A simple sensitivity analysis of the turbulence-induced flocculation model of cohesive sediment

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ABSTRACT

In this study, the local and global sensitivity analyses of the Winterwerp model to the input parameters have been carried out using the Garson algorithm and the PaD2 method by virtue of an artificial neural network. The main results of the sensitivity analyses are that the model is most sensitive to the breakup parameter and that only two parameters (the floc aggregation and breakup parameters) are significant. The result that the model output is less sensitive to the choice of fractal dimension seems to imply that the modification work on the fractal dimension might be unnecessary.

Key words | cohesive sediment, flocculation, sensitivity analysis, turbulence

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INTRODUCTION

When fine-grained sediment particles are transported into estuarine and coastal waters, they continually flocculate into different-sized flocs due to small-scale particle–particle interaction, and some flocs may break into smaller fragments/particles caused by flow shear (breakup or disaggregation) (Dyer 1989; Winterwerp 1998; Kranenburg 1999), thereby changing their sizes, excess densities and setting velocities (Kumar *et al.* 2010; Keyvani & Strom 2014). Since the vertical flux of sediment is a function of floc size and settling velocity distribution, flocculation of cohesive sediment plays an important role in the morphodynamic changes in estuarine and coastal regions through the complex processes of sediment transport, deposition, erosion and consolidation (Maggi 2007; Manning & Dyer 2007; Markussen & Andersen 2014). The presence of cohesive sediment also largely influences the typical dynamic processes of the coastal engineering practice, for example, the scouring at underwater pipelines (e.g. Postacchini & Brocchini 2015).

It has been acknowledged that the sediment flocculation is governed by three processes (Winterwerp 1998; Thomas *et al.* 1999): Brownian motion, differential settling and/or turbulence. This study focuses on the turbulence-induced flocculation process of cohesive sediment. There have been many studies that have investigated the flocculation process of cohesive sediment due to the flow shear, among which the simplified Lagrangian flocculation model is an important topic. The original form of this kind of model was proposed by Winterwerp (hereafter referred to as the Winterwerp model) (Winterwerp 1998; Son & Hsu 2008, 2009).

In the Winterwerp model, sediment flocs are treated as a fractal object and are assumed to be composed of mono-sized primary particles. Thus, the effective density of floc could be calculated as (Jiang & Logan 1991; Kranenburg 1999)

$$\rho_f - \rho_w = (\rho_s - \rho_w)\left(\frac{D}{D_p}\right)^{n_f-3} \tag{1}$$

where ρ_f, ρ_s and ρ_w are the densities of floc, primary particle and water, respectively, D and D_p are a characteristic size of floc and size of primary particle, respectively, and n_f is the fractal dimension of the floc. For cohesive sediment, the volumetric concentration, ϕ, could be expressed by mass concentration, c, and the number of floc per unit fluid volume, n, as follows (Winterwerp 1998),

$$\phi = \left(\frac{\rho_s - \rho_w}{\rho_f - \rho_w}\right)\frac{c}{\rho_s} = f_s n D^3 \tag{2}$$

where f_s is a shape factor taken to be $\pi/6$ for spherical particles. Based on the aggregation model of particles in a turbulent fluid proposed by Levich (1962), Winterwerp

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(1998) developed an equation representing the evolution of the number of flocs due to aggregation:

$$\frac{dn}{dt} = -k_a \frac{m_p}{\rho_s} G \left(\frac{D}{D_p}\right)^3 n^2 \quad (3)$$

where m_p is the mass of primary particle; G is the shear rate or shear velocity gradient of the turbulent flow, a parameter commonly used for characterizing the shear flow (Thomas *et al.* 1999); k_a is a dimensionless floc aggregation parameter and t is the flocculation time. Based on a dimensional analysis for the breakup of floc, Winterwerp (1998) introduced the following equation to describe the evolution of the number of flocs due to floc breakup when the flow shear stress exerted on the floc exceeds the yield strength of the floc:

$$\frac{dn}{dt} = k_b \sqrt{\frac{\mu}{F_y}} G^{\frac{3}{2}} D \left(\frac{D}{D_p} - 1\right)^{3-n_f} n \quad (4)$$

where k_b is a dimensionless floc breakup parameter, μ is the dynamic viscosity of the fluid, and F_y is the yield strength of flocs. Using a linear combination of the aggregation and breakup processes (Equations (3) and (4)), a complete Lagrangian flocculation model could be obtained:

$$\frac{dn}{dt} = -k_a \frac{m_p}{\rho_s} G \left(\frac{D}{D_p}\right)^3 n^2 + k_b \sqrt{\frac{\mu}{F_y}} G^{\frac{3}{2}} D \left(\frac{D}{D_p} - 1\right)^{3-n_f} n \quad (5)$$

