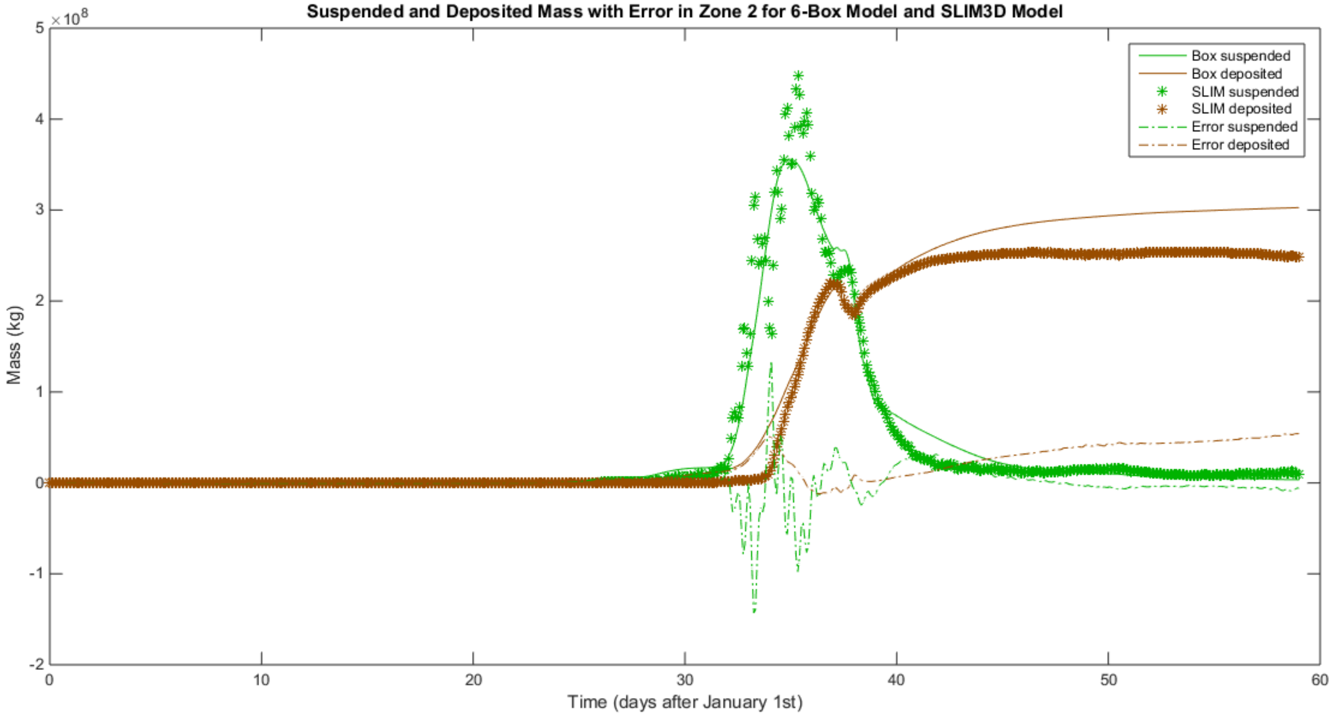


Figure 3: Plot comparing the suspended and deposited mass in zone 2 of the 14-box model to that of the SLIM 3D model. Positive error markings indicate too much mass predicted by box model.

