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懸浮泥砂之對流、擴散及隨機運動機制之探討

A probabilistic description of suspended sediment transport: advection, diffusion and random movement

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國立臺灣大學碩士學位論文
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A probabilistic description of suspended sediment transport: advection, diffusion and random movement

本論文係吳棕翰君（R03521318）在國立臺灣大學土木工程學系碩士班完成之碩士學位論文，於民國 105 年 07 月 18 日承下列考試委員審查通過及口試及格，特此證明

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中文摘要

泥砂運輸與人類的生活息息相關，例如橋墩沖刷、水質估計等等，故泥砂運輸的研究是一直以來都是一個很重要的議題。泥砂顆粒在水中除了隨著水流方向運動之外，也會因為受到紊流的影響而向周圍不規則擴散，此外，其運動的行為可以馬可夫鏈(Markov chain)來近似，因此本研究將泥砂顆粒的運動視為一個隨機過程。本文以力學原理結合序率方法(Stochastic method)來模擬泥砂顆粒在水中的運動軌跡，亦即增強隨機微分方程中的物理性質，使之更貼近自然情形。

為模擬泥砂顆粒的運動行為，本文以朗之萬方程(Langevin equation)為原型所推導出的隨機擴散粒子追蹤模型(Stochastic Diffusion Particle Tracking Model)呈現顆粒運動因紊流而造成的不確定性。其中，隨機擴散粒子追蹤模型主要包含兩種基本元素：平均漂移項(Mean drift term)，即為顆粒隨著水流方向運動；紊流項(Turbulence term)，即顆粒受到紊流作用而有不規則的運動，也稱為布朗運動(Brownian motion)，係利用維納過程(Wiener process)來模擬。

本研究利用隨機擴散粒子追蹤模型來模擬在一般流況下泥砂顆粒的運動軌跡，分別使用兩種隨機擴散粒子追蹤模型: 單顆粒粒子追蹤模型(One-particle Particle Tracking Model)和雙顆粒粒子追蹤模型(Two-particle Particle Tracking Model)去模擬。其中，雙顆粒粒子追蹤模型比單顆粒粒子追蹤模型多考慮了顆粒在距離相近時候的變化,因為大尺度的渦流(Large scale turbulence)的關係可能使彼此相近的顆粒具有相似的隨機運動。另外，以巨觀的角度去觀察顆粒整體的運動，可以計算出水中的泥砂濃度，且因為泥砂顆粒受到紊流擾動的影響，使得泥砂的濃度也具有不確定的變化。因此本文呈現顆粒軌跡和泥砂濃度的平均值和標準差來表示泥砂顆粒在水中的不確定性。本研究首先和實驗資料比對單顆粒和雙顆粒粒子模型所估計的濃度以驗證模型的可行性，最後使用此模型分別探討層流流場中和紊流流場中顆粒隨機運動的情形，結果顯示在紊流流場中顆粒的隨機運動比較明顯，因此在高雷諾數(Reynolds number)的流場中估計泥砂濃度時,應考慮漩渦對泥砂顆粒所造成的隨機變化，並給予濃度變動範圍較為恰當。此外，泥砂顆粒運動具有馬可夫特性也在本文中證實。然而，如本文結果所顯示，泥沙顆粒的移動距離卻不是和時間呈線性的正比關係，並不符合菲克擴散(Fickian diffusion)。泥砂顆粒具

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有再懸浮的現象可能導致泥砂擴散為反常擴散(non Fickian diffusion or anomalous diffusion)。

關鍵字：隨機微分方程、序率模式、顆粒軌跡模型、泥砂運動、雙顆粒模型、馬可夫特性、反常擴散

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ABSTRACT

Sediment transport is an important issue for human. It is closely related to human society, such as bridge scour and water quality. A sediment particle in flow not only follows the flow direction, but also diffuses through the surrounding water due to turbulence. Markov chain is used to approach the movement of sediment particles. From this perspective, particle movement is regarded as a stochastic process in our study; moreover, the proposed models simulate particle trajectories based on stochastic methodologies and physical mechanisms, underscoring mechanics in the stochastic differential equation.

To simulate sediment particle movement, the stochastic diffusion particle tracking model (SD-PTM) has been derived from the Langevin equation, which is able to show the random characteristics of sediment movement. SD-PTM has two basic elements, the mean drift term and the turbulence term. One of the particle characteristics, the mean drift term, is that particles follow the flow direction; another one is called the turbulence term that describes random behaviors caused by turbulence diffusion. This movement is known as Brownian motion. In general, the diffusion movement is modeled by the Wiener process.

The aim of this study is to simulate sediment particle trajectories under the normal flow condition by the SD-PTMs, one-particle PTM and two-particle PTM. The difference between the single particle model and the paired particle model is that the paired particle model accounts for large eddy turbulence. In other words, the paired particles may have similar random movement if the locations of particles are in the immediate vicinity of each other. Besides, to observe assemblage of particles' motion in the macroscopic manner, the sediment concentrations can be estimated. Moreover,

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sediment concentrations involve the property of uncertainty on account of sediment particles' stochastic trajectories. Therefore, to demonstrate such uncertainty of sediment particles, the ensemble means and ensemble standard deviations of sediment trajectory as well as concentrations are presented in the study respectively. The proposed models are validated against experimental data by ensemble mean velocity and sediment concentrations. Moreover, this study also discussed the random movement of sediment particles under various flow conditions, laminar cavity flow and fully developed turbulent open channel flow. Results show that the random movement of sediment particles is significant in turbulent flow. Thus, it is appropriate to consider the fluctuation of sediment concentrations under high Reynolds number flow conditions. Besides, the Markovian property of the PTMs is validated in our study. However, the variance of particle displacement and time are not a linear proportion as the result. Resuspension of sediment particles may cause particle movement to be anomalous diffusion.

Keyword: stochastic differential equation, stochastic model, particle tracking model, sediment transport, two-particle model, Markovian property, anomalous diffusion.

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Chapter 1 Introduction

Irregular movement of particles owing to turbulence has been studied for many years. The drag force of turbulence fluid is a main factor that causes a particle to move randomly. For instance, hydraulic and environmental engineers have been highly concerned with sediment transport caused by turbulence. This is important for designing flow structure, water quality management and ecological environment. According to the particle properties, sediment particles can be classified into suspended load and bed load in flow. In general, a particle floating in the water column is classified as suspended load; bed load is defined as a particle moving near the bed. To study sediment transport, researchers and engineers used to concentrate on deterministic methods. There are many kinds of modeling approaches, such as the sediment-transport balance method and the sediment-divided method. Sediment-transport balance method is a method that offers the sediment balance equation derived from the sediment transport formula. In sediment-divided method, different particle movement is considered in order to decide whether a suspended load model or bed load model needs to be applied. The aforementioned models are mainly focused on particle concentration, i.e. particles in the Eulerian model seem to be presented by concentrations. However, more detailed information on trajectories of particles is preferred. Consequently, simulating sediment transport by Lagrangian models became more and more popular recently and were promoted in various fields such as hydraulics, marine, environment, economics, physics etc.(Man *et al*., 2007; Spivakovskaya *et al*., 2007; Oh and Tsai, 2010; Shah *et al*., 2011)

In order to study bed-load transport, Einstein (1942) established the foundation of

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the applicability of probabilistic concepts. The entrainment probability function is innovated in sediment entrainment to bed load. In other words, stochastic properties have been suggested for the transport of sediment particles. A new viewpoint for stochastic models for sediment transport has been implemented ever since.

One category of the stochastic models is particle tracking models (PTM), also known as “Random walk models’’. This type of model can be treated as the transport of a constituent of large number of moving particles which can be simulated as discrete particles. Because of discrete particle characteristics, this stochastic process might be regarded as a Markov-process theory, meaning that particle position only depends on the present state instead of all past history. The PTM normally employs two terms: the mean drift term and random term. This stochastic transport model based on physical mechanisms are called the stochastic diffusion particle tracking model (SD-PTM), which is built on stochastic differential equations (SDE). Since SD-PTM, a type of Langevin equation is equivalent to the Fokker-Planck equation (FPE) derived from the advection-diffusion (ADE) equation for suspended sediment transport. The detail of model development will be introduced in chapter 4. In addition to this, turbulence flow plays an essential role because we are focused on the sediment transport in open channel flows. Unfortunately, turbulence in the open channel flows is not completely understood even in recently. Because of insufficient knowledge about turbulence, there exists uncertainty when attempting to modeling particle movement in flows. As such, the stochastic method is an appropriate way to describe the movement of sediment particles in this study.

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1.1 Problem statement

The problem of sediment transport is closely related to the environment such as water quality, estuary improvement, environmental protection and estuary surrounding construction. In order to reach the above objectives, it is important to study the law of natural environment. With an enhanced understanding of sediment transport mechanisms, hydraulics constructions or engineering management can operate more effectively based on this scientific information. However, the natural environment is too difficult to simulate, as it involves multiple interacting factors. In other words, it is impossible to have complete information on all the factors in the natural process. Moreover, sediment motion in the flow and eddies are a complex process, which can be regarded as a stochastic process. Most sediment transport models such as ADE or the Exner equation are deterministic models, meaning that if a model with the same input(s) will yield the same results. These deterministic models simplify the uncertain variables (e.g. sediment properties, and flow discharge) to deterministic values and neglect the irregular eddy effect. Stochastic models for complicated and random natural process are thus developed. These stochastic methods such as uncertainty analysis that considers uncertainties incurred in data by considering their probability of occurrences. Yen (2002) discussed the hydraulic problems with stochastic perspectives, which can be briefly summarized as follows.

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Input	*System*	*Output*
Deterministic	Deterministic	Deterministic
Deterministic	Stochastic	Stochastic
Stochastic	Deterministic	Stochastic
Stochastic	Stochastic	Stochastic

Table 1.1 Different types of model (modified from Yen, 2002)

In this study, we consider the stochastic model-- SD-PTM to describe sediment particle movement in the open channel flows. A different concept of SD-PTM, two-particle PTM, is proposed by Spivakovskaya and Heemink (2006). Unlike traditional SD-PTM, the two-particle PTM suggested that the behavior of sediment particles caused by turbulence flow is correlated in space. Therefore, to more comprehensively model sediment particles, it is desirable to develop the two-particle PTM considering the effect of spatial correlation of particle behavior.

1.2 Research Hypotheses

Motion of sediment particles caused by turbulence is an irregular motion, which is difficult to describe exactly. This study raises two main hypotheses in the PTMs.

Markovian property

Sediment particles in open channel flows are poorly understood because of its random motion. Therefore, sediment particle motions are regarded as a memoryless stochastic process. The memoryless behavior is called as Markovian property. Based on

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this, the FPE is used to describe particles' movement. In the other words, sediment particles relates to the present state rather than the previous state.

Fickian law

Turbulent diffusivity plays an important role in the high Reynolds number flow. For instance, in turbulent flow, the effect of turbulence is more significant than that of the molecular diffusion. As will be introduced in chapter 4, turbulent diffusion is also considered as some form of random motion. The behavior of turbulence flow is analogous to Fickian diffusion. In Fickian law, the variance of particles displacement is defined to be linearly proportional to time. Figure 1.1 presents the flow chart of the PTMs. The difference between one-particle and two-particle PTMs is in the stochastic diffusion process. The two-particle PTM emphasizes the inter-particle relationship.

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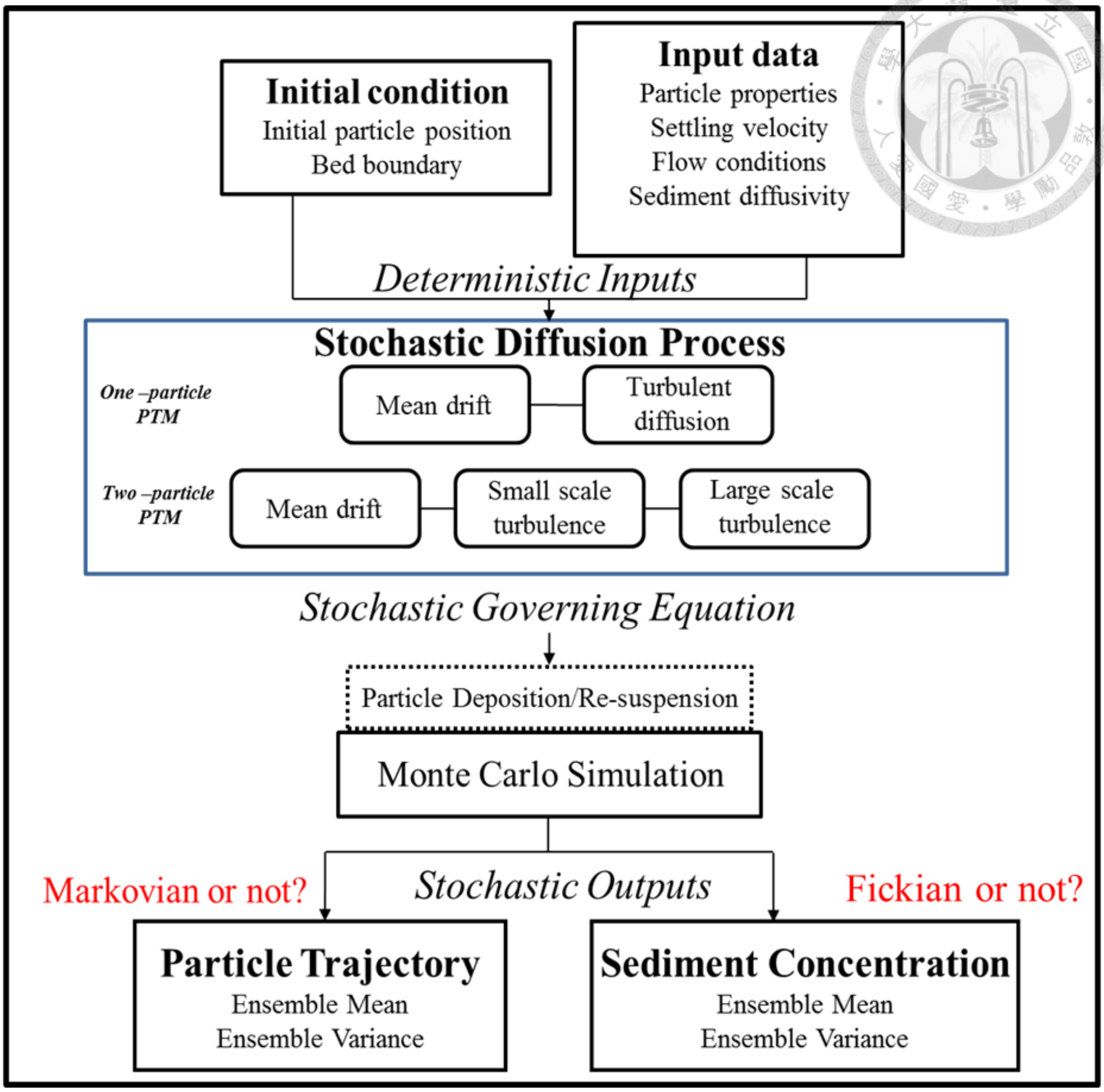

Figure 1.1 Flow chart of two-particle PTM

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1.3 Objectives of Study

This study is intended to develop a refined stochastic diffusion particle tracking model for sediment transport in open channel flows to estimate sediment concentrations. The main objectives are

i. to incorporate a more sophisticated turbulent diffusivity formula and a recently developed mechanism of re-suspension into the proposed stochastic particle tracking model;

ii. to simulate the movement of sediment particles under various flow conditions;

iii. to verify the proposed model by comparing the quantified sediment concentrations and velocity with experimental data;

iv. to compare and discuss the difference of the concentration fluctuations by proposed one-particle and two-particle models.