Simply consider the stationary state in which the floc population and size remain constant. Letting $dn/dt = 0$ in Equation (5) yields the following implicit definition of the floc equilibrium size D_∞:

$$D_\infty \left(1 - \frac{D_p}{D_\infty}\right)^{3-n_f} = \frac{k_a c}{k_b \rho_s} \sqrt{\frac{F_y}{\mu G}} \quad (6)$$

More details regarding Equations (5) and (6) can be found in the original paper of Winterwerp (1998).

The weaknesses of the Winterwerp model are that only a characteristic floc size is addressed, and a constant fractal dimension of flocs has been adopted; therefore, the floc size distribution and a detailed evolution process of particle number and volume is not obtained from this model. Considering that the flocs could have a variable fractal dimension with floc size during flocculation and a simple power law could be used to describe it as proposed in Khelifa & Hill (2006) and Maggi (2007), Son & Hsu (2008) further extended the floc dynamic equation of Winterwerp for variable fractal dimensions. However, Son & Hsu (2008) showed that neither of the two flocculation models of Winterwerp and Son & Hsu (2008) are in satisfactory agreement with experimental results for floc size evolution in mixing tanks. Further, Son & Hsu (2009) modified the Winterwerp model by considering a variable yield strength of the floc (that is, F_y term in Equation (5)), and as a result the model accuracy for the prediction of flocculation process is improved. Vahedi & Gorczyca (2012) argued that the reason why the flocs of the same size settled at different velocities lies in the variety of fractal dimensions for a floc size. Thus, they suggested a normal distribution of the fractal dimensions of a given floc size. Xu & Dong (2017) further modified the Winterwerp model by considering the fractal dimensions for a given floc size to be normally distributed, and the proposed model performed better in predicting the temporal evolution of floc size than that based on a single power law fractal dimension. In another aspect, there were works to modify the Winterwerp model for the polydisperse case. By considering a sequence of stochastic aggregation and breakup events among particles, Maggi (2008) developed a stochastic Lagrangian model to describe the flocculation of suspended cohesive sediment, and this model could be used to investigate floc mobility with the population size spectrum. Further, Shin *et al.* (2015) theoretically developed a new stochastic approach to modify the floc breakup parameter term of the Winterwerp model (that is, k_b term in Equation (5)), and this modified model has the capability to replicate a size distribution of flocs reasonably well under different sediment and flow conditions.

However, it might be important to analyse the identifiability of the Winterwerp model before some modifications of it are performed. At present, the sensitivity of the model result to the input parameters still remains unclear. In a sensitivity analysis, local sensitivity analysis refers to the case in which the influence of variations in the parameters (one at a time) was observed around a reference point. Thus, the conclusion drawn from the local sensitivity analysis around a given reference point might be modified by the consideration of another reference point (Cai *et al.* 2007; Hu 2010). In contrast, global sensitivity analysis aims to investigate the function form of the model rather than the behaviour around a particular reference point, and the influence of the parameters is considered jointly over the entire range of all the parameters. Detailed introductions to local and global sensitivity analysis can be found in the literature

(Helton *et al.* 2006; Cai *et al.* 2007; Hu 2010). In this study, we performed the local and global sensitivity analysis towards the Winterwerp model for a unique characteristic floc size and a constant fractal dimension. Four input parameters were considered – the size of primary particles, D_p; the fractal dimension of flocs, n_f; the floc aggregation parameter, k_a; and the floc breakup parameters, k_b – and the model output result refers to the characteristic floc size, D.

The next section introduces the method to perform the local and global sensitivity analyses of the model, and the literature survey for the range of variations in the flocculation model parameters. The sensitivity analysis results of the Winterwerp model to input parameters and some simple discussions are then presented. The final section gives some concluding remarks.

SENSITIVITY ANALYSIS METHODOLOGY AND THE MODEL PARAMETERS

Methodology introduction

Sensitivity analysis refers to the determination of the contributions of individual uncertain inputs to the uncertainty in the analysis result (Helton *et al.* 2006). There are many methods for sensitivity analysis, and review works can be found in the references (Saltelli *et al.* 2004; Cai *et al.* 2007). For local sensitivity analysis, we simply choose the Garson algorithm based on the artificial neural network (ANN) here (Garson 1991). The objective of this study is to study the sensitivity of floc size with respect to all of the input parameters.