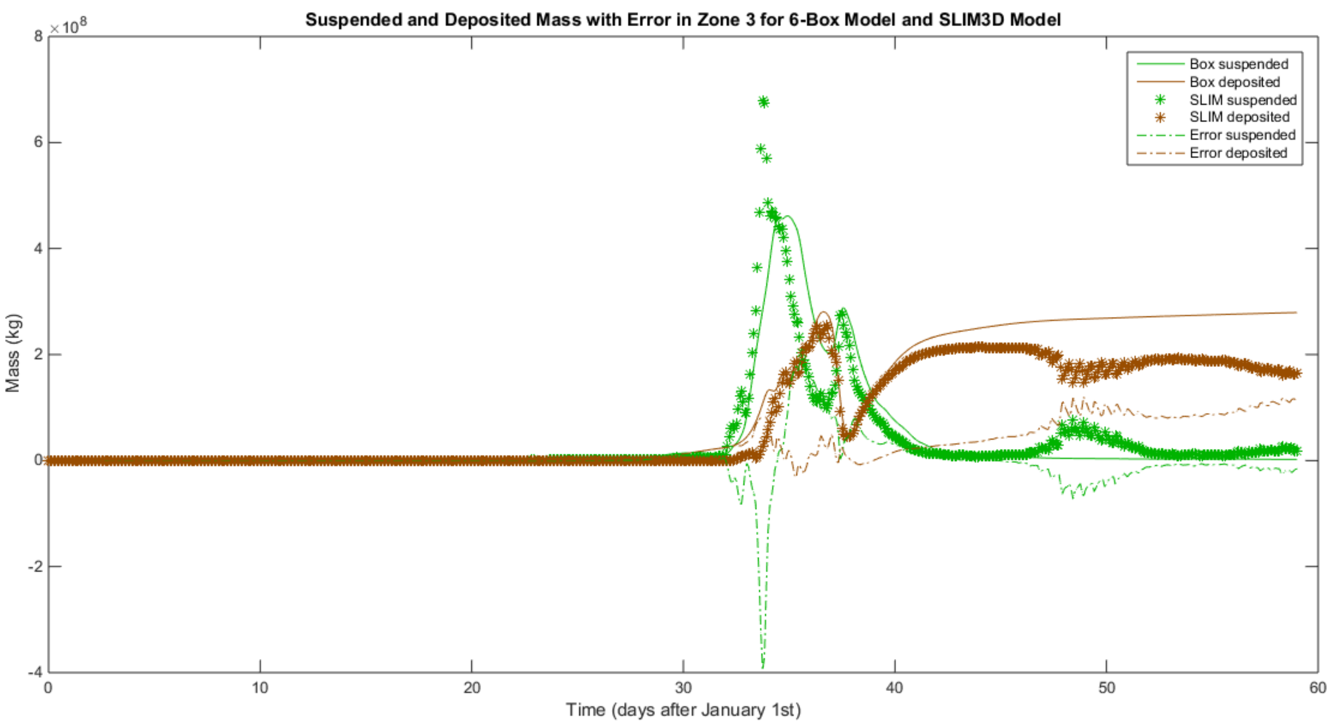


Figure 4: Plot comparing the suspended and deposited mass in zone 3 of the 14-box model to that of the SLIM 3D model. Positive error markings indicate too much mass predicted by box model.

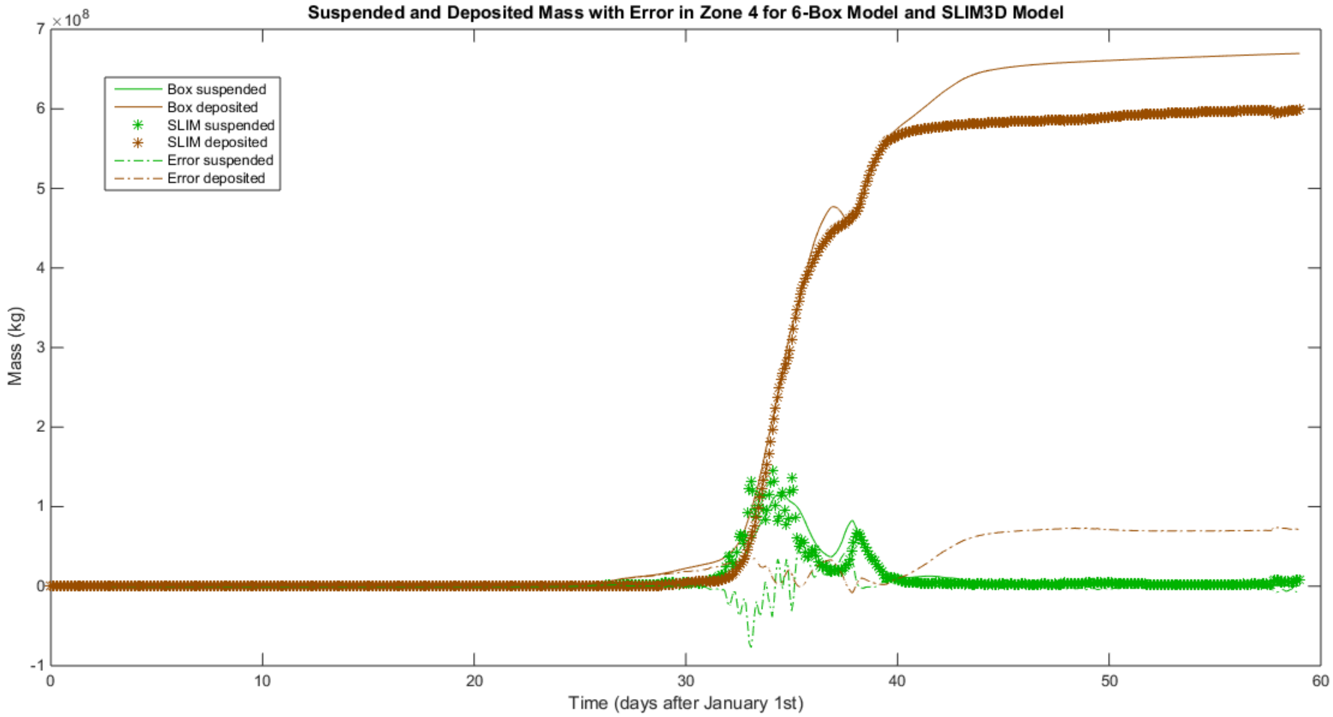


Figure 5: Plot comparing the suspended and deposited mass in zone 4 of the 14-box model to that of the SLIM 3D model. Positive error markings indicate too much mass predicted by box model.