1.4 Overview of Thesis

This thesis includes two main hypotheses which are previously defined. Chapter 2 is a literature review about different opinions of quantitative sediment particles, and the important hydraulics parameters to the proposed models. In chapter 3, the foundation of stochastic theories and numerical schemes are presented. Chapter 4 is the development of the SD-PTM, including the derivation of SD-PTM from ADE and the equivalent equation, FPE, as well as the definition of hydraulics parameters. Chapter 5 demonstrates three applications by the proposed models with comparison of experimental data and the various flow field data, respectively. Lastly, Chapter 6 supplies a summary of the findings, contributions, and recommendations for future studies in this field.

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Chapter 2 Literature Review

2.1 Stochastic Methods

Sediment transport model can be basically divided into two categories, the Lagrangian methods and the Eulerian methods. These kinds of methods are used to quantify particles in the flow. However, the erratic movement of particles which caused by flow eddies brings challenge for hydraulic engineers. In 1827, Brown first found that this phenomenon on microscopic scale, and named it "Brownian motion". In 1905, Albert Einstein explained the physical mechanisms of Brownian motion and then Wiener built up the mathematical theory for such motion. Particle movement with Brownian motion can be regarded as a stochastic process. A stochastic process includes a group of random variables, which represents the evolution of a random variable over time (i.e. $\{X_t, t \in T\}$ and $\{t_1 < ... < t_n\} \subset T$). Despite the results of deterministic models, the outcomes of the stochastic models are random, though the same initial and boundary conditions are used. It indicates that stochastic models are more realistic in many cases, especially for "large numbers" problems. However, it is generally easier to analyze the problem by deterministic models rather than stochastic ones. This study focuses on implementing stochastic models to sediment transport

In 1980, Durbin proposed a new definition of concentration in turbulent flows with a stochastic two-particle model. It demonstrates the difference of the predictions of concentration fluctuation by the two-particle model and those by one-particle model. The difference between one-particle model and two-particle model such as the production of fluctuations is related to dispersion of the blob's mass center by large

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scale turbulence. Durbin indicates that the process of blob mixing is with uncertainty. In other words, whether the behavior of turbulent eddies mixing two blobs together would occur depended on the probability. Therefore, the blobs' dispersion is relative to each other. With this new concept, Spivakovskaya *et al*. (2007) predicted the probable concentrations of the contaminant in order to reduce the possible environmental damage. In addition, the multiple particle model is constructed and the forward-reverse estimator is used to estimate the ensemble mean and standard deviation of the concentration of contaminant with the given number of critical locations. The following sections will describe the common methods to quantify particles in the flow.

2.1.1 The Eulerian model

In the Eulerian model, particles are treated as a continuum. In order to quantify particles, concentration is defined as the particles average spacing. The mathematical formulation of Eulerian model is governed by the advection-diffusion equation:

$$\frac{\partial c}{\partial t}+\nabla\cdot\left(Uc\right)-\nabla\cdot\left(D\nabla c\right)=0\,. \tag{2.1}$$

Where c is the ensemble mean of sediment particle concentration; ∇ is the divergence operator $\left(\partial/\partial x,\partial/\partial y,\partial/\partial z\right)$; D indicates the diffusion coefficient in the streamwise $\left(D_x,D_y,D_z\right)$; and ∇c is the gradient vector of sediment concentration. For incompressible fluids, $\nabla\cdot u$ =0, equation(2.1) becomes:

$$\frac{\partial c}{\partial t}+\mathrm{U}\cdot\nabla c-\nabla\cdot\left(D\nabla c\right)=0\,. \tag{2.2}$$

In general, this partial differential equation can be solved by numerical techniques such as finite differences, finite elements or finite volumes.

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2.1.2 The Lagrangian model

Unlike the Eulerian model, the Lagrangian model focused on the movement of individual particles, easily applying stochastic concept to each other (i.e. the collision of inter-particle). The basic ideas of Lagrangian models are from the random-walk particle tracking models. The random-walk model accurately simulates the turbulent dispersion with mathematical expression described by stochastic diffusion equations (Gardiner, 1985). In this model, the diffusion processes affect particle trajectories and is regarded as stochastic processes (i.e. the governing equation is stochastic). To avoid the inaccurate result by advection-diffusion equation in regions where the gradient of concentration tends to be high, the stochastic differential equations can be applied to such transport problems so the concentration with the probability function can be generated. The Fokker-Plank equation, known as the forward Kolmogorov equation (Tsai, 2012), is applied to develop the particle tracking models by defining the partial differential equation for the conditional probability density function

$$\frac{\partial f(x,t|x_0,t_0)}{\partial t} = -\sum_i \frac{\partial f\bar{u}_i(x,t)}{\partial x_i} + \frac{1}{2}\sum_{i,j}\frac{\partial^2 f(\sigma\sigma^T)_{i,j}}{\partial x_i \partial x_j}. \tag{2.3}$$

where $i = 1,2,3$; $j = 1,2,3$; $f(x,t|x_0,t_0)$ denotes the probability density function which initial position is x_0 at time t_0 ; $\bar{u}_i$ is mean and $\sigma\sigma^T$ is variance. To describe Brownian motion, there is a stochastic diffusion equation such as Langevin equation. The Fokker-Plank equation derivate from the Langevin equation in Ito scheme gives the form as equation(2.3) which has the property of Markovian chain. The numerical techniques for parabolic stochastic partial differential equation are suggested to tackle more sophisticated sediment transport problem. The detailed introduction about Langevin equation is presented in the following chapter

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2.2 Pickup Probability

The incipient motion of a sediment particle on a stream bed may occur in a form or forms like rolling, sliding, and saltation, which depends on the characteristics of near bed load flow. Einstein (1905) took bed load particles as stochastic process and defined pickup probability in this issue, giving incipient problem a new concept. Although the methods of stochastic have been applied to model the hydraulics of open-channel flow and sediment transport for a long time, there still remains much space for advancement in stochastic modeling like the initial entrainment and particles motion near the bed. However, most Researchers have investigated the critical shear stress by experimental or theoretical methods. Lee and Balachandar (2011) proposed the theoretical prediction of the threshold for incipient motion which is based on a force or momentum balance (i.e. the force balance relations such as hydrodynamic drag, lift force gravitational and frictional forces are considered). On the other hand, Wu and Lin (2002) laid the foundation of the positive fluctuations of the streamwise velocity nearing the bed to decide pickup probability. Instead of previous assumption that velocity fluctuation obeys the normal distribution, the streamwise instantaneous velocity is based on lognormal distributions. In this foundation, the instantaneous velocity follows the lognormal distribution from zero to infinite.

Different from previous studies that were based on the normal and the lognormal distribution, Bose and Dey (2010) suggested a probability function with the Gram-Charlier series expansion according to the two-sided exponential or the Laplace distribution. They indicated that the velocity fluctuations (u', w') comply with Gram Charlier-based two-sided exponential or Laplace distributions. The streamwise velocity fluctuations can be expressed as a probability density function by assuming $\hat{u} = u' / \sigma_1$

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and $\hat{w} = w' / \sigma_2$, where σ_1, σ_2 are root-mean square of u' and w', respectively,

$$p_{\hat{u}}(\hat{u}) = \frac{1}{2\pi}\sum_{j=0}^{\infty} \mathrm{i}^j C_{j0} I_j(\hat{u}) = \frac{1}{2}\left[1 + \frac{1}{2}C_{10}\hat{u} - \frac{1}{8}C_{20}(1+|\hat{u}|-\hat{u}^2) - \frac{1}{48}C_{30}\hat{u}(3+3|\hat{u}|-\hat{u}^2)+...\right]\exp(-|\hat{u}|) \tag{2.4}$$

where the coefficients C_{jk} is related to the m_{jk}, $C_{10} = m_{10}$; $C_{20} = -1 + (m_{20}/2)$; $C_{30} = -2m_{10} + (m_{30}/6)$. The probability density function $p_{\hat{v}}(\hat{v})$ of vertical velocity fluctuations is similarly given by an expression in which substituting $\hat{u}$ for w', and C_{10}, C_{20} and C_{30} by C_{01}, C_{02} and C_{03}, respectively. The moments m_{j0} and m_{0k} related to the C_{j0} and C_{0k}, respectively, can be shown as,

$$m_{j0} = \int_{-\infty}^{\infty} \hat{u}^j p_{\hat{u}}(\hat{u})\,\mathrm{d}\hat{u}, \quad m_{0k} = \int_{-\infty}^{\infty} \hat{v}^k p_{\hat{v}}(\hat{v})\,\mathrm{d}\hat{v} \ , \tag{2.5}$$

Owing to experimental data, the coefficients C_{j0} and C_{0k} can be estimated. The integral in equation(2.4), one can write

$$I_j(x) = \int_{-\infty}^{\infty} \frac{\xi^j \exp(\text{-i}x\xi)}{(1+\xi^2)^{j+1}}\mathrm{d}\xi \ . \tag{2.6}$$

Thanks to the smallness or dividing by a large number, the coefficients in equation(2.4) can be neglected and reduced to

$$p_{\hat{u}}(\hat{u}) = \frac{1}{32}(17+|\hat{u}|-\hat{u}^2)\exp(-|\hat{u}|)\ . \tag{2.7}$$

Bose and Dey (2013) raised the hypothesis that the sediment particles can be transported not only bedload motion by the velocity fluctuations in turbulent flows, but also as suspended load. Cheng and Chiew (1999) assumed that only the suspended particles are replaced with the bed load, and the wash load is egligible. It is said that the suspended particles at the top of the bed-load layer occur resuspension when the vertical

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velocity fluctuations w' of the turbulent flow exceeds the settling velocity w_s of particles. Following this discussion, the vertical velocity fluctuations' PDF, equation(2.4) obeyed the one-sided exponential-based Gram-Charlier series can be shown as

$$
\begin{aligned}
&P_{v'}(w' \geq 0) = \frac{1}{16}\left(17 + \hat{w} - \hat{w}^2\right)\exp(-\hat{w}) \\
&P_{v'}(w' < 0) = 0
\end{aligned}
\tag{2.8}
$$

Namely, they supposed that the instantaneous hydrodynamic force acting on a particle of the near bed velocity fluctuations is an important mechanism toward the sediment entrainment. In this assumption, the submerged weight of a particle is considered as a constant for a given particle size. Here, the probability of vertical velocity fluctuations contacts with the value of σ_2, and the value of σ_2 is related to the bed layer. Table 2.1 shows the comparison of previous studies. They also obtained the following expression for the relationship between σ_2 and bed layer property. For the bed layer is very thin, the bed is regarded as rough (Grass, 1971), it is

$$\sigma_2 \approx u_* . \tag{2.9}$$

On the contrary, the bed is considered as smooth for thicker bed layer by Grass (1971), one can be written as

$$\frac{\sigma_2}{u_*} = 1 - \exp\left[-0.093\left(\frac{u_* d}{\nu}\right)^{1.3}\right]. \tag{2.10}$$

where u_*, d and ν are shear velocity, particle diameter and kinematic viscosity of fluid, respectively.

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Published year	Authors	PDF of turbulence fluctuations	Entrainment type	Thresholds for entrainment	Bedload type
1998	Cheng and Chiew	Gaussian (streamwise velocity)	Lifting	$F_L > W$	Rough bed
1999	Cheng and Chiew	Gaussian (vertical velocity)	Suspended particles	$w' > w_s$	Smooth bed and Rough bed
2002	Wu and Lin	Log-normal (streamwise velocity)	Lifting	$F_L > W$	Rough bed
2003	Wu and Chou	Log-normal (streamwise velocity)	Lifting and Rolling	$F_D L_D + F_L L_L > W L_W$ and $F_L > W$	Smooth bed, transition bed and Rough bed
2007	Wu and Jing	Gram-Charlier joint probability (streamwise and vertical velocity)	Lifting and Rolling	$F_D L_D + F_L L_L > W L_W$ and $F_L > W$	Smooth bed, transition bed and Rough bed
2013	Bose and Dey	Gram-Charlier expansion based on the Laplace-type (streamwise and vertical velocity)	Suspended particles	$w' > w_s$	Rough bed and Smooth bed

Table 2.1 Summary of previous study

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2.3 Turbulent diffusion and dispersion

There are two categories of mixing process in a flow, diffusion and dispersion (Chien and Wan, 1999; Elder, 1958; Fisher *et al*, 1979; French, 1985). Diffusion can be used to describe the random scattering of particles, which is caused by molecular motion or eddy fluctuations, in the laminar flow field and the turbulent flow field, respectively. In contrast to diffusion, the variation of velocity distribution over the cross section leads to dispersion. In other words, dispersion is the scattering of particles associated with shear and transverse turbulent diffusion.

In this thesis, our focus is on the diffusion process. Following Roberts and Webster (2002) and Kirmse (1964), the velocity fluctuations of a turbulent flow have efficiently transport of momentum and heat. Comparing to molecular diffusion, the turbulent transport has more significant effect since the magnitude of eddy size is larger than molecular (i.e. turbulent energy is larger than molecular energy). The eddies are considered as continuous evaluation in time and its eddies range in size from Integral scales down to Batchelor scales. Pope (2000) indicated that even the flow with small length scale, the order of small length scale turbulence exceeds three or more orders of magnitude to the length scale of molecule. Figure 2.1 illustrates that the highest energy has the largest length scale, and also indicates that the Batchelor scale is much smaller than an order of magnitude than Kolmogorov scale.

The behavior of suspended particles is related to turbulent flow structure. The important concept in sediment theory is that the vertical concentration distribution is related to the ratio of turbulent sediment diffusion to momentum diffusion coefficient

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(Cellino, 1998; Rouse, 1937; Tsujimoto, 2010). The ratio is a value which represents the difference between the diffusion of sediment particles and the diffusion of fluid particles (e.g. the molecule of water) in a flow. In 1937, Rouse obtained the turbulent sediment diffusion coefficient under the assumption of the log law for open channel turbulent flow. Without the supposition of log law profile, Absi *et al*. (2011) used the accurate analytical formulation for turbulent kinetic energy and eddy viscosity which calibrated by DNS data to calculate the coefficient of turbulent diffusion.