An ANN is composed of three layers: the input layer, hidden layer and output layer. The ANN assumes that the numbers of neurons in these three layers are N, L and M, respectively. $(x_1, \cdots, x_N)$ is the input variable and $(y_1, \cdots, y_M)$ is the output variable. $w = (w_{ij})_{N\times L}$ is the link weight between the input layer and hidden layer, and $\upsilon = (\upsilon_{jk})_{L\times M}$ is the link weight between the hidden layer and output layer. Garson (1991) proposed to use the product of the link weight to estimate the influence of the input variable on the output variable as follows,

$$Q_{ik} = \frac{\sum_{j=1}^{L}(|w_{ij}\upsilon_{jk}|)/\sum_{r=1}^{N}(|w_{rj}|)}{\sum_{i=1}^{N}\sum_{j=1}^{L}\left(|w_{ij}\upsilon_{jk}|/\sum_{r=1}^{N}(|w_{rj}|)\right)} \tag{7}$$

with $i = 1, \cdots, N$; $k = 1, \cdots, M$; and Q_{ik} is the defined sensitivity coefficient of an input variable x_i on an output variable y_k. By fixing the output variable (that is, a fixed k), we could estimate the sensitivity degrees of each of the input variables to the given output variable using Equation (7).

For the global sensitivity analysis, we simply choose the PaD2 method proposed by Gevrey *et al.* (2006). This method aims to study the influence of the interaction of two input variables on the output variable. We assume that the expression for the ANN is as follows,

$$y = g\left(\sum_{j=1}^{L}\upsilon_j f\left(\sum_{n=1}^{N} w_{jn}x_n + b_{1j}\right) + b_2\right) \tag{8}$$

where $g()$ and $f()$ are the input layer function and the hidden layer function, respectively, and b_1 and b_2 are constants. Here, simply consider $g(x) = x$, $f(x) = \tanh(x)$, as suggested by Cai *et al.* (2007), and Equation (8) becomes $y = \sum_{j=1}^{L}\upsilon_j \tanh\left(\sum_{n=1}^{N} w_{jn}x_n + b_{1j}\right) + b_2$. Taking the derivative of this equation with respect to an input variable x_k, we can estimate the influence of the chosen input variable x_k on the output result y as follows: $\frac{\partial y}{\partial x_k} = \sum_{j=1}^{L}\upsilon_j w_{jk}\tanh^{(1)}\left(\sum_{n=1}^{N} w_{jn}x_n + b_{1j}\right)$, where $\tanh^{(1)}(x)$ is the first-order derivative of the function $\tanh(x)$. Again taking the derivative of this equation with respect to another input variable x_i, we can estimate the influence of two input variables (x_k and x_i) on the output result y as follows: $\frac{\partial^2 y}{\partial x_k \partial x_i} = \sum_{j=1}^{L}\upsilon_j w_{jk} w_{ji}\tanh^{(2)}\left(\sum_{n=1}^{N} w_{jn}x_n + b_{1j}\right)$, where $\tanh^{(2)}(x)$ is the second-order derivative of the function $\tanh(x)$.

More detailed introductions regarding the Garson algorithm and the PaD2 method can be found in the review work of Cai *et al.* (2007).

Description of the model parameters

The input parameters of the Winterwerp flocculation model are the size of primary particles, D_p, the fractal dimension of flocs, n_f, the floc aggregation parameter, k_a, and the floc breakup parameter, k_b. For simplicity, we just concentrate on the equilibrium floc size D_∞ in Equation (6) as the output variable and carry out the sensitivity analysis of D_∞

to D_p, n_f, k_a, and k_b in this study, as adopted by some authors (Son & Hsu 2008, 2009).

The first step for the sensitivity analysis is to choose the appropriate probability function for the input parameters. The adopted method is simply to consider a database of experimentally identified values of these input parameters from the literature. Table 1 reports the values of these input parameters found in different literature sources. Regarding the fractal dimension, some studies adopted $D_f = 2$ as the average fractal dimension of relatively large flocs (Winterwerp 1998; Kumar *et al.* 2010). For the sake of the sensitivity analysis in this study, a range of the variation in floc fractal dimension reported in some of the literature is collected and shown in Table 2. From these tables, the maximum and minimum values of input parameters could be determined; in this study, we simply adopt the uniform probability distributions of these parameters across their ranges, as used by some studies (Zhang & Li 2003; Li *et al.* 2004).