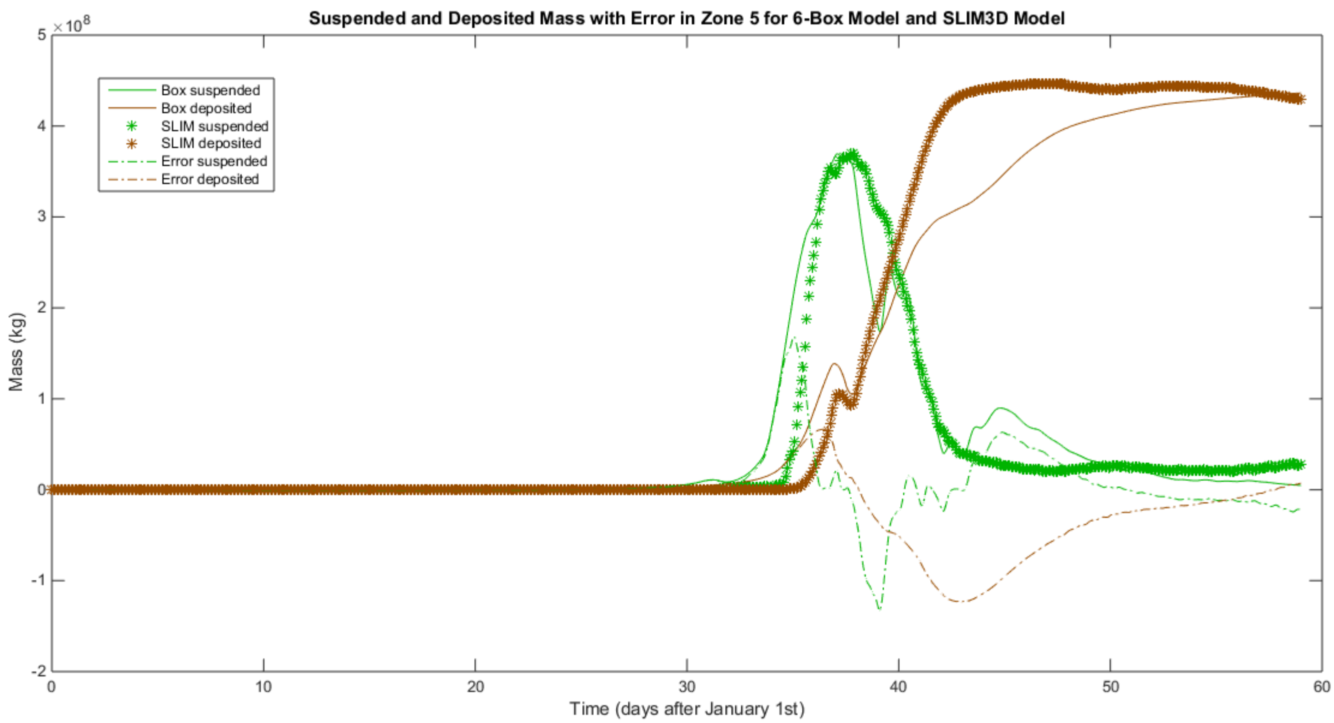


Figure 6: Plot comparing the suspended and deposited mass in zone 5 of the 14-box model to that of the SLIM 3D model. Positive error markings indicate too much mass predicted by box model.