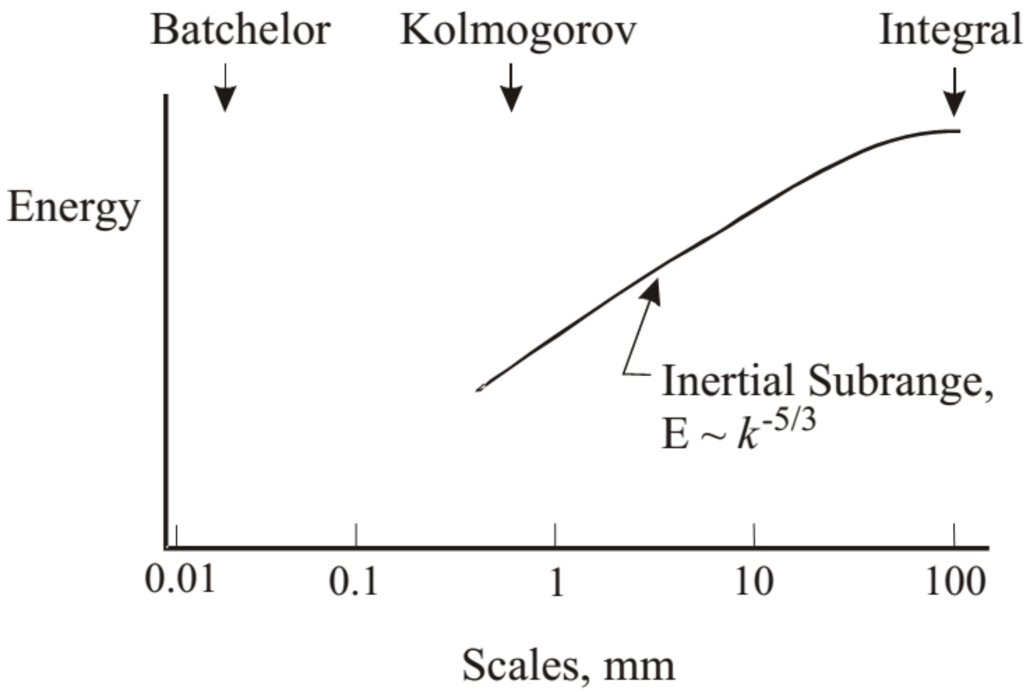

Figure 2.1 The classic turbulence energy spectrum versus to length scales for the open channel flow (Roberts and Webster, 2002).

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2.4 Summary

In this chapter, different types of quantitative sediment transport methods are introduced (e.g. the Eulerian and the Lagrangian model). However, this study is focused on the Lagrangian model instead of the Eulerian model. Mechanisms such as sediment entrainment probability and diffusion coefficient are introduced in this section and more details will be mentioned in chapter 4. The aforementioned techniques will be applied to simulate sediment transport in chapter 5.

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Chapter 3 Stochastic Theories

The specific objective in this thesis is to explore sediment transport in regular flow through an analysis of stochastic methods. Particles' erratic behavior in fluid can be considered as stochastic, which may be caused by flow turbulence or particle interaction. The Lagrangian model is used in this study in order to describe more details about particle motion. Moreover, different from the Eulerian model, the Langrangian model is more suitable and efficient to simulate the problem if the observer only concentrates on a particular region rather than the whole domain. Therefore, the particle tracking model based on the Lagrangian concept and the uncertainty characteristic is introduced. The abovementioned method is known as the stochastic diffusion process. Besides, there is another stochastic method called the stochastic jump diffusion process, which can be applied to condition of extreme flow events. This chapter introduces the simulation techniques of the stochastic theory such as the Markov process (or Markov chain) and the Wiener process (or Brownian motion) for particle tracking model. In addition, the numerical form for the stochastic differential process is also presented.

3.1 Markov Process

The Markov process is a stochastic process on a finite or countable number of possible values (Ross, 2007). In general, the possible value of the process is regarded as nonnegative integers (e.g. $\{0,1,2,...\}$). The Markov chain in mathematical form can be given as

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$$P\left\{X_{n+1}=j \middle| X_n=i, X_{n-1}=i_{n-1},\ldots,X_1=i_1,X_0=i_0\right\}=P_{ij}\,. \tag{3.1}$$

It indicates that in the process there is a sate i which will correspond to a fixed probability P_{ij}. In other words, the property of Markov chain can be said that the future state is independent of the past states and will be influenced only by the present state. In this point, movement of a particle in a water system is assumed to be followed by the Markov process. For assumptions of the stationary process and Markovian property, there is a random walk theory of stochastic processes available to describe the state of sediment transport.

3.2 Brownian Motion

A pollen grain moved randomly in water is observed by Robert Brown in 1827, who named this phenomenon as Brownian motion. Regarding to molecular diffusion, a pollen grain has a stochastic trajectory. This phenomenon is based on the theory of random walk. Each particle moves left or right with the same probability $\frac{1}{2}$, and obeys the well-known equation, Fick's law. It can be noted that the motion of particle is independent because of the dynamic balance of retarding force and heat fluctuations. In spite of considering one-dimensional Fick's law usually, the flux in an arbitrary direction is corresponding only to the concentration gradient in a specific direction, three-dimensional Fick's law can be directly derived. For the concentration changing with time, the solution of unsteady state diffusion can be obtained as follows

$$c(x,t)=\frac{1}{\sqrt{4\pi Dt}}\exp\left(-\frac{x^2}{4Dt}\right) \tag{3.2}$$

where $c(x,t)$ is concentration; D is diffusion coefficient; t is observation time.

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This distribution is the normal distribution with a zero mean and a variance of $2Dt$. By means of the aforementioned concept, it can be easily assumed that the moving distance of a particle is the Gaussian distribution also with the same statistic properties (e.g. zero mean, standard divination, $\sqrt{2Dt}$).

Thanks to the contribution of Wiener and Levy, the mathematical expression of Brownian motion is also named the Wiener process or the Wiener-Levy process. The random walk theory is employed. Considering that the particle is released at origin, the position at time t can be shown as

$$X(t) = \Delta x\left(X_1 + ... + X_{[t/\Delta t]}\right) \tag{3.3}$$

in which $\left[t/\Delta t\right]$ is the largest integer less than or equal to $t/\Delta t$, and the X_i are assumed as independent values, obeying the same probability of moving left or right. It can be concluded that the Wiener process follows few conditions such as

i) W(0) = 0 with probability 1.

ii) If $0 < s < t < T$, then the random variable $\Delta W = W(t) - W(s)$ is the Gaussian distribution with mean and variance of 0 and (t - s) respectively, thus, the mathematical form can be written as $\Delta W = \sqrt{t-s}\mathcal{N}(0,1)$

iii) The property of stationary independent increments. If $0 < s < t < u < v < T$, $\Delta W_1 = W(t) - W(s)$ and $\Delta W_2 = W(t) - W(s)$ are independent.

Figure 3.1 displays part of simple simulations of particle trajectory starting at $X_1 = 0$ and predicting the possible scenarios. In this example, time step Δt is given as

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0.5 seconds, and the end of time is 1 second. The particles interaction is neglected, which means that particles have independently motions. We released 3000 particles at the origin, and the ensemble mean is calculated. The figure also shows that the trajectories' variance is increasing with time.

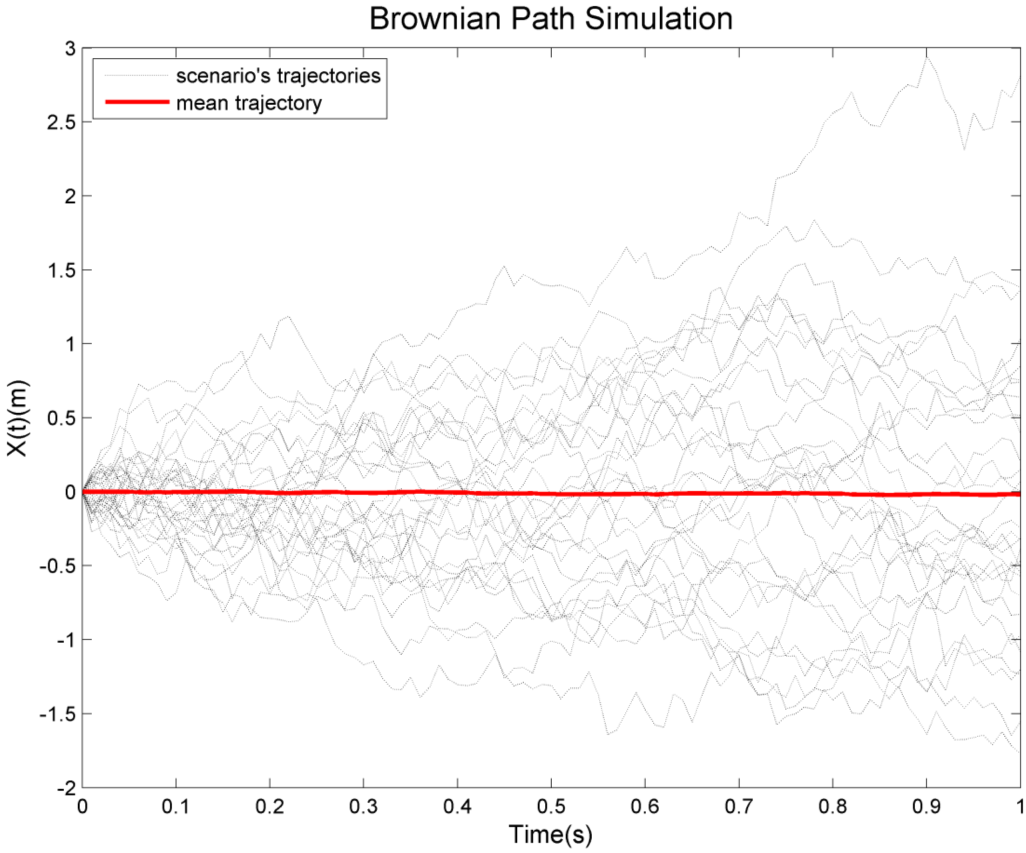

Figure 3.1 Simulation of 3000 samples of the Wiener process

3.3 Stochastic Diffusion Process

The aim of differential equations is to describe the system of the time evolution. For instance, the variable which is the function of time $x(t)$ within deterministic function is ordinary differential equations (ODE). In contrast, the system of the time evolution in the stochastic manner can be expressed by the stochastic differential

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equation (SDE). The stochastic diffusion process is a type of stochastic differential equations, which can be expressed as follows.

$$\frac{dX_t}{dt} = f(X_t, t) + g(X_t, t)\dot{W}_t \tag{3.4}$$

where $X_t = X(t)$ is the realization of a stochastic process; $f(X_t, t)$ is the drift term, which is presented as the deterministic part of the SDE and has the meaning of local trend; $g(X_t, t)$ is the diffusion term, influencing the size of fluctuations in the SDE; $\dot{W}_t$ is the Gaussian White noise process, which represents dW_t / dt. However, paths of the Wiener process are not differentiable. Depending on the choice of τ_j (i.e. the integral manner of "left-hand" sum or "midpoint" sum), leading to the stochastic process to different kinds of stochastic calculus: Ito and Stratonovich; where τ_j is in the time interval $[t_j, t_{j+1}]$ as shown in following sections.

Ito calculus

$$\tau_j = t_j \tag{3.5}$$

Stratonovich calculus

$$\tau_j = \frac{\left(t_j + t_{j+1}\right)}{2} \tag{3.6}$$

Using the symbol "o" in the Stratonovich concept to distinguish between SDEs interpreted in Ito and Stratonovich opinions, one obtain

$$\frac{dX_t}{dt} = f(X_t, t) + g(X_t, t) \circ \dot{W}_t \tag{3.7}$$

The stochastic integral between the Ito and Stratonovich calculus can be obtained respectively,

$$\int_0^T W(t)\,\mathrm{d}W(t) = \frac{1}{2}\left[W(T)^2 - W(0)^2 - T\right] \tag{3.8}$$

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and

$$\int_0^T W(t) \circ \mathrm{d}W(t) = \frac{1}{2}\left[W(T)^2 - W(0)^2\right] \tag{3.9}$$

Since the Ito and Stratonovich interpretations do not converge to the identical form, using Ito's formula to find a transformation from Ito to Stratonovich. The form equivalent to equation (3.4) can be given as

$$\frac{dX_t}{dt} = \left(f(X_t,t) - \frac{1}{2} g(X_t,t)\partial_x g(X_t,t) \right) dt + g(X_t,t) \circ dW_t \tag{3.10}$$

in which the modified drift term is called the noise-induced drift.

Although the Stratonovich interpretation is considered to be used within the physical property, the Ito interpretation is used in this study owing to the Markovian property (i.e. the future stat is only dependent on the present state).

3.4 Numerical Approximation for Stochastic Differential Equations

The Ito integral was introduced in the previous section. The numerical methods are introduced for solving equation(3.4) since most SDEs are unsolvable analytically. Moreover, equation(3.4) can be rewritten in the differential form as

$$dX_t = f(X_t,t)dt + g(X_t,t)dW_t \tag{3.11}$$

Note that the initial position is $X(0) = \mathrm{X}_0$ and that the time region is between **0** and ***T***. To apply the numerical methods such as the Euler-Maruyama (EM) method and Milstein method, first we need to discretize the interval. Assuming that the time increment $\Delta t = T / L$ for some positive integers L and $\tau_j = j\Delta t$, then we can have

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the numerical form of the EM method and Milstein method.

EM method

$$X_j = X_{j-1} + f(X_{j-1})\Delta t + g(X_{j-1})\left(\mathrm{W}(\tau_j) - \mathrm{W}(\tau_{j-1})\right),\ j = 1, 2, ..., L \tag{3.12}$$

Milstein method

$$\begin{aligned} X_j &= X_{j-1} + f(X_{j-1})\Delta t + g(X_{j-1})\left(\mathrm{W}(\tau_j) - \mathrm{W}(\tau_{j-1})\right) \\ &\quad + \frac{1}{2} g(X_{j-1}) g'(X_{j-1})\left(\left(\mathrm{W}(\tau_j) - \mathrm{W}(\tau_{j-1})\right)^2 - \Delta t\right),\ j = 1, 2, ..., L \end{aligned} \tag{3.13}$$

Both of these methods are the results of the Ito stochastic Taylor expansion by using the Taylor approximation. Here, the EM approximation in the Ito sense is a one-step approximation method, and converges with order 0.5 and 1 in the strong and weak sense, respectively. By adding all the stochastic increments, both of Milstein's methods converge with order 1.

The strong and weak convergence definitions are as follows, and their convergence is equal to γ.

Strong convergence

$$\mathrm{E}\left|X_n - X(\tau)\right| \le C\Delta t^{\gamma} \tag{3.14}$$

in which C is a constant; E is the expected value; X_n and $X(\tau)$ are random variables, respectively; Δt is sufficiently small which fixs $\tau = n\Delta t$ in the region of 0 to T.

