Application of a Bayesian Method for Investigating the Probability and Uncertainty of a Two-Class Flocculation Kinetic Model

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Many cohesive sediment transport models adopt empirical flocculation equations based on the correlation between settling velocity (or floc size) and hydrodynamic and biochemical conditions of the water. Those empirical flocculation equations are robust in computation, but they disregard flocculation kinetics (i.e. time-dependent rate of floc growth and breakup). More realistic cohesive sediment transport model, with adoption of flocculation kinetics based on population balance equations have been developed (Winterwerp, 1998; Verney et al., 2011; Lee et al., 2014; Shen et al., 2018), and have been applied and validated in idealized 0 or 1 dimensional vertical test cases. Recently, Sherwood and coworkers applied and validated a flocculation kinetic and sediment transport model for an estuarine and coastal area (Sherwood et al., 2018). The drawback of flocculation kinetic models is the high complexity generated by the dozen of model parameters, which is the bottleneck for practical, realistic application, especially in large scale application. To the authors' opinion, the flocculation kinetic model parameters should be estimated with great attention, before being adopted to large-scale, multi-dimensional simulation. Various curve-fitting methods, such as linear, non-linear regression and genetic algorithm, are available for parameter estimation. Those curve-fitting methods find a specific set of the best-fit model parameters, but they can hardly estimate the probability and uncertainty of the model parameters. Bayesian methods instead have been applied not only to find the best-fit parameters but also to investigate the probability and uncertainty of and the correlation between model parameters. Throughout this research, we applied and tested a Bayesian method coupled with a flocculation kinetic model, and thus we could explore a highly complex flocculation kinetic model in a systematic manner.

A 1DV cohesive sediment transport model, with adoption of a two-class flocculation kinetic equation, was coupled with a Bayesian method (Vrugt, 2016). Experimental data measured in the Belgian coastal area were applied to parameter estimation of the flocculation kinetic and sediment transport model (Fettweis et al., 2014). The aggregation efficiency factor (*alpha*), breakup efficiency factor (*Eb*), breakup exponent constant (*q*), fractal dimension (*Df*), erosion rate constant (*M*), and critical shear stress (tau,c) were selected as the curve-fitting parameters. Four thousands numerical simulations were performed with different sets of the model parameters, based on the Markov chain Monte Carlo theory. Afterwards, the simulation results were statistically analyzed regarding their probability, uncertainty and correlation. As shown in Figure 1, each parameter composes a statistical distribution with their median and standard deviation, indicating the most probable value and the uncertainty of a parameter. The Bayesian method also show the correlation between the model parameters. For example, the correlation between the aggregation efficiency and breakup efficiency factors (*alpha* and *Eb*) and between erosion rate constant and critical shear stress (*M* and *tau,c*) could be identified by the Bayesian method. Therefore, the Bayesian method gives us better insight into the complex flocculation kinetic model, regarding the parameters' probability and uncertainty and the correlation between model parameters. The Bayesian method combined with the 1DV flocculation kinetic and cohesive sediment transport model will be further applied to various measured data sets in different seasonal and spatial conditions. The Bayesian method will eventually help us understand flocculation kinetics and set a realistic, rigorous cohesive sediment transport model.