All of the sensitivity calculations in this study were done with $G = 10\ \text{s}^{-1}$, and $c = 1$ g/L as adopted in some studies (Biggs & Lant 2000; Son & Hsu 2008, 2009). They were repeated with different pairs of values with no qualitative influence on the results. The other numerical parameters were $F_y = 10^{-10}$ (kg·m)/s^2, $\mu = 10^{-3}$ kg/(m·s), and $\rho_s = 2{,}650$ kg/m^3, as used by some authors (Son & Hsu 2008, 2009).

Table 1 | The values of three flocculation model parameters found in different literature sources

Reference	k_a	k_b ($\times 10^{-5}$)	D_p (μm)
Winterwerp (1998)	0.31	3.5	4
Manning & Dyer (1999)	0.3, 0.33	1.1, 1.4	15
Biggs & Lant (2000)	0.008	1.3	15
Bouyer *et al.* (2004)	1.02	0.4	5
Maggi *et al.* (2007)	0.46	24	6
Maerz *et al.* (2011)	0.18, 0.4	2.9, 11.5	4

Table 2 | Range of floc fractal dimension found in different literature sources

Reference	n_f
Bouyer *et al.* (2004)	1.35–2.3
Khelifa & Hill (2006)	2–3
Hsu *et al.* (2007)	2.15
Maerz *et al.* (2011)	1.5–2.4

Calculation procedure

All of the sensitivity analyses are performed based on the platform of Matlab software (Matlab version7.0.0.19920 (R14), produced by MathWorks Corporation, Natick, MA, USA) in this study. It simply contains three steps: (1) the first step is to acquire the sample; a large sample number often consumes a longer computational time; (2) the second step is to carry out the neural network training, and during this process great attention should be paid to restricting the training error and (3) the last step is to estimate the sensitivity of the output result to each of input parameters using the Garson algorithm and PaD2 as mentioned above, based on the neural network training results. In this study, three 'm files' are written in the Matlab platform corresponding to the above three steps: 'acquire-sample.m', 'training.m', and 'sensitivity.m'. All of the details regarding the coding of these 'm files' can be found in the supplementary file, available with the online version of this paper.

SENSITIVITY ANALYSIS RESULT AND SIMPLE DISCUSSION

In the ANN calculation, the acquired sample number in the first step (acquire-sample.m file) is 300,000 and the trained sample number is 270,000 in the second step (training.m file). In the neural network training, the chosen neuron number in the hidden layer is 12, and the epoch takes 19,025 cycles. The training performance error is small, and the prediction effect is good, as shown in Figure 1(a) and 1(b), respectively. Table 3 shows the ranges of the parameters used to train and test the ANN model. Table 4 presents the statistical measurement values of the ANN in the prediction of training and testing data. Here CC denotes the correlation coefficient, MSE denotes the mean square error. They, as well as BIAS value, are determined as follows (Pourzangbar *et al.* 2017): $\text{CC} = \frac{\sum_{i=1}^{N}(O_i - \overline{O_m})(P_i - \overline{P_m})}{\sqrt{\sum_{i=1}^{N}(O_i - \overline{O_m})^2 \times \sum_{i=1}^{N}(P_i - \overline{P_m})^2}}$, $\text{MSE} = \sqrt{\sum_{i=1}^{N}(P_i - O_i)^2}$, $BIAS = \frac{\sum_{i=1}^{N}(P_i - O_i)}{n}$, where O_i and P_i represent the observed and predicted values respectively, N is the number of observed data, and $\overline{O_m}$ and $\overline{P_m}$ are the mean values of the observed and predicted parameters respectively. It was found that the ANN model adopted in this study is reliable.