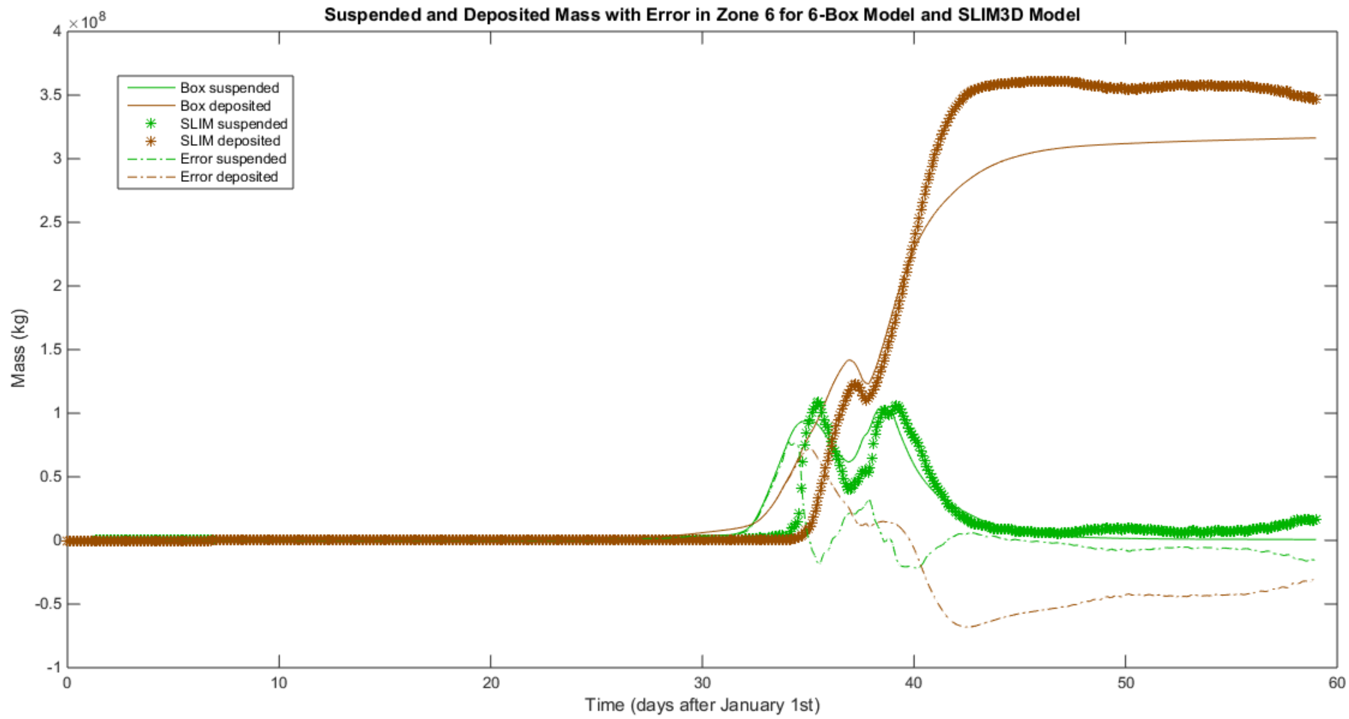


Figure 7: Plot comparing the suspended and deposited mass in zone 6 of the 14-box model to that of the SLIM 3D model. Positive error markings indicate too much mass predicted by box model.