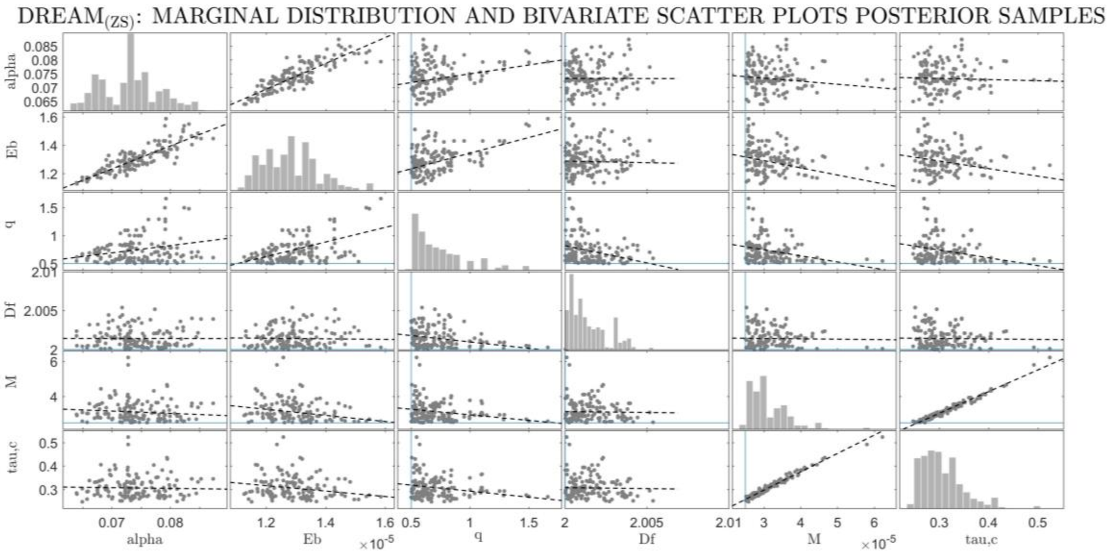

Fig. 1. Histograms of the marginal posterior distribution of the two-class flocculation kinetic model parameters, aggregation efficiency factor (*alpha*), breakup efficiency factor (*Eb*), breakup exponent constant (*q*), fractal dimension (*Df*), erosion rate constant (*M*), and critical shear stress (*tau,c*),

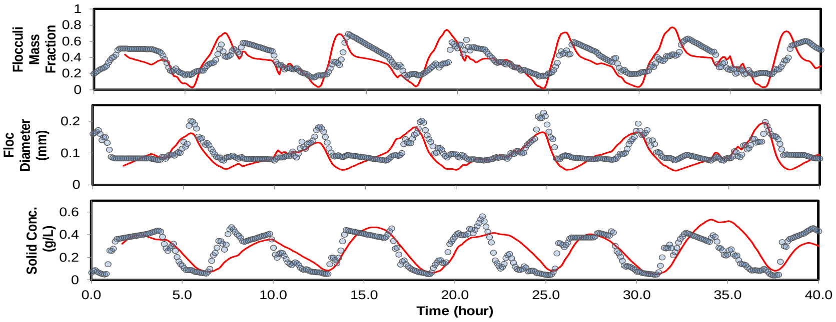

Fig. 2. Simulation result with the best-fit model parameters estimated by the Bayesian method with the 1DV flocculation kinetic and cohesive sediment transport model

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References

Fettweis M., Baeye M., Van der Zande D., Van den Eynde D., Lee B.J. (2014). Seasonality of floc strength in the southern North Sea. J. Geophys. Res. Oceans 119, 1911-1926.

Lee B., E. Toorman, and M. Fettweis (2014). Multimodal particle size distributions of fine-grained sediments: mathematical modeling and field investigation. Ocean Dynamics 64(3), 429–441.

Shen, X., E. Toorman, B. Lee, and M. Fettweis (2018), Biophysical flocculation of suspended particulate matters in Belgian coastal zones. Journal of Hydrology, 567, 238-252.

Sherwood, C., A. Aretxabaleta, C. Harris, J. Rinehimer, R. Verney, and B. Ferre (2018). Cohesive and mixed sediment in the Regional Ocean Modeling System (ROMSv3.6) implemented in the Coupled Ocean–Atmosphere–Wave–Sediment Transport Modeling System (COAWSTr1234), Geosci. Model Dev. 11, 1849-1871.

Verney, R., R. Lafite, J. Claude Brun-Cottan, and P. Le Hir (2011), Behaviour of a floc population during a tidal cycle: Laboratory experiments and numerical modelling, Continental Shelf Research, 31(10), S64–S83.

Vrugt, J. (2016). Markov chain Monte Carlo simulation using the DREAM software package: Theory, concepts, and MATLAB implementation, Environmental Modelling & Software 75, 273–316.

Winterwerp, J. (1998), A simple model for turbulence induced flocculation of cohesive sediment, Journal of Hydraulic Engineering, 36(3), 309–326.