Weak convergence

$$\left|\mathrm{E}p\left(X_n\right) - \mathrm{E}p\left(X(\tau)\right)\right| \le C\Delta t^{\gamma} \tag{3.15}$$

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where the functions $\boldsymbol{p}$ in equation(3.15) obeys the conditions of smoothness and polynomial growth;

The above convergence definitions measure the rate of decay as $\Delta t \to 0$. As we can see, the convergence of strong measures the proportion of decay of "mean of error". In contrast, the convergence of weak is to measure the proportion of decay of "error of means". Therefore, it can be concluded that weak convergence only takes into account the mean of solution. For instance, if the increment is $\sqrt{\Delta t}\mathcal{N}(0,1)$ it can be replaced by any random variable which obeyed the same mean and variance such as sign function "$\operatorname{sgn}(x)$", where x is a random number. There is a simple example to show the difference between the strong and weak convergence (Higham, 2001). The EM method is applied to the following equation in the linear form,

$$dX_t = \lambda X_t + \mu X_t dW_t \tag{3.16}$$

Equation(3.16) has an exact solution written as,

$$X_t = X_0 \exp\left(\left(\lambda - \frac{1}{2}\mu^2\right)t + \mu W_t\right) \tag{3.17}$$

The initial conditions and parameters in equation(3.16) in this example are shown in Table 3.1.

Parameter	X_0	λ	μ	**T**	**dt**
Value	1	2	0.1	1	$2^{-9}, 2^{-8}, 2^{-7}, 2^{-6}, 2^{-5}$

Table 3.1 Some parameters and initial conditions in the example

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Figure 3.2 shows the comparison of one of scenarios with strong and weak solutions by using the time step 2^{-9}. In this figure, it can be observed that the strong solution gives more information of paths than the weak solution. However, both of them have same statistic properties such as mean and variance. In Figure 3.3, the trajectories are almost the same if averaging the trajectories of both convergences. On the other hand, by using a least squares method, the convergence can be solved. In the strong solution, the convergence value is producing $0.5384 \approx 0.5$ with a least squares value of 0.0266. The weak solution gives the convergence value $0.9858 \approx 1$ with a least squares value 0.0508.

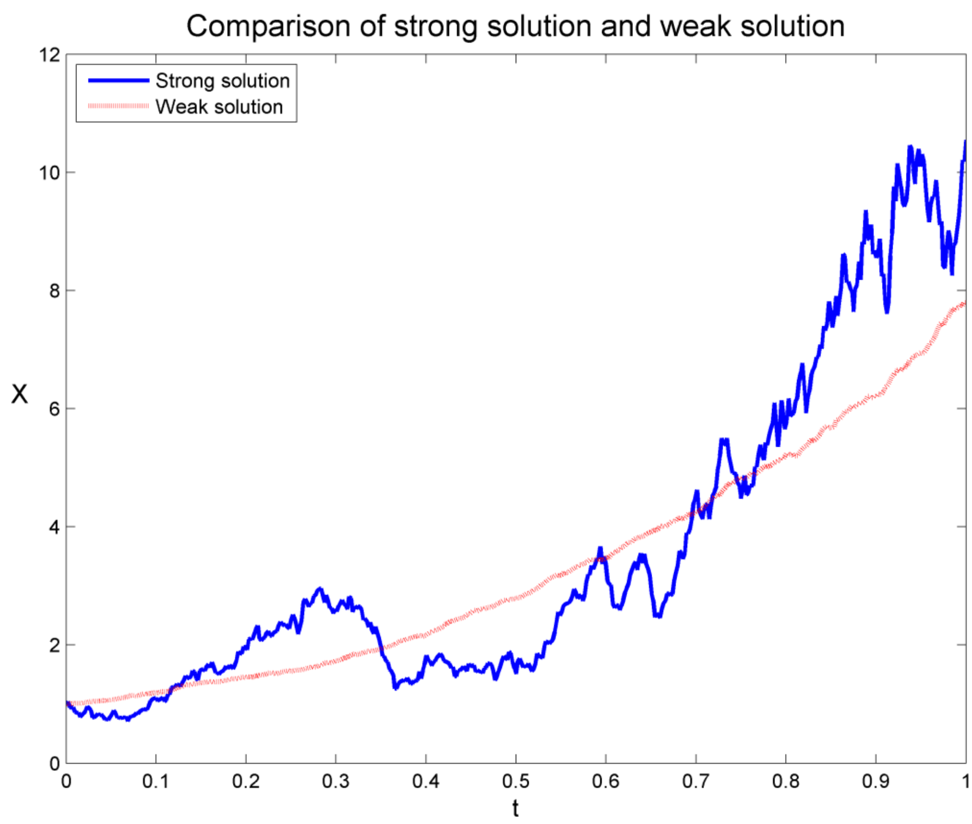

Figure 3.2 Comparing with Weak solution, strong solution emphases the information of path

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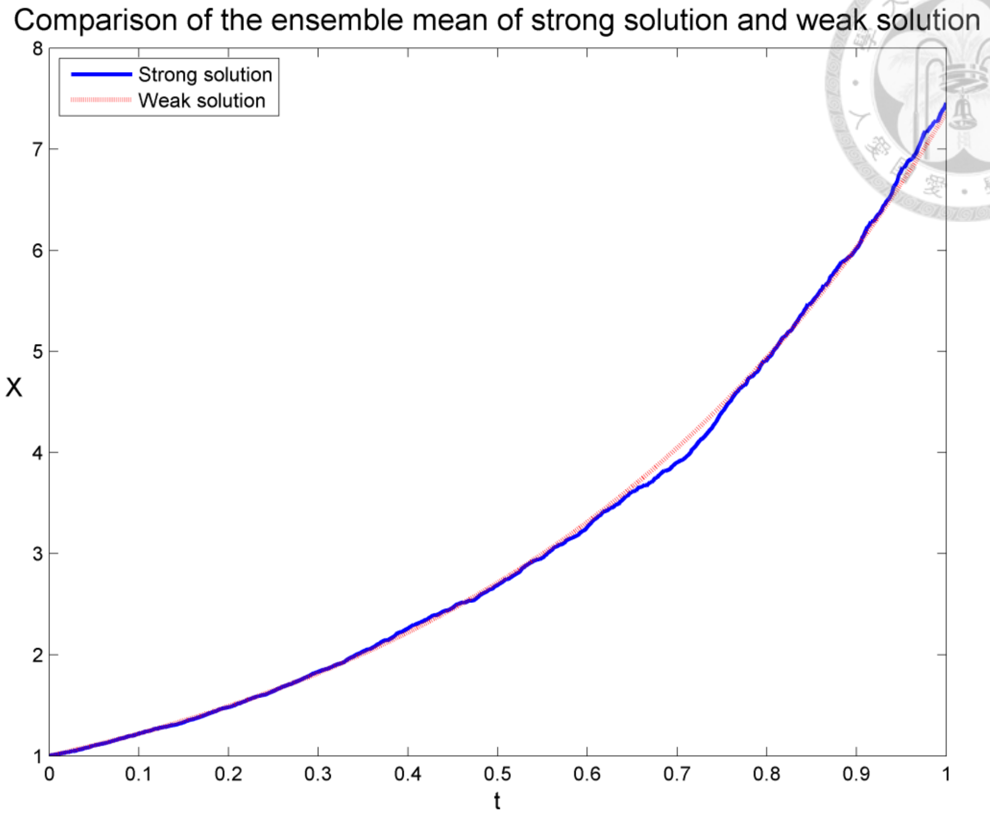

Figure 3.3 Ensemble mean of strong solution and weak solution

3.5 Summary

The backgrounds of stochastic theories are introduced in this chapter. At first, the Markov theory is presented herein. The important mathematical form of the Wiener process (or Brownian motion) is also applied in the PTMs. With the aforementioned concepts, the stochastic differential equation can be constructed. Different types of mathematical interpretations such as the Ito scheme and Stratonovich scheme are appropriate in the respective problems. However, in this study, the Ito calculus is utilized since the hypothesis of Markovian property that the future state is only related to the present state. At the end of this chapter, different numerical schemes which enhance the numerical accuracy are also introduced. The EM method is ubiquitous and well-accepted. Therefore, the EM method is still the best candidate in our study.

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Chapter 4 Development of Stochastic Particle Tracking Model of Suspended Sediment Transport

4.1 Introduction

Sediment particle movement in turbulent flow is difficult to describe exactly because of a large number of molecules in the flow and small particles' collision. It takes longer to solve the equations of motion for all the molecules in the flow and for small particles. Moreover, the unknown of initial values of all the molecules in the flow and different motion of the small particles also puzzle the problem. To treat this problem in a simple way, the stochastic force is employed to describe the effect caused by molecules in flow and small particles' collision (Risken, 1989). In other words, sediment particles or fluid particles in turbulent flow can be considered as a stochastic process. Based on the Markovian theory, the Fokker-Planck equation describes the conditional probability density for the fluid particle's velocity and position as the evolution of time (Risken, 1989; Sawford and Borgas, 1994; Sharma and Patel,2010).

In general, the suspended sediment transport is simulated by the advection-diffusion equations by means of the deterministic solution of the Eulerian model. However, Dimou and Adams (1993) suggested that there are several reasons to use the Lagrangian model instead of the Eulerian model. Firstly, it is easier to represent sources in the Lagrangian model or the particle tracking model. The numerical problem of an Eulerian model is difficult to solve with a high gradient concentration. Secondly, it

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is more obvious to represent the region where most particles are located in the Lagrangian model rather than in the Eulerian model where all regions of the computational domain are considered equally. Thirdly, it is more effective to represent properties of the individual particles (e.g. particle diameter, settling velocity) in the Lagrangian model. To combine the characteristic of stochastic and the Lagrangian model, the Fokker-Planck equation which derived from Langevin equation (Gadiner, 1985) is used. Langevin equation describes the detail of individual particles in the Lagrangian framework instead of an assemblage of many particles. Since we cannot consider all the forces by molecules or particles collisions, by assuming these forces are random, the stochastic differential equation is constructed of deterministic forces. Random force is introduced. Furthermore, the Fokker-Planck equation in the concept of the Markovian property, and the large number of particles at a very small time step corresponds to the advection-diffusion equation. However, some researchers have shown that it is not enough for considering a single particle model (Durbin, 1980; Thomson, 1990; Borgas and Sawford, 1991; Borgas and Sawford, 1994). Durbin (1980) suggested that the autocorrelation of concentrations is needed for a complete stochastic theory of concentration fluctuations. The development of a particle tracking model is introduced in this chapter.

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4.2 Model Assumptions

Assumptions regarding the particle tracking models are described as follows:

One-particle PTM

The SD-PTM is constructed based on the foundation of the random walk model. The assumption is that particles are moved by the collision against adjacent fluid particles under a stochastic process, which is independent of the original position. Random motion of sediment particles is described by the Wiener process. More details of the Wiener process are introduced in chapter 3.

Two-particle PTM

Different from one-particle PTM, this model tends to distinguish the effect by multiple scales of turbulence to describe more details of particle motion. The basic concept is that if their distance is close to zero, the motion of sediment particles is highly related to other particles caused by large scale turbulence. Particles can be separated by molecular diffusion if particles are in the immediate neighborhood. On the contrary, if their distance is large, sediment particles move independently. However, it is difficult to define how sediment particles move in response to various scales of eddies. For simplification, it is hypothesized that the spatial correlation of sediment particles can be primarily attributed to large scales of eddies. As such, dependent Brownian motion can be used to simulate spatial correlation of particles constrained by large eddies. On the other hand, movement of sediment particles caused by molecular diffusion or smaller scales of turbulence is modeled by the independent Brownian motion.

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4.3 Model Development

4.3.1 Stochastic Diffusion Model – One-Particle Particle Tracking Model

An aggregation of many particles is commonly employed instead of an individual particle. Fisher *et al*. (1979) applied an analysis of the concentration with no sources or sinks based on the deterministic continuity equation. Therefore, the equation with spatially varying coefficient in uniform flow can be written as

$$\frac{\partial c}{\partial t}+\underbrace{\bar{U}\frac{\partial c}{\partial x}+\bar{V}\frac{\partial c}{\partial y}+(\bar{W}-w_s)\frac{\partial c}{\partial z}}_{\text{change owing to advection}} = \underbrace{\frac{\partial}{\partial x}\left(\varepsilon_x\frac{\partial c}{\partial x}\right)+\frac{\partial}{\partial y}\left(\varepsilon_y\frac{\partial c}{\partial y}\right)+\frac{\partial}{\partial z}\left(\varepsilon_z\frac{\partial c}{\partial z}\right)}_{\text{change owing to diffusion}} \quad (4.1)$$

where c is concentration changing with time and space; $\bar{U}$, $\bar{V}$, $\bar{W}$ are the direction of x, y and z mean flow velocities, respectively, w_s is particle settling velocity, and ε_x, ε_y, ε_z are the sediment diffusion which represent all of the mechanisms causing mixing in the respective directions.

In 1985, Gardiner proposed that the random walk model which describes the position of each particle in Langevin framework, can be shown as

$$\frac{dx}{dt}=\underbrace{A(x,t)}_{\text{deterministic forces}}+\underbrace{B(x,t)\frac{dB_t}{dt}}_{\text{random forces}} \quad (4.2)$$

where $A(x,t)$ represents the deterministic forces, $B(x,t)$ is the random forces; and dB_t/dt is a Gaussian White noise which represents the uncertainty nature of motion (Gardiner, 1985). Under the concept of Ito calculus, equation(4.2) can be rewritten as the form of a stochastic differential equation

$$dx = A(x,t)dt + B(x,t)dB_t \quad (4.3)$$

where dB_t is the Wiener process which can be simulated as $\sqrt{dt}\mathcal{N}(0,1)$. The next

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step is to determine $A(x,t)$ and $B(x,t)$, for a given turbulent flow field in Eulerian statistics. Wilson and Sawford (1995) pointed out that A and B represent drift and diffusion term, respectively.