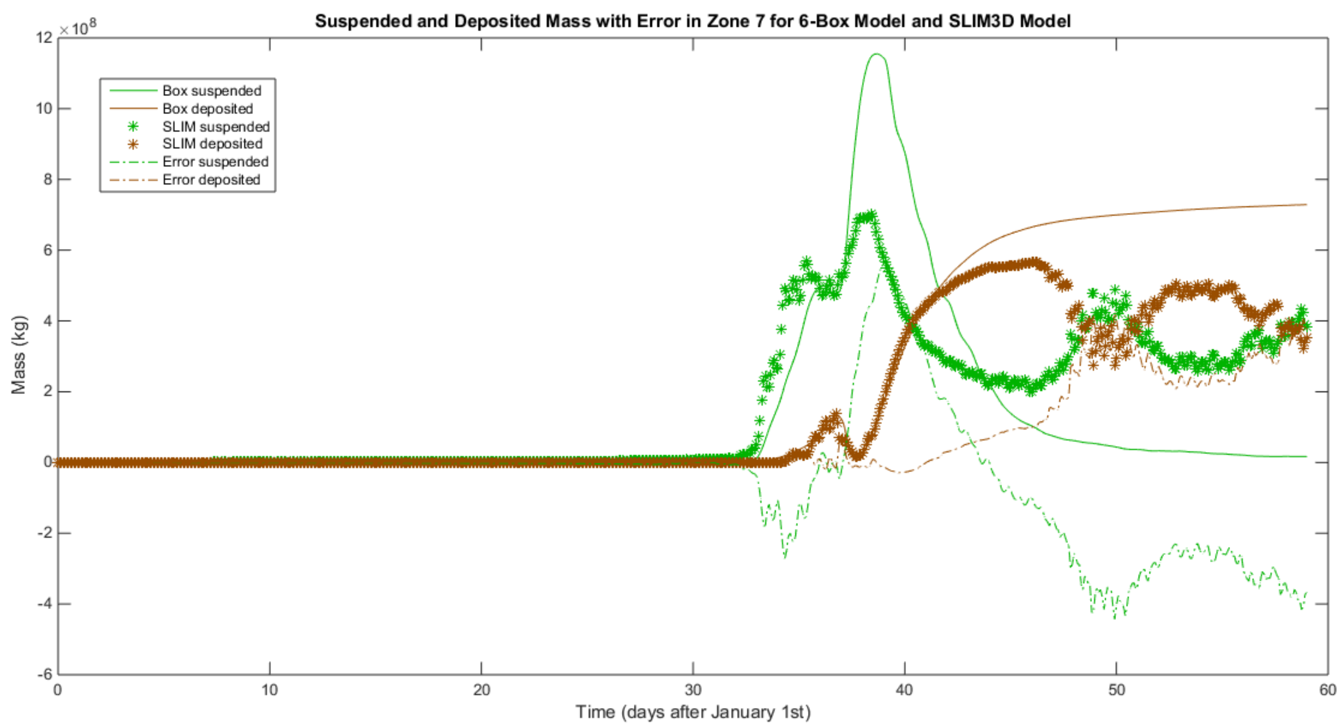


Figure 8: Plot comparing the suspended and deposited mass in zone 7, which contains all remaining zones, of the 14-box model to that of the SLIM 3D model. Positive error markings indicate too much mass predicted by box model.

The sediment and erosion parameters were analyzed for any dependence on bathymetry or surface area. Only the sediment coefficients correlated with bathymetry and surface area. The exact nature of the relationship e.g. power, exponential, linear, etc. is unclear because the coefficients of determination were too similar. Removing one data point drastically changed the least squares regression line, making finding an equation unreliable. There appears to be the strongest correlation between bathymetry and the sediment coefficient, the next strongest with volume, and the weakest with surface area. Based on the way the boxes were divided, there is a moderately strong correlation between average bathymetry in a zone and the surface area of that zone. With this, it is hard to tell whether the surface area is directly affecting the sediment coefficient or whether its relationship with bathymetry is the culprit.

Since the box model was built one zone at a time, observations on the differences in the box model with different numbers of boxes were able to be made. Parameters changed with increasing number of boxes, and sometimes a model with fewer boxes matched the SLIM 3D results better than one with more boxes. One reason for this could be that the error of the specified zones averages out when they are combined into one large remainder zone, giving the illusion of fitting the data better. For example, the model with seven zones arguably is worse than the model with three zones, which can be seen in figures 9-11. Mass flow direction was able to be qualitatively observed, for with an increase in zone precision comes more information about where mass comes from and goes to.