The sensitivity analysis result of the equilibrium floc size D_∞ with respect to all input flocculation parameters using the

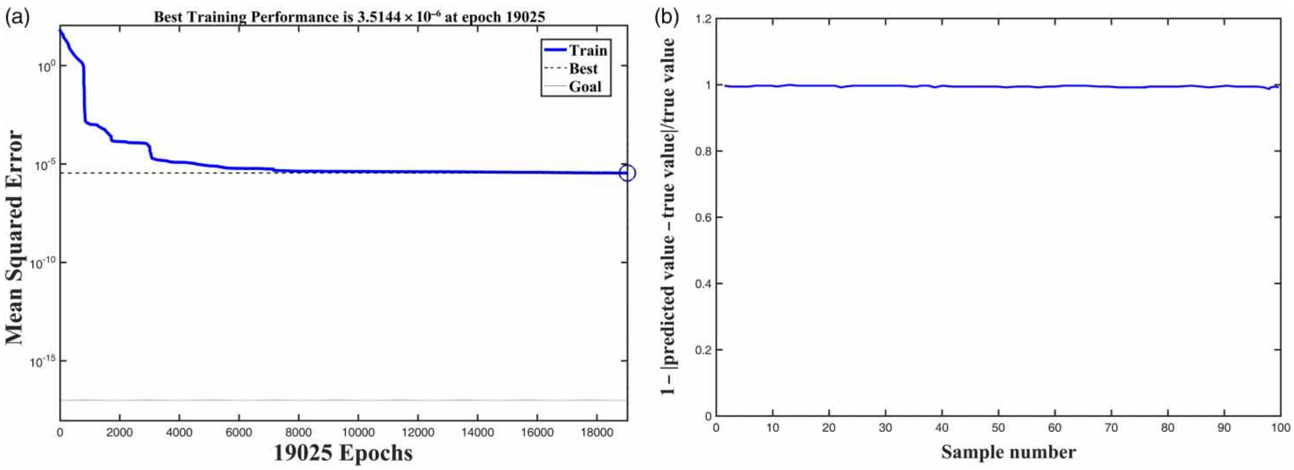

Figure 1 | Training error (a) and the prediction effect (b) during the neural network training in this study.

Table 3 | Ranges of the parameters employed to train and test the ANN model

Parameters	Test data range	Full data range	Minimum	Average	Maximum
D_p (μm)	4–15	4–15	4	9.5	15
n_f	1.4–3	1.35–3	1.35	2.175	3
k_a	0.01–1.01	0.008–1.02	0.008	0.514	1.02
k_b ($\times 10^{-5}$)	0.42–22	0.4–24	0.4	12.2	24

Table 4 | Statistical measurements of ANN in the prediction of training and testing data set

Number of hidden layer neurons	Training data set			Testing data set		
	CC	MSE	BIAS	CC	MSE	BIAS
12	0.941	10^{-5}	0.008	0.953	$5*10^{-6}$	0.005

Table 5 | Sensitivity index of the equilibrium floc size D_∞ with respect to all of the input flocculation parameters using the Garson algorithm

	Statistical parameter			
	D_p	n_f	k_a	k_b
Sensitivity index	5.2852×10^{-5}	1.4953×10^{-4}	5.2544×10^{-4}	0.9993

Garson algorithm is presented in Table 5. The first-order and second-order sensitivity analysis results of the equilibrium floc size D_∞ with respect to all of the input flocculation parameters using the PaD2 method are presented in Tables 6 and 7, respectively. It can be found from Tables 5 and 6 that the most influential parameter for the output result of the Winterwerp flocculation model is the floc breakup parameter k_b, whereas the model output result is less sensitive

Table 6 | First-order sensitivity indices of the equilibrium floc size D_∞ with respect to all of the input flocculation parameters using the PaD2 method (the first-order derivative)

	Statistical parameter			
	D_p	n_f	k_a	k_b
First-order sensitivity index	5.1257×10^{-4}	1.3541×10^{-4}	1.1132×10^{-4}	0.9992

to D_p, n_f, and k_a. From Table 7, it is evident that the floc aggregation parameter k_a is also influential to the output result, but only through its influence coupled together with the floc breakup parameter k_b. The model output result is subtly sensitive to joint variations in n_f and k_b (n_f–k_b) and in D_p and k_b (D_p–k_b) since the output result of the Winterwerp model is strongly sensitive to the variation in k_b.

The sensitivity analysis result regarding k_b and k_a presented in this study seems to be in agreement with some previous studies. Zhang & Li (2003) and Li *et al.* (2004) showed the obvious influence of different function forms of the floc breakup model on the flocculation dynamics. Mietta *et al.* (2008) presented different flocculation modelling results with respect to different function forms of the floc breakup. In the work of Maggi (2008), both the floc aggregation parameter k_a and the floc breakup parameter k_b are treated as stochastic variables, and the developed stochastic flocculation model could be used to investigate floc mobility with the population size spectrum. By fixing k_a as a constant while considering k_b as a stochastic variable, Shin *et al.* (2015) developed a new stochastic flocculation model and this modified model has the capability to replicate a size distribution of flocs reasonably well under different sediment and flow conditions.