Following the Strong Law of Large Numbers, when the time step is nearly zero, equation(4.1) is equivalent to the Fokker-Planck equation

$$\frac{\partial f}{\partial t}+\frac{\partial}{\partial x_i}\left(A_i f\right)=\frac{\partial}{\partial x_i x_j}\left(\frac{1}{2}B_{ik}B_{jk}f\right) \tag{4.4}$$

where $f\left(x,t\middle|x_0,t_0\right)$ denotes the conditional probability density function for x at time t, from the initial position x_0 at time t_0. In order to compare with equation(4.4), noting that

$$\frac{\partial^2}{\partial x^2}\left(\varepsilon_x c\right)=\frac{\partial}{\partial x}\left(\varepsilon_x\frac{\partial c}{\partial x}+c\frac{\partial \varepsilon_x}{\partial x}\right) \tag{4.5}$$

and adding the flow continuity equation into equation(4.1)

$$\frac{\partial \overline{U}}{\partial x}+\frac{\partial \overline{V}}{\partial y}+\frac{\partial \overline{W}}{\partial z}=0 \tag{4.6}$$

Equation(4.1) can then be rewritten as

$$\begin{aligned}\frac{\partial c}{\partial t}&+\frac{\partial}{\partial x}\left[\left(\overline{U}+\frac{\partial \varepsilon_x}{\partial x}\right)c\right]+\frac{\partial}{\partial y}\left[\left(\overline{V}+\frac{\partial \varepsilon_y}{\partial y}\right)c\right]+\frac{\partial}{\partial z}\left[(\overline{W}-w_s+\frac{\partial \varepsilon_z}{\partial z})c\right]\\&=\frac{\partial^2}{\partial x^2}\left(\varepsilon_x c\right)+\frac{\partial^2}{\partial y^2}\left(\varepsilon_y c\right)+\frac{\partial^2}{\partial z^2}\left(\varepsilon_z c\right)\end{aligned} \tag{4.7}$$

It can be seen that equation(4.4) and equation(4.7) are equivalent if

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$$A = \begin{bmatrix} \overline{U} + \dfrac{\partial \varepsilon_x}{\partial x} \\ \overline{V} + \dfrac{\partial \varepsilon_y}{\partial y} \\ \overline{W} - w_s + \dfrac{\partial \varepsilon_z}{\partial z} \end{bmatrix}, \ \frac{1}{2}BB^T = \begin{bmatrix} \varepsilon_x \\ \varepsilon_y \\ \varepsilon_z \end{bmatrix}, \ f = c \tag{4.8}$$

Thus, the stochastic differential equation becomes (Heemink 1990; Dimou and Adams, 1993; Man and Tsai, 2007; Oh and Tsai, 2010; Tsai *et al*., 2014)

$$\begin{aligned} dX_t &= \left(\overline{U} + \frac{\partial \varepsilon_x}{\partial x} \right) dt + \sqrt{2\varepsilon_x}\, dB_t \\ dY_t &= \left(\overline{V} + \frac{\partial \varepsilon_y}{\partial y} \right) dt + \sqrt{2\varepsilon_y}\, dB_t \\ dZ_t &= \left(\overline{W} - w_s + \frac{\partial \varepsilon_z}{\partial z} \right) dt + \sqrt{2\varepsilon_z}\, dB_t \end{aligned} \tag{4.9}$$

Equation(4.9) is also called a stochastic diffusion equation, which can be described as particle movement, for instance particles do random motion in the turbulent flow (Oh and Tsai, 2009). Thanks to a multitude of factors such as eddy diffusion and inter-particle collisions, sediment transport can be treated as a stochastic process in open channel flow (Yen , 2002). This equation is a governing equation of the particle tracking model in streamwise, transverse and vertical direction respectively, to delineate sediment particle trajectory.

4.3.2 Stochastic Diffusion Model – Two-Particle Particle Tracking Model

A Lagrangian framework of the stochastic diffusion model for the trajectory by one-particle model was introduced in the previous section. However, one-particle model is good at estimating the ensemble mean of concentrations but not the ensemble variance of concentrations. Turbulent properties such as different size of eddies in a flow and mixing process (e.g. many turbulent eddies mix together) cause the

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fluctuations of concentrations. Namely, the stochastic model that considers paired particle motion can give a more realistic description of the natural process, as concentration variance is associated with statistics of particle trajectories produced by the two-particle model. Based on this definition, Durbin (1980) proposed a two-particle model that contained multiple scales of turbulent eddies. After this idea was established, many authors have explored to develop the two-particle model (Thomson, 1990; Borgas and Sawford, 1994; Reynolds, 1998; Spivakovskaya and Heemink, 2006). In this section, the major concept of a two-particle model is built upon Spivakovskaya and Heemink (2006). The spatial correlation of particle behavior related to turbulence is applied in this section. The assumption of the two-particle model is that the inter-particle correlation is dependent on the distance between two particles. Thus, it can be observed that particles have very similar motion (i.e. highly correlated) if the location of particles is the immediate vicinity of each other. On the contrary, motion of particles becomes more independent when particles are away from each other. Spivakovskaya and Heemink (2006) agreed with the argument that the effect of molecular diffusion is important in a two-particle model. The difference between the single particle model and paired particle model is that one neglects molecular diffusion, as the order of molecular diffusion is much smaller than the turbulent diffusion. On the other hand, the effect of molecular diffusion is considered. The particles can be separated by the molecular diffusion if the particles are in the immediate neighborhood.

Based on the above theoretical considerations, the one-particle model can be modified and the two-particle model equations (equation(4.10)) in two-dimension uniform flow are given as

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$$\begin{bmatrix} dX_1(t) \\ dX_2(t) \end{bmatrix} = \begin{bmatrix} \overline{U_1} + \dfrac{\partial \varepsilon_{x1}}{\partial x_1} \\ \overline{U_2} + \dfrac{\partial \varepsilon_{x2}}{\partial x_2} \end{bmatrix} dt + \begin{bmatrix} \sqrt{2\varepsilon_{x1}} \left(\sqrt{1-\beta^2} dB_{x1}(t) + \beta dB_{x1}{}'(t) \right) \\ \sqrt{2\varepsilon_{x2}} \left(\sqrt{1-\beta^2} dB_{x2}(t) + \beta dB_{x2}{}'(t) \right) \end{bmatrix}$$

$$\begin{bmatrix} dZ_1(t) \\ dZ_2(t) \end{bmatrix} = \begin{bmatrix} \overline{W_1} - w_{s1} + \dfrac{\partial \varepsilon_{z1}}{\partial z_1} \\ \overline{W_2} - w_{s2} + \dfrac{\partial \varepsilon_{z2}}{\partial z_2} \end{bmatrix} dt + \begin{bmatrix} \sqrt{2\varepsilon_{z1}} \left(\sqrt{1-\beta^2} dB_{z1}(t) + \beta dB_{z1}{}'(t) \right) \\ \sqrt{2\varepsilon_{z2}} \left(\sqrt{1-\beta^2} dB_{z2}(t) + \beta dB_{z2}{}'(t) \right) \end{bmatrix} \quad (4.10)$$

where $\overline{U}$, $\overline{W}$ is mean flow velocity; w_s is particle settling velocity dependent on the particle; ε is diffusion coefficient of sediment particle; β is the diffusion effect which can be chosen between 0 to 1; B is the standard Brownian motion simulated as a single particle model; B' is a correlated Brownian motion independent of B; $\sqrt{1-\beta^2}B(t)$ is the diffusion due to molecular diffusion and small scale turbulence and $\beta B'(t)$ is the diffusion due to large scale turbulence.

In the two-particle model, large scale turbulence is to be simulated as the correlated Brownian motion. The Brownian motion are correlated with covariance matrix as follows

$$E\left[dB_1'(t)\ dB_2'(t)\right] = f(r_{12})I_2 \quad (4.11)$$

where $f(r)$ is a correlated coefficient related to distance between particles. Moreover, the covariance is assumed to obey several conditions, for instance, the function of correlated coefficients is adequately smooth (i.e. the second derivative is continuous and bounded); the covariance matrix is a positive matrix. If particle distance is very close ($\Delta x \to 0$), the correlated coefficient is defined as one (e.g. $\lim_{x\to 0} f(x) = 1$). In contrast, if particle distance is very far ($\Delta x \to \infty$), the correlated coefficient is defined as zero (e.g. $\lim_{x\to\infty} f(x) = 0$). In this thesis, we follow the function proposed by Diamant *et al.*, (2005).

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$$f(r) = \frac{1}{r^2} \tag{4.12}$$

The following is the procedure for producing correlated Brownian motion (Bolin, 2009).

(1) Generating two independent Brownian motion dependent on the Integral scale, which represents the large turbulence scale.

$$B = \begin{bmatrix} B_1 \\ B_2 \end{bmatrix}$$

(2) Producing the covariance matrix according to the distance of particles.

$$cor = \begin{bmatrix} 1 & f(r) \\ f(r) & 1 \end{bmatrix}$$

(3) Applying the Cholesky factorization to decompose the correlation matrix.

$$cor = LL^T$$

(4) Obtaining newly correlated Brownian motion based on particle distance.

$$B_{cor} = \begin{bmatrix} B_{cor1} \\ B_{cor2} \end{bmatrix} = L^T B$$

4.4 Determination of Hydraulic Parameters in Open Channel Flow

4.4.1 Velocity Profile

Turbulent flow plays an important role in open channel flow, since the flow we investigated commonly has a large Reynolds number. Turbulent flow has the random property, which is difficult to measure. Based on Reynolds' equation, the velocity field can be represented as follows

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$$u = \bar{u} + u' \tag{4.13}$$

where $\bar{u}$ is mean velocity; u' is velocity fluctuations caused by turbulent eddies. This equation can be used to describe the random process of turbulence. The velocity fluctuation properties can be predicted by the Gaussian statistical theory in general. Following Spurk (2008), the mean velocity profile has been driven by the assumption of Prandtl's mixing length. The turbulent shear stress τ_t is connected with mixing length l under Prandtl's mixing length formula, which can be shown as

$$\tau_t = -\rho \overline{u'w'} = \rho l^2 \left(\frac{d\bar{u}}{dz} \right)^2 = \rho l^2 \left| \frac{d\bar{u}}{dz} \right| \frac{d\bar{u}}{dz} \tag{4.14}$$

Although the mixing length is considered as experimental investigation, herein the assumption of shear stress is constant. Thus, the mixing length is thought to be proportional to z

$$l = \kappa z \tag{4.15}$$

where κ is the von Karman constant. Since the shear stress is equivalent to the wall shear stress $\left(\tau_w = \rho u_*^2\right)$, combining equation(4.14) and equation (4.15), the shear velocity u_* can be written as

$$u_* = \kappa z \frac{d\bar{u}}{dz} \tag{4.16}$$

The velocity and water depth can be obtained by integrating equation(4.16), the velocity distribution in turbulent flow is

$$\bar{u} = \frac{u_*}{\kappa} \ln z + C \tag{4.17}$$

The mean velocity is zero at the location of z_0 in the turbulent flow, so the constant C of integration in equation(4.17) can be shown as

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$$C = -\frac{u_*}{\kappa} \ln z_0 \tag{4.18}$$

Thus, it becomes

$$\bar{u} = \frac{u_*}{\kappa} \ln\left(\frac{z}{z_0}\right) \tag{4.19}$$

Flow velocity over the bed will be used to determine the roughness Reynolds number ($\mathrm{Re}_{k_s} = k_s u_* / \nu$). In other words, it depends on the characteristic of hydrodynamic boundary (e.g. smooth boundary and rough boundary). Figure 4.1 and Figure 4.2 show the picture of smooth turbulent flow and rough turbulent flow, respectively. An expression for z_0 can be given,

Smooth boundary $$z_0 = \frac{\nu}{9u_*},\ \frac{u_* k_s}{\nu} < 5 \tag{4.20}$$

Rough boundary $$z_0 = \frac{k_s}{30},\ \frac{u_* k_s}{\nu} > 70 \tag{4.21}$$

where ν is kinematic viscosity, δ_s is the height of laminar sublayer, and k_s is roughnees height.

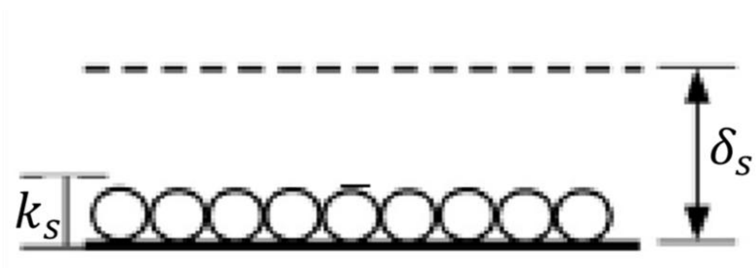

Figure 4.1 Turbulent flow under the condition of the smooth bed boundary (modified by MIT note).

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Figure 4.2 Turbulent flow under the condition of the rough bed boundary (modified by MIT note).

4.4.2 Particle Settling Velocity

In the settling process, a particle settles quickly at beginning and reaches steady state under the force balance condition when its gravity force is equivalent to the drag force. However, compared to the observation time step, the time to reach steady velocity is very short. In general, the particle settling velocity can be treated as a constant in the modeling of sediment transport (Chen and Wang, 1999). Another important factor of sediment particles is particle geometric shape. The geometric shape will result in different degrees of drag force in the descending process in flow. Since the drag force is varying, a particle in flow might not retain its original orientation and fall steadily. Furthermore, the diameter of a particle is a significant factor by no means peculiar to the particle shape. Chien and Wan (1999) have given a suggestion about the effect of finer sediment diameter. Finer sediment particles move in flocs because of the physic-chemical effect on the particle surface. This process gathers the fine sediment particles into a floc and increases their effective diameter. According to previous experimental results, it can be suggested that sediment particle flocculation may not have a significant impact on the particle deposition process when their size is larger than 0.01mm.

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In addition to flocculation, sediment concentrations also have influences on the settling velocity. The fluid specific density increases when the sediment concentration increases. This phenomenon also increases buoyance, decreasing the settling velocity. The following equations which defined low and high sediment concentration respectively are arranged by Chen and Wang (1999).

Low concentration (S_v<2.25%):

$$\frac{w_{s_0}}{w_s} = 1 + 1.24 k S_v^{\frac{1}{3}} \tag{4.22}$$

in which w_{s_0} is the settling velocity of sediment particle at zero concentration, w_s is the settling velocity of sediment particle at concentration S_v; k is the coefficient of experimental investigation. Cai (1956) gives a value 0.75 for k by considering the force conservation (Chien and Wan, 1999).

High concentration (S_v>2.25%):

$$\frac{w_{s_0}}{w_s} = \left(1 - S_v\right)^m \tag{4.23}$$

in which m is the parameter to be determined.

On the other hand, Sadat *et al*. (2009) provided the settling velocity based on the previous study. Depending on different size of particles, the settling velocity has the relationship with the effective diameter D_{gr}.

For the effective diameter D_{gr} is less than or equal to 10, the settling velocity can be expressed as

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$$w_{s_0} = 0.33\frac{\nu}{d}\left(\frac{d^3 g\left(S-1\right)}{\nu^2}\right)^{0.963} \quad (4.24)$$

For the effective diameter D_{gr} larger than 10, the settling velocity can be expressed as follows

$$w_{s_0} = 0.51\frac{\nu}{d}\left(\frac{d^3 g\left(S-1\right)}{\nu^2}\right)^{0.553} \quad (4.25)$$

in which D_{gr} is defined as $d\left(\frac{g\left(S-1\right)}{\nu^2}\right)^{\frac{1}{3}}$; d is particle diameter; g is gravity acceleration; and S is specific gravity.