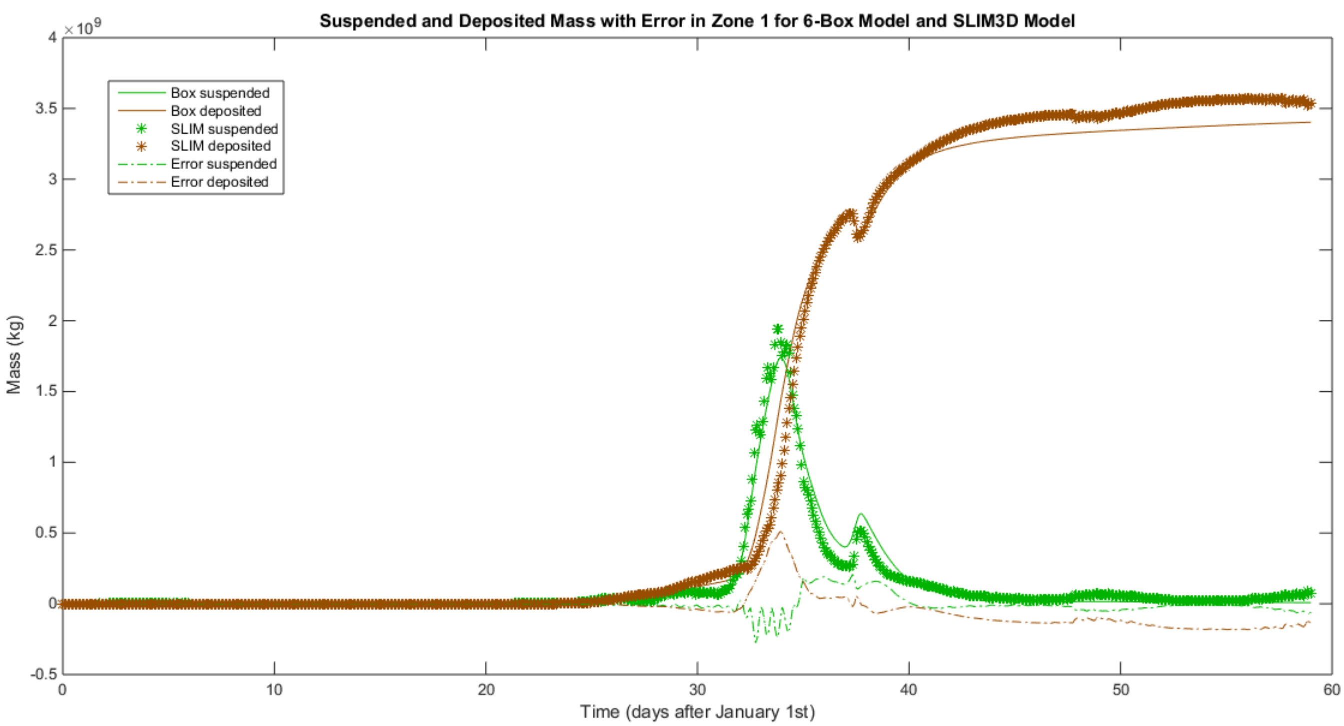


Figure 9: Plot comparing the suspended and deposited mass in zone 1 of the 6-box model to that of the SLIM 3D model. Positive error markings indicate too much mass predicted by box model.

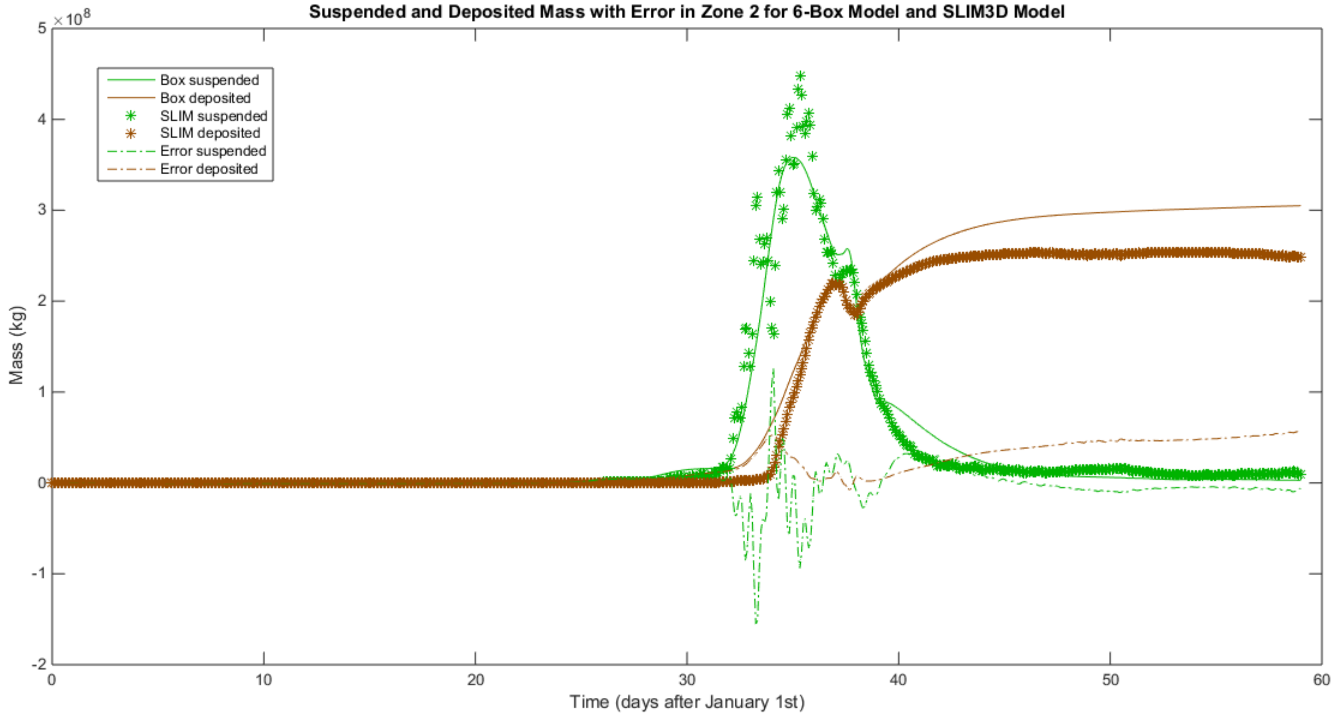


Figure 10: Plot comparing the suspended and deposited mass in zone 2 of the 6-box model to that of the SLIM 3D model. Positive error markings indicate too much mass predicted by box model.