Table 7 | Second-order sensitivity indices of the equilibrium floc size D_∞ with respect to all of the input flocculation parameters using the PaD2 method (the second-order derivative)

	Statistical parameter					
	D_p–n_f	D_p–k_a	D_p–k_b	n_f–k_a	n_f–k_b	k_a–k_b
Second-order sensitivity index	7.0268×10^{-7}	6.8133×10^{-6}	0.0223	9.9353×10^{-6}	0.0820	0.8957

Son & Hsu (2008) showed that the variation in the size of primary sediment particle leads to a constant equilibrium floc size. This qualitatively agrees with the sensitivity result of the model output with respect to D_p presented in this study.

To the best of our knowledge, at present there are conflicting results regarding whether the floc fractal dimension could be treated as a constant during flocculation. Based on some published works, Khelifa & Hill (2006) suggested that the fractal dimension will decrease as the floc size increases, and further presented a power law to describe the relationship between fractal dimension and floc size. A similar power law relationship was also derived in Maggi (2007) by laboratory optical observation of floc structure. This relationship has been adopted by some authors to model the turbulence-induced flocculation process (Cai *et al.* 2007; Maggi *et al.* 2007; Son & Hsu 2008; Shen & Maa 2015). Kumar *et al.* (2010) made a simple modification to this relationship and proposed an alternative model for a variable fractal dimension during flocculation. However, in some published studies, a fixed constant value for the fractal dimension was still adopted to model the flocculation process. Xu *et al.* (2008) developed a size-resolved flocculation model to simulate the variations in floc size by adopting the fixed fractal dimension as 2. A fixed fractal dimension value was also used in Keyvani & Strom (2014) and Shen & Maa (2015). However, it should be pointed out that in the work of Son & Hsu (2008), the Winterwerp model has been modified by adopting a power law variable fractal dimension. However, they showed that this modified model is not in satisfactory agreement with the experimental results. This qualitative conclusion seemingly agrees with the sensitivity result with respect to n_f in this study. Our sensitivity analysis result indicating that the model output is less sensitive to the choice of fractal dimension seems to imply that further modification efforts towards the fractal dimension might be unnecessary in terms of improving the model accuracy.

Keyvani (2013) has analyzed the sensitivity of all key parameters to equilibrium floc size in the Winterwerp model by testing different values of a parameter while holding the rest of the parameters constant. Some findings from the study of Keyvani (2013) are as follows.

(1) Increasing fractal dimension only slightly reduces the equilibrium floc size, which is in accordance with our sensitivity result that the model output is less sensitive to the variation of fractal dimension.
(2) Increasing the primary particle size only slightly increases the equilibrium floc size, which agrees with the sensitivity result in this study that the model output is not sensitive to primary particle size.
(3) An increase in the floc breakup parameter leads to a reduction in equilibrium floc size. This is consistent with the main result of the sensitivity analysis in this study, that the model is most sensitive to the breakup parameter.
(4) Keyvani (2013) also showed that the floc aggregation parameter affects the final equilibrium floc size. This seems to be in accordance with our global sensitivity analysis result that the floc aggregation parameter k_a coupled with the floc breakup parameter k_b is influential to the model output result. However, our local sensitivity analysis result showed that the model result is less sensitive to the variation in the floc aggregation parameter. Additionally, it seems necessary to state that the sensitivity analysis refers to the calculation of the parameters' importance within the specific developed model (not in general). A deep study regarding the reliability analysis of the proposed model can be found in the work of Pourzangbar *et al.* (2017).

CONCLUDING REMARKS

In this study, we performed a local and global sensitivity analysis of the Winterwerp model that has been commonly used to describe the flocculation dynamical process of cohesive sediment in some rivers, reservoirs, lakes and estuarine waters. The adopted methods were the Garson algorithm for the local sensitivity analysis and the PaD2 method for the global sensitivity analysis based on an ANN. The input parameters of the Winterwerp flocculation model were the floc aggregation and breakup parameters, the floc fractal dimension and the size of primary particles, and the output parameter of interest was the equilibrium floc size at steady state flocculation in this study.

The main results of the sensitivity analyses are that the flocculation model is most sensitive to the breakup parameter, and only two parameters (the floc aggregation and breakup parameters) are significant. Further, the result that the model output is less sensitive to the choice of fractal dimension seems to imply that further modification efforts towards the fractal dimension might be unnecessary.

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