4.4.3 Diffusion Coefficient

Similar to the diffusion in air or the diffusion in turbulent flow, particle diffusion in fluid also can be described as Brownian motion. Particle diffusion in turbulent flow is related to the surrounding fluid so that the motion of particle diffusion can be also regarded as following eddy diffusion. The floc diffuses with surrounding fluid at the beginning and then mix with ambient flow after moving for a distance l_3. Based on the definition of mixing length, if the momentum exchange coefficient ε_m is equivalent to diffusion coefficient ε_z, the diffusion coefficient ε_z can be expressed

$$\varepsilon_z = \sqrt{\overline{w'^2}}\, l_3 \quad (4.26)$$

in which $\sqrt{\overline{w'^2}}$ is the turbulent intensity. The coefficient of diffusion is associated with the length scale of turbulence in different directions. The relative magnitude of diffusion coefficient in longitudinal, transverse, vertical direction respectively, has an expression as follows

$$\varepsilon_x > \varepsilon_y > \varepsilon_z \quad (4.27)$$

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Lateral diffusion

It is difficult to quantify the lateral or longitudinal diffusion in natural flows, because of the complex terrain. Previously we focus more on the turbulent diffusion in simple channel flow such as straight and uniform channel flow. Herein, there is no transverse velocity profile on average available from laboratory experiment. Ficher et al. (1979) indicated that in the uniform straight channel the average transverse turbulent diffusion coefficient can be given as

$$\varepsilon_y = 0.15 u_* h \tag{4.28}$$

In natural streams, Fisher et al. (1979) suggested that transverse mixing in the uniform depth is,

$$\varepsilon_y = 0.6 u_* h \tag{4.29}$$

Longitudinal diffusion

Following Socolofsky and Jirka (2005), by assuming no boundary effects in the transverse or longitudinal directions, one can demonstrate that the longitudinal turbulent diffusion can be equivalent to transverse diffusion.

$$\varepsilon_x = \varepsilon_y \tag{4.30}$$

Vertical diffusion

Following Cellino (1998), the vertical concentration distribution is related to sediment turbulent diffusion. However, the sediment turbulent diffusion is to be described by the momentum diffusion, which means the diffusion of fluid particles in the flow. In previous studies, the momentum diffusion is determined by the log law velocity profile and has a relation with the sediment diffusion and the momentum diffusion as follows

$$\varepsilon_s = \beta \varepsilon_m \tag{4.31}$$

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where β is the proportion of the sediment diffusion coefficient to the momentum diffusion coefficient; ε_s is the diffusion coefficient of sediment; ε_m, the coefficient of momentum diffusion is given by

$$\varepsilon_m = \kappa u_* z\left(1-\frac{z}{H}\right) \tag{4.32}$$

In open channel flow, the momentum coefficient of turbulence and shear stress are zero as described by equation(4.33). Since suspended particles follow closely with turbulent motion, suspended particles may be subject to non-negligible transport on flow surface. In view of this, the turbulent diffusion coefficient of suspended particles ε_s is proposed Absi *et al*., 2011). It can be shown as

$$\varepsilon_s = \frac{1}{Sc_t}\nu_t \tag{4.33}$$

in which Sc_t is Schmidt number; ν_t is the eddy viscosity or the diffusivity of momentum. The turbulent Schmidt number is given as

$$Sc_t = \left(\frac{St}{\left(1-\rho_f/\rho_s\right)}+\frac{1}{1+St}\right) \tag{4.34}$$

The Stokes number St is defined as

$$St = \frac{\tau_p}{\tau_t} = \frac{w_s}{\left(1-\rho_f/\rho_s\right)g}\frac{k}{\alpha_0\nu_t} \tag{4.35}$$

where τ_p is the particle timescale; τ_t is the integral turbulence timescale or large eddy's turnover time; ρ_f and ρ_s are the density of fluid and solid, respectively; g is acceleration of gravity; α_0 is a coefficient for two-equation ($k-\varepsilon$ model), which is defined as α/C_μ. In this study, α and C_μ are given as $o(10^0)$ (empirical

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coefficient) and 0.09 (Toorman, 2008), respectively; k and ν_t are the turbulent kinetic energy (TKE) and the eddy viscosity respectively, defined by analytical formulations and calibrated by direct numerical simulation (DNS) data.

The turbulent kinetic energy (TKE)

$$k = \frac{u_*^{\ 2}}{\sqrt{C_\mu}} e^{-\frac{y^+ - a_k^{\ +}}{A_k^{\ +}}} \text{, } for\ y^+ > 40 \tag{4.36}$$

in which the dimensionless distance from the channel bed $y^+ = yu_* / \nu$; $A_k^2 = 0.58\,\mathrm{Re}_\tau - 17$ for $\mathrm{Re}_\tau \geq 650$; $a_k^+ = 0.3\,\mathrm{Re}_\tau - 100$ for $\mathrm{Re}_\tau > 700$; and Re_τ is the friction Reynolds number.

The eddy viscosity

$$\nu_t = \nu y^+ e^{-\frac{y^+ + a_\nu^+}{A_\nu^+}} \text{, } for\ y^+ > 40 \tag{4.37}$$

in which $A_\nu^+ = 0.46\,\mathrm{Re}_\tau - 5.98$; $a_\nu^+ = 0.34\,\mathrm{Re}_\tau - 11.5$.

Figure 4.3 shows the comparison of the Rouse model governed by equation(4.31) and the experimental data presented by Coleman (1970). Figure 4.4 illustrates that Absi et al. (2011) method agreed with the experimental data well on the region of near surface instead of the Rouse method. In this study, the Absi et al. (2011) method is employed in the particle tracking model.

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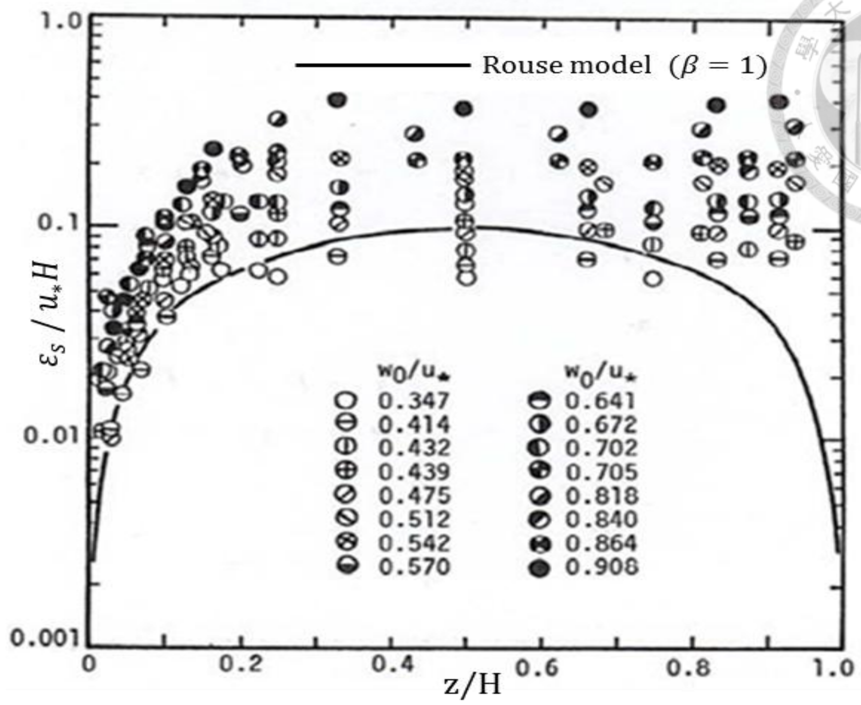

Figure 4.3 Comparison between vertical distribution of suspended sediment diffusion coefficient and experimental data (Tsujimoto, 2010).

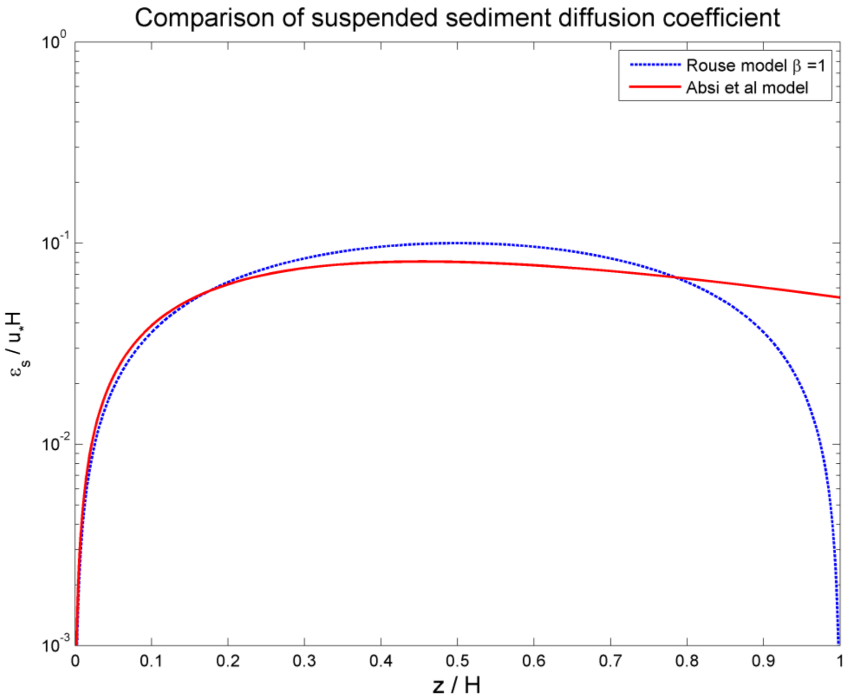

Figure 4.4 Comparison of different sediment suspended diffusion model.

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4.4.4 Re-suspension Mechanism

Sediment transport can be divided into two categories, bed load and suspended load transport. Cheng and Chiew (1998, 1999) proposed the pick-up probability for sediment entrainment to bed load and the probability for threshold a condition of sediment particles remaining in suspension, respectively. Figure 4.5 displays the first proposition considering the motion of individual particles in bed load. The incipient motion of sediment particles is determined by the criteria whether the instantaneous lift force acting on the particle exceeds the submerged weight force of the particle. However, as Bose and Dey (2013) said, “the mechanism of the particle motion from the bed layer to the suspension state is not yet well understood”. The near-bed characteristic of turbulence is a one of the factors that makes the process complicated.

This study focuses primarily on suspended sediment transport. As shown in Figure 4.6, following Cheng and Chew (1999), sediment particles will remain in suspension except if the vertical velocity fluctuations w' exceed the settling velocity w_s of particles. Herein, the thickness of bed load layer is given as two times the particle diameter $2d$, and the theoretical bed level is defined as lower than the top of the bed particles of $0.25d$. Therefore, the lowest center of a sediment particle in suspension (i.e. the top center of sediment particles of bed load layer) can be determined as a distance $2.75d$ above the bed level.

Following Bose and Dey (2013), the fluctuations of vertical velocity can be written as the following PDF,

$$\begin{aligned} &P_{v'}(w' \geq 0) = \frac{1}{16}\left(17 + \hat{w} - \hat{w}^2\right)\exp(-\hat{w}) \\ &P_{v'}(w' < 0) = 0 \end{aligned} \tag{4.38}$$

The derivation of equation(4.38) has been mentioned in the previous section, which is a

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theoretical analysis based on a simple one-sided exponential probability function. Moreover, the threshold of sediment suspension is determined by vertical velocity fluctuations w' and settling velocity w_s. Once $w' > w_s$, the surrounding fluid brings sediment particles into suspension.

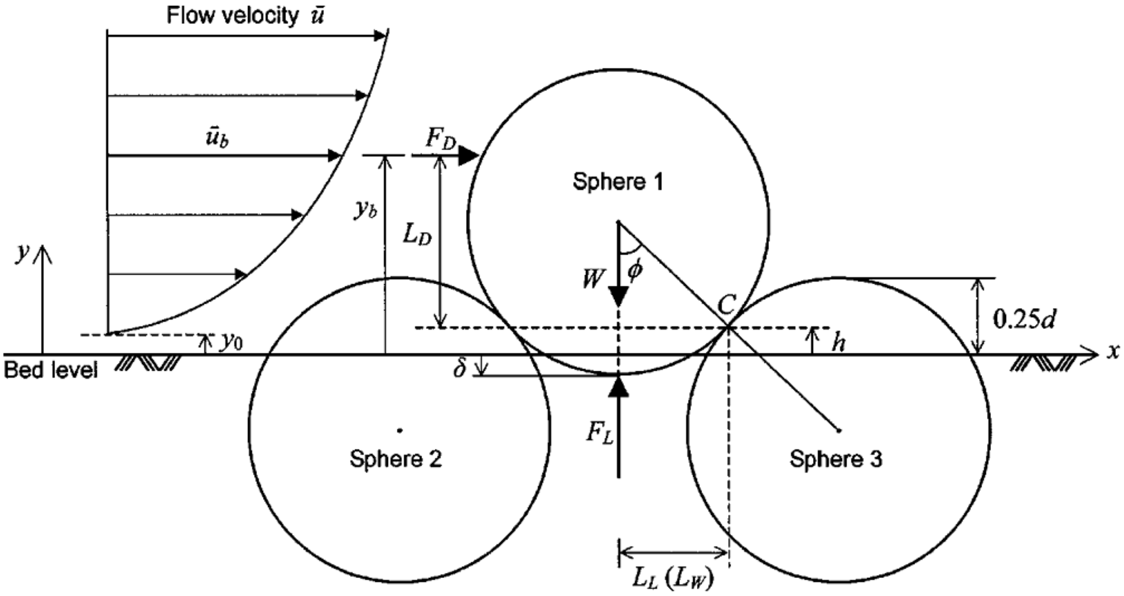

Figure 4.5 The conservation of forces acting on individual sediment particles in bed load (Wu and Chou, 2003).

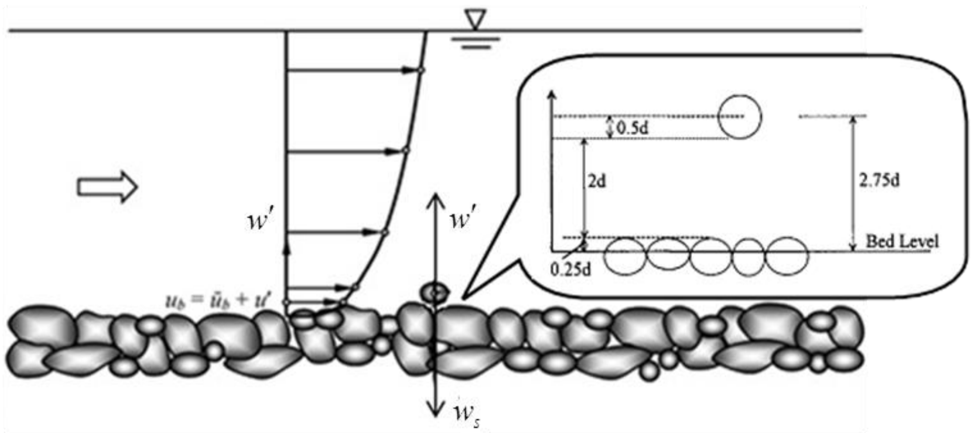

Figure 4.6 The condition for incipient motion of sediment particles is that the upward velocity of turbulent eddies w' exceeds particles' settling velocity w_s (modified from Chen and Chew, 1999 and Bose and Dey, 2013).