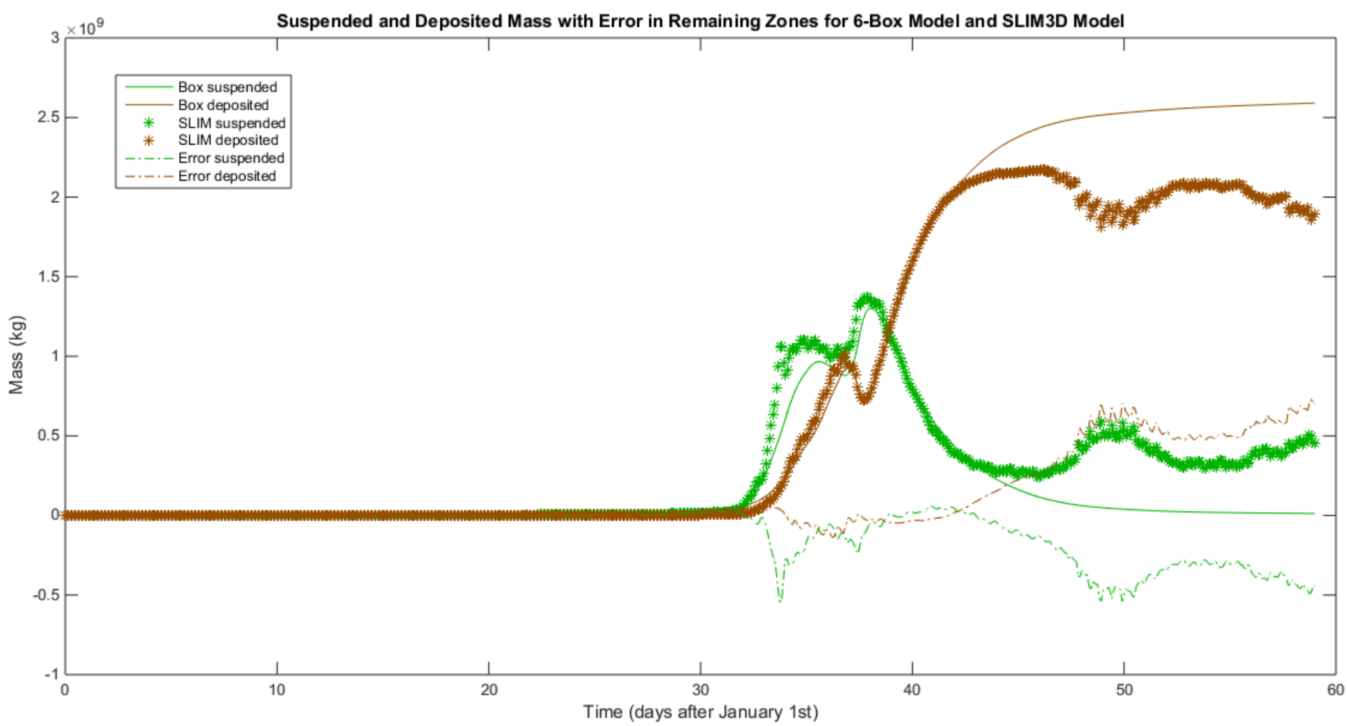


Figure 11: Plot comparing the suspended and deposited mass in the remaining zones of the 6-box model to that of the SLIM 3D model. Positive error markings indicate too much mass predicted by box model.

Discussion

The success of the box model in replicating the SLIM 3D model's results is a boon for the notion that simple physical concepts govern the major aspects of physical movement. The only terms used to model the movement were ones for flux between zones, wind forcings to aid in extra or diminished transport, and sediment vs. re-suspension within a zone. Wind forcings contributed the most towards moving mass in the lagoon, signifying that more movement can be expected during storms and the rainy season.

Despite reaching some important conclusions about the fundamentals of fine sediment transport in the Great Barrier Reef lagoon and about the benefits and disadvantages of the box model in helping to reach these conclusions, there still remain issues that warrant further research. The first issue is that the box model is unable to pick up the re-suspension event in several zones that occurs around the 50 day mark. Introducing a separate wind threshold for re-suspension that differs from deposition helped somewhat for the six-box model, although the effects are small and can only be seen in the end behavior for the remaining zones as shown in figure 12. Introducing this same tactic for the fourteen-box model did not help, and further research should be done into having an optimal sedimentation and re-suspension wind threshold for each zone.

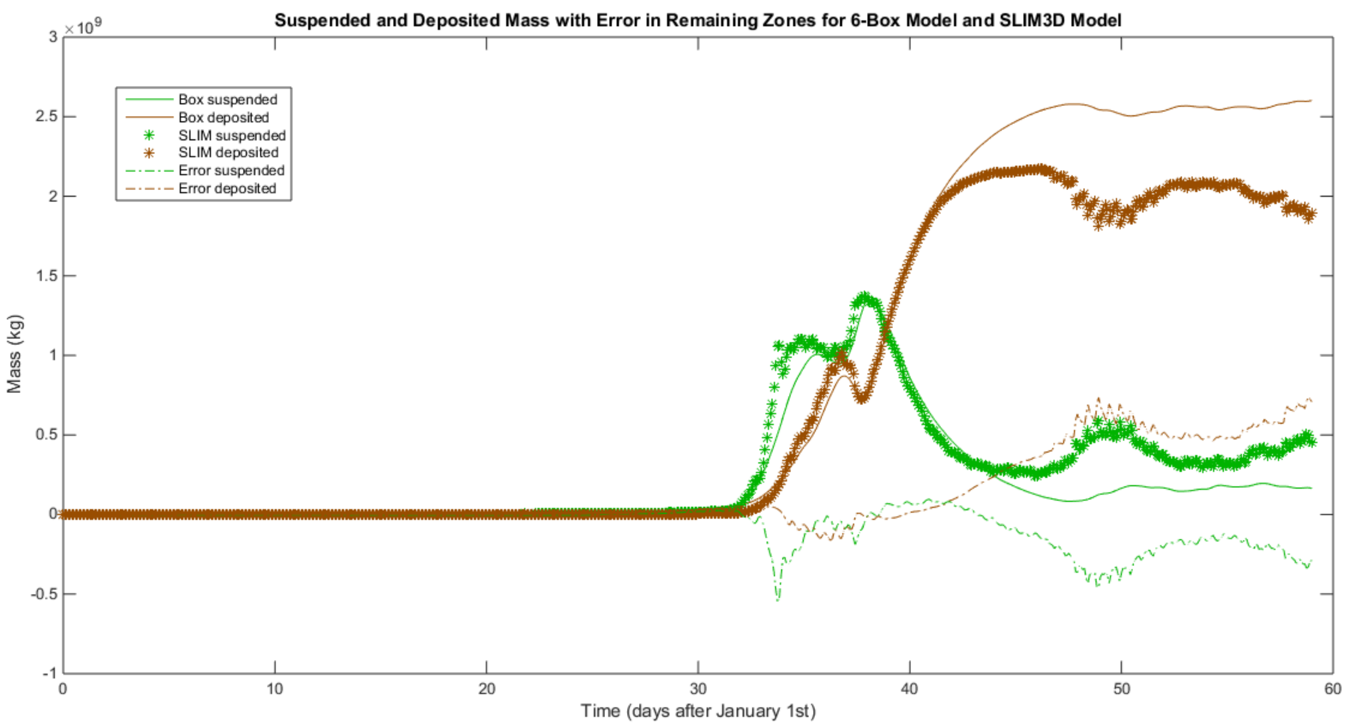


Figure 12: Plot comparing the suspended and deposited mass in the remaining zones of the 6-box model to that of the SLIM 3D model where the box model includes a separate re-suspension wind threshold. Positive error markings indicate too much mass predicted by box model.

Another issue that was briefly investigated was taking the Coriolis force into consideration to produce Ekman transport. Some initial experiments were conducted to see whether the net mass flux between zones would in fact be at an angle to the wind and if so to see what that angle would be. Little effect was had on the six-box model. For the fourteen-box model, some zones were affected greatly, whereas some zones were not affected at all. This could be because the boundary lines are more important with smaller boxes, and adding in an angle due to Ekman transport has the same mathematical effect in our model as changing the boundary direction, causing big changes in where mass is being transported. Further research should be conducted into the importance of Ekman transport in our model and to see what role bathymetry plays on the angle of the transport.

On a numerical modelling note, it was observed that the box model with three zones modelled movement more precisely than the model with seven zones. This speaks to the fundamental purpose of the box model, which is to model a complicated process in a very simple way. Every model is at heart a box model, although some models have orders of magnitude more boxes. The more boxes we add to our box model, the closer we approach to a detailed mesh. Further research on optimizing the number of boxes needed to best model movement should be conducted. Much of the problem in adding too many boxes is taking into account boundary conditions. Part of the success of the flux expression lies in being able to say that dispersion will always occur out of one box, meaning that mass will not naturally flow back into it, with the exception being if the wind blows in that direction. The more finely we divide our domain, the more we have to consider that there will be a flux going back and forth between zones. More time must be spent making educated guesses and running experiments to determine the true net flux direction in these cases.

Acknowledgements

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Delandmeter, P., Lewis, S., Lambrechts, J., Deleersnijder, E., Legat, V., Wolanski, E., 2015. The transport and fate of riverine fine sediment exported to a semi-open system. Submitted to Estuarine, Coastal and Shelf Science.