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4.5 Simulation Results

This section attempts to distinguish the difference between one-particle PTM and two-particle-PTM by using a simple test. The objective is to observe movement of sediment particles with turbulent diffusion that considers spatial correlation versus that with primarily independent turbulent diffusion. Table 4.1 shows the environmental conditions of this test. In this case study, it is assumed that flow is stationary and isotropic. The gravity effect is neglected. Sediment particles are released from the origin. In this case, the time step is 0.05 and total time is 15s. Equation(4.9) and equation(4.10) are the governing equations of the one-particle PTM and two-particle PTM respectively, and equation(4.39) and equation(4.40) are the discretized equations by using the EM method.

One-particle PTM

$$\begin{cases} X_{n+1} = X_n + \sqrt{2\varepsilon_x}\Delta B_t \\ Y_{n+1} = Y_n + \sqrt{2\varepsilon_y}\Delta B_t \end{cases} \tag{4.39}$$

Two-particle PTM

$$\begin{cases} X^j{}_{n+1} = X^j{}_n + \sqrt{2\varepsilon_x}\left(\sqrt{1-\beta^2}\Delta B_t + \beta\Delta B_t'\right) \\ Y^j{}_{n+1} = Y^j{}_n + \sqrt{2\varepsilon_y}\left(\sqrt{1-\beta^2}\Delta B_t + \beta\Delta B_t'\right) \end{cases} \tag{4.40}$$

where ΔB_t is the independent Gaussian distribution; $\Delta B_t'$ is the dependent Gaussian distribution. X_{n+1} is the particle position in the x-direction at time t_{n+1}. X_n is the particle position in the x-direction at time t_n. Y_{n+1} is the particle position in the y-direction at time t_{n+1}. Y_n is the particle position in the y-direction at time t_n. ε_x and ε_y are the turbulent diffusion coefficient in x and y direction, respectively; j is 1 and 2 distinguishing the number of paired particles in the two-particle PTM. Figure 4.7

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is the averaged correlation of paired particles in the two-particle PTM, which shows that sediment particles correlation decrease very soon. Equation(4.12) is the correlation function of sediment particles. In other words, spatially correlated eddies have a significant effect only in the initial time period. In this case, 2,000 particles are released at the origin 1,000 times. Figure 4.8 shows 1,000 and 500 realizations of the one-particle PTM and two-particle PTM, respectively. However, the spatial correlation of sediment particles cannot be observed explicitly. Thus, to characterize the spatial correlation of sediment particles, the principal axis transformation of paired particles (e.g. particle 1's x-axis versus particle 2's x-axis) as in Figure 4.9 and Figure 4.10 needs to be done. It can be obviously seen that sediment particles have high correlation at 0.1s but the correlation decreases very quickly.

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Environmental condition	*Value*
Diffusivity coefficient(m^2/s)	0.001
Particle specific gravity	1.025
Particle diameter(m)	0.00025

Table 4.1 Environment conditions in simple test and parameters in model

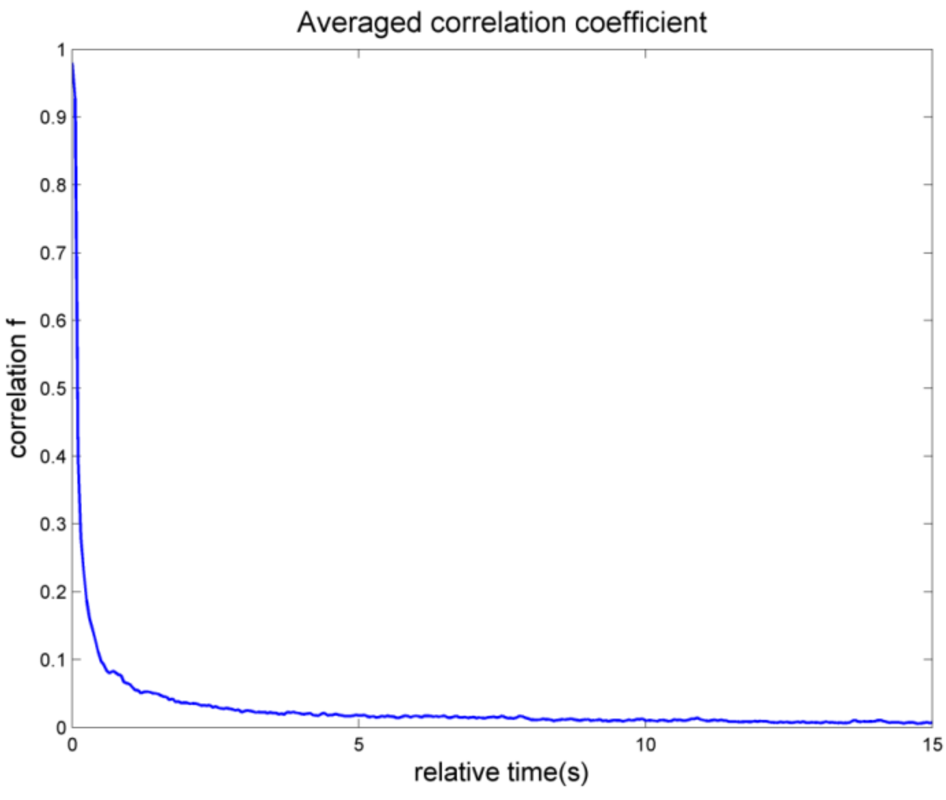

Figure 4.7 The averaged particle correlation versus relative time

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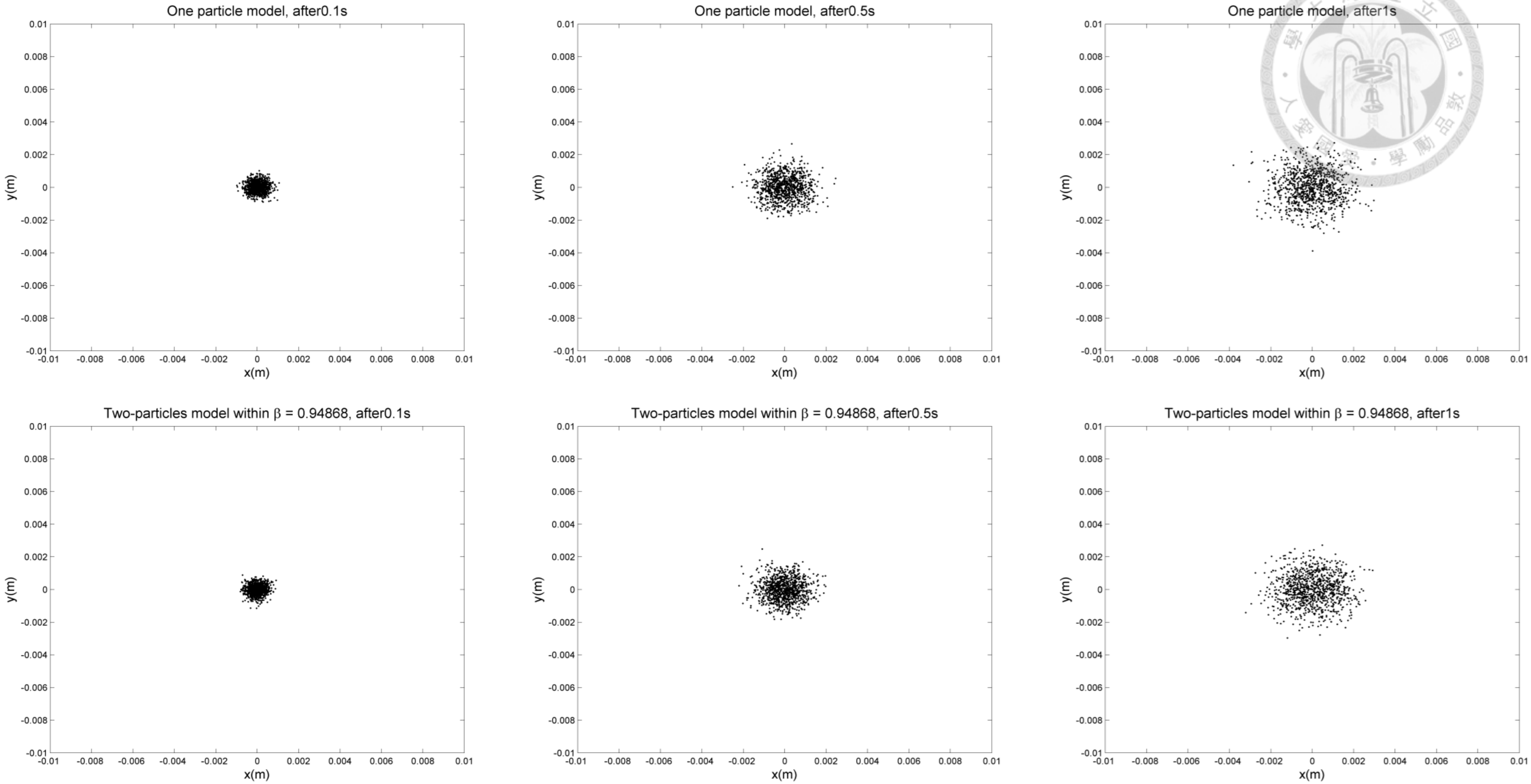

Figure 4.8 Sediment particles released from original by the one-particle PTM and two-particle PTM at time 0.1, 0.5, 1s, respectively

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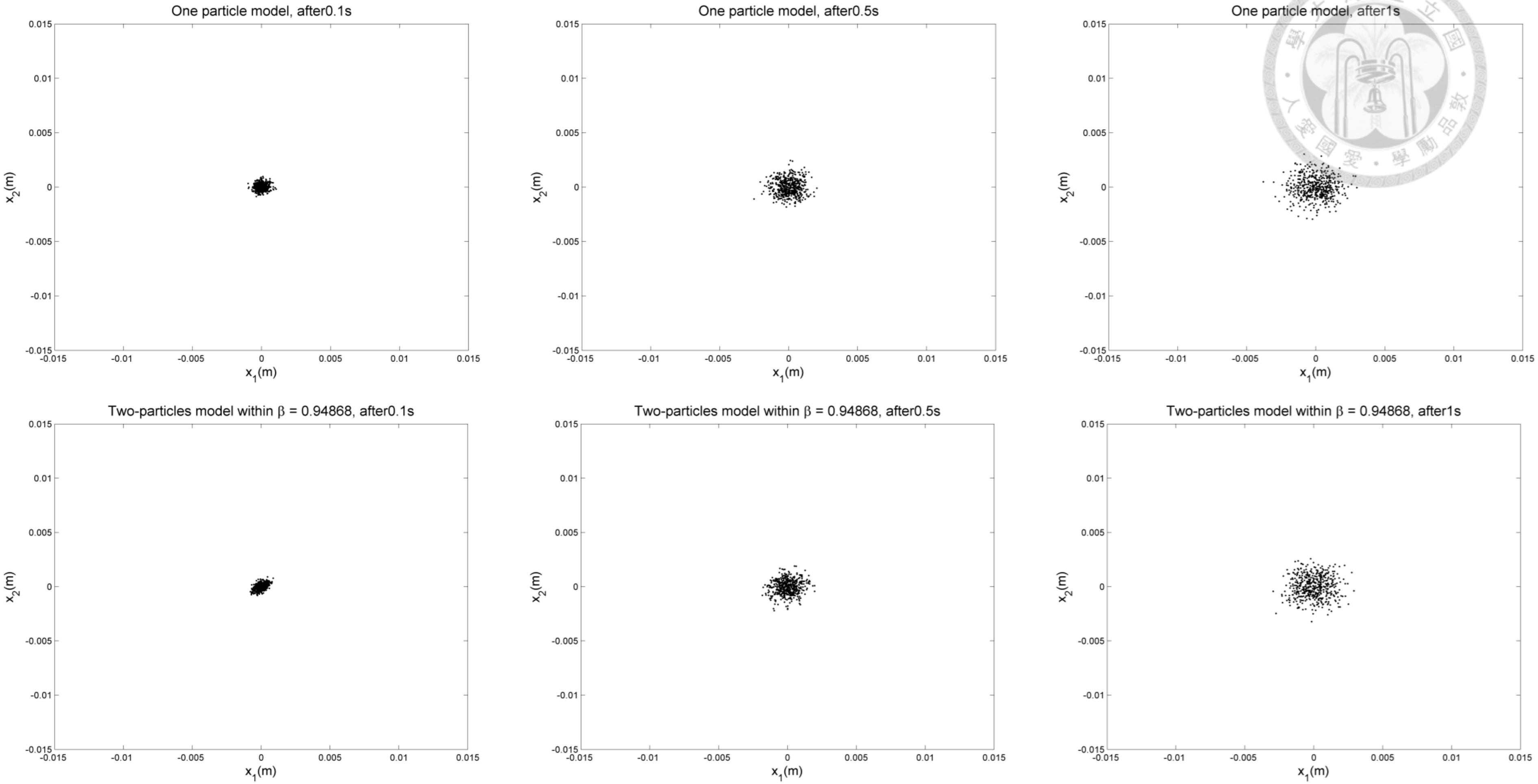

Figure 4.9 The correlation with x direction of different two sediment particles by the one-particle PTM and two-particle PTM

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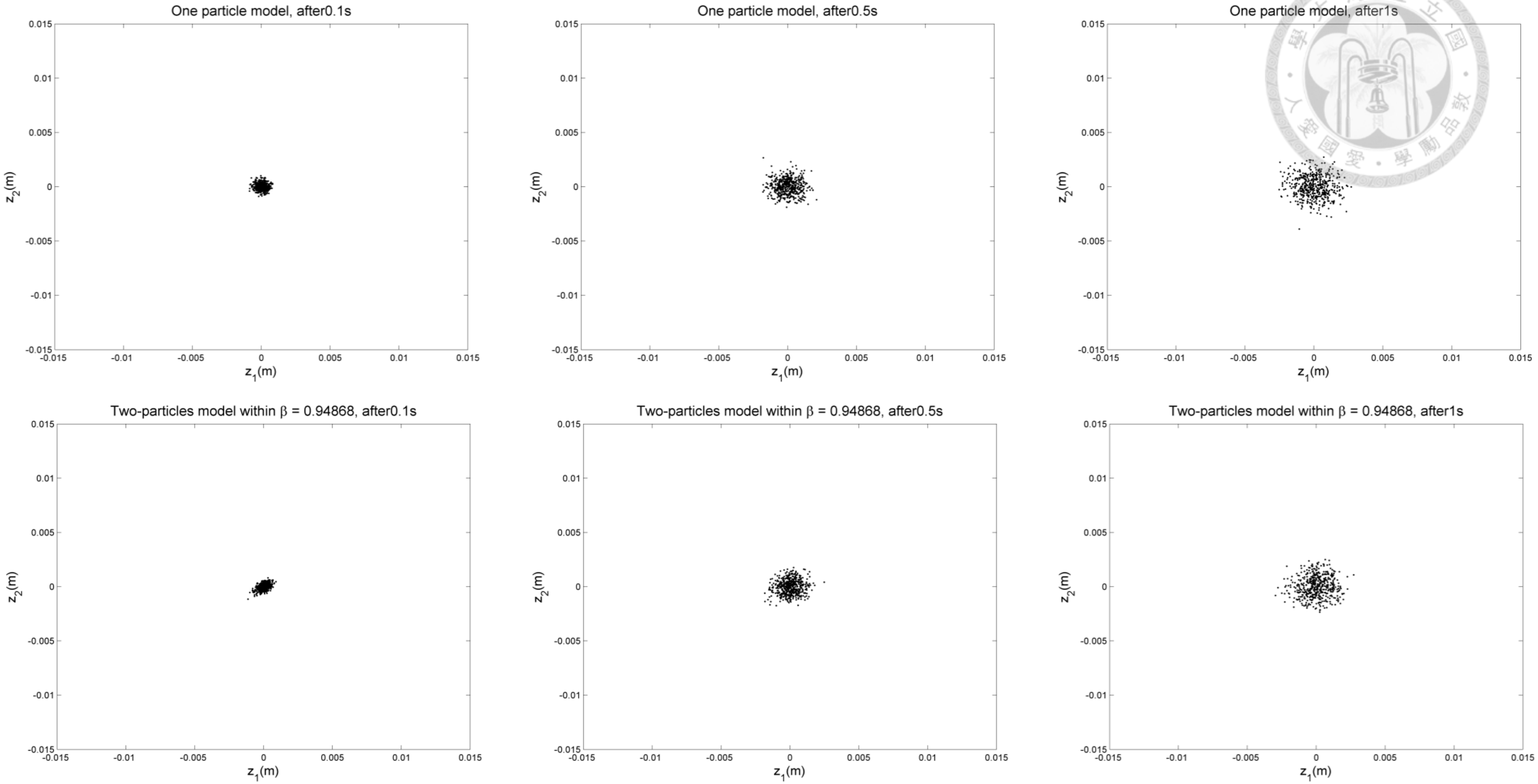

Figure 4.10 The correlation with z direction of different two sediment particles by the one-particle PTM and two-particle PTM

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4.6 Summary and Conclusions

This chapter documents the development of the PTMs. The assumption of dependent Brownian motion in the two-particle PTM is presented before the description about the spatial turbulence correlation. The PTM is derived from the ADE, which is equivalent to the FPE in the Langevin equation. The details of model development are introduced in this chapter. After that, hydraulic parameters are defined for given flow conditions.

First, the vertical diffusion coefficient proposed by Absi et al. (2011), instead of Rouse' diffusion coefficient formula, is employed in the PTMs. This can be attributed to the fact that Absi's method is able to describe the smaller scale turbulent diffusion on the water surface while Rouse's formula is not.

Second, the settling velocity as a function of sediment concentration is used in this model, as sediment particles will be affected by other particles. To illustrate in details, settling particles squeeze surrounding fluid particles and water around sediment particles and subsequently lift them up. This will impede particle's settling process and the settling velocity will decrease.

Last but not least, the mechanism of re-suspension is taken into consideration in this model. Sediment particles near the bed will be brought up by turbulent fluctuations. This model is inherently used to describe the movement of suspended sediment particles. Consequently, the threshold of suspended load, rather than that of bed load, is employed in this study. According to Chen and Chew (1999), suspended particles mostly interchange with bed load.

In addition to the hydraulic parameters, a simple test is introduced in this section to display the difference between the one-particle and two-particle PTM. The apparent

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difference only exists at the beginning in the simulation, which might be caused by the correlation function. The aim of this example is to test the effect of dependent Brownian motion. It is expected that the correlation function decays with time with an infinite boundary in this example. Sediment particles will diffuse and then become independent eventually. Dependent Brownian motion in the two-particle PTM will be applied in the next chapter.

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Chapter 5 Application of The Stochastic Particle Tracking Model

5.1 Introduction

In this chapter, the stochastic particle tracking model is applied. To ensure both the one-particle PTM and two-particle PTM are acceptable models, the first case study presents the model validation with experimental data such as velocity and sediment concentrations. The Markovian property and Fickian law are demonstrated. The PTMs are not only used in turbulence flows. There is an example of laminar flow filed in the next case study. To model a more realistic flow field, the last case study is to simulate the movement of sediment particles by the PTMs under a more complicated flow condition simulated by computational fluid dynamics (CFD). Equation(5.1) and equation(5.2) show the numerical discretization of PTMs using the Euler Maruyama method (EM method),

One-particle PTM
$$\begin{cases} X_{n+1} = X_n + \left(\bar{U} + \dfrac{\partial \varepsilon_x}{\partial x}\right) + \sqrt{2\varepsilon_x}\Delta B_t \\ Z_{n+1} = Z_n + \left(\bar{W} - w_s + \dfrac{\partial \varepsilon_z}{\partial z}\right) + \sqrt{2\varepsilon_z}\Delta B_t \end{cases} \tag{5.1}$$

Two-particle PTM
$$\begin{cases} X_{n+1} = X_n + \left(\bar{U} + \dfrac{\partial \varepsilon_x}{\partial x}\right) + \sqrt{2\varepsilon_x}\left(\sqrt{1-\beta^2}\Delta B_t + \beta \Delta B_t'\right) \\ Z_{n+1} = Z_n + \left(\bar{W} - w_s + \dfrac{\partial \varepsilon_z}{\partial z}\right)\sqrt{2\varepsilon_z}\left(\sqrt{1-\beta^2}\Delta B_t + \beta \Delta B_t'\right) \end{cases} \tag{5.2}$$

where $\bar{U}$ and $\bar{W}$ are mean flow velocities; w_s is particle settling velocity; ΔB_t is

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independent Gaussian distribution; $\Delta B_t'$ is the dependent Gaussian distribution. X_{n+1} is the particle position in the x-direction at time t_{n+1}. X_n is the particle position in the x-direction at time t_n. Z_{n+1} is the particle position in the z-direction at time t_{n+1}. Z_n is the particle position in the z-direction at time t_n. ε_x and ε_z are the turbulent diffusion coefficient in the x, z direction, respectively; j is 1 and 2 for distinguishing the paired particles in two-particle PTM. Argall et al. (2004) suggested that the time step can be roughly constrained by $w_s \Delta t / h < 0.01$ for numerical stability.

5.2 Case study of validating with experimental data

Muste et al. (2009)

Muste et al. (2009) presented the velocity of dilute particle suspensions by means of image velocimetry enabling simultaneous. Two kinds of particles are examined in the experiment, natural sand (NS) and naturally-buoyant sand (NBS). Their specific gravity is 2.65 and 1.025 for natural sand and crushed Nylon (NBS), respectively. In this section, only the NBS is used for validation, as this study primarily focuses on suspended particles (Rouse number < 0.5). Table 5.1 shows the flow and particles characteristic in the NBS flows.

Figure 5.1 presents the mean longitudinal velocity of 2,000 times with normalized depth. It can be seen that the estimated ensemble mean NBS particles velocities agree well with the measured particle velocity. In this case, β is $\sqrt{0.9}$.

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Environmental conditions	*Value*
Flow depth (m)	0.021
Reynolds number	16317
Shear velocity (m/s)	0.041
Karman coefficient	0.405
Particle specific gravity	1.025
Settling velocity (m/s)	0.0006
Particle diameter (m)	0.00023

Table 5.1 The environmental conditions in the NBS flows

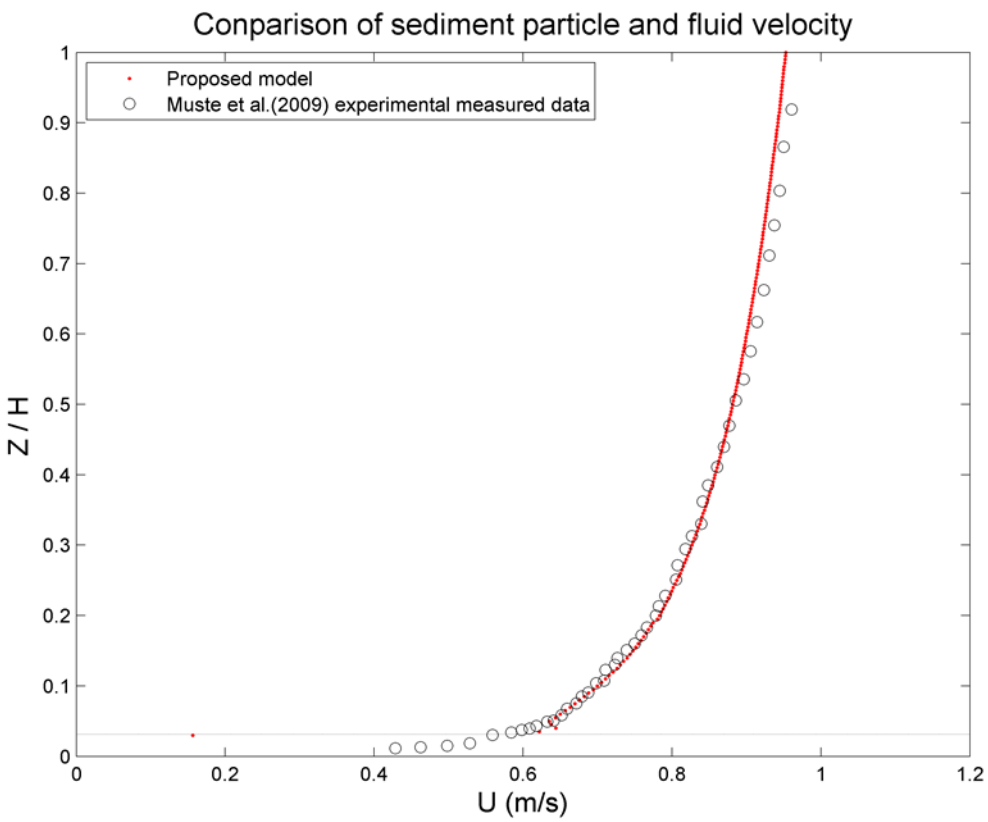

Figure 5.1 Comparison of mean particle velocities with NBS particle

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Coleman (1986)

The sediment particle trajectory is related to sediment concentration. With the position of sediment particles, sediment concentration can be estimated. In this study, the suspended load is not concerned with the effect of bed forms (e.g. no wash bed). This experiment is established under a uniform flow at a constant discharge, depth and energy gradient. The particle diameter in this experiment is 0.105, 0.210, and 0.420mm, respectively. In this section, finer particles are selected for comparison. Results from PTMs are compared with both the Rouse profile and Coleman run C02 data as shown in Table 5.2. Figure 5.2 displays the comparison between the Rouse profile, the one-particle PTM and two-particle PTM. 400 particles are simulated by one-particle PTM based on 500 simulation times, and 200 particles are simulated by two-particle PTM based on 500 simulation times. The PTMs are shown to compare well with the Rouse profile. It should be noted that the reference height is not needed as Rouse profile in PTM. It shows that ensemble mean concentrations of the one-particle PTM and two-particle PTM are similar. The difference between two PTMs lies in the concentration fluctuations such as the ensemble variance of concentrations. As in Table 5.3, the variances of concentration of two-particle PTM are slightly higher than those of one-particle PTM, especially for the region below the middle height. The effect of dependent Brownian and independent Brownian motion might give more uncertainty. In other words, the two-particle PTM with consideration of multiple scaled eddies are more uncertain than the one-particle PTM that considers merely a specific scale of eddies.

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Environmental conditions	*Value*
Flow depth (m)	0.171
Reynolds number	179775
Shear velocity (m/s)	0.041
Mean von Karman coefficient	0.433
Particle specific gravity	2.65
Particle diameter (m)	0.00015
Mean concentration along the depth	0.0305%

Table 5.2 Flow and sediment characteristics in Coleman (1986)

Normalize Depth	*Variance (one-particle)*	*Variance (two-particle)*
0.05	0.68	0.70
0.15	0.43	0.46
0.25	0.27	0.32
0.35	0.22	0.24
0.45	0.19	0.20
0.55	0.16	0.14
0.65	0.11	0.12
0.75	0.09	0.09
0.85	0.07	0.07
0.95	0.06	0.05

Table 5.3 The variance of sediment concentration by one-particle PTM and two-particle PTM

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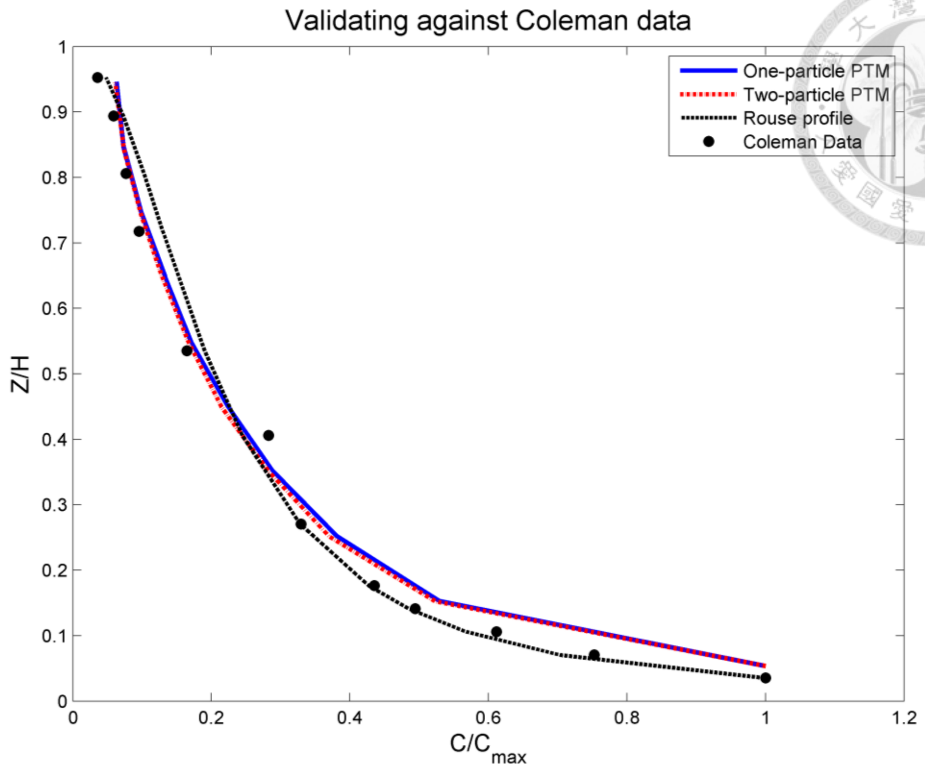

Figure 5.2 Comparison of sediment concentration with Coleman measured data (with diameter 0.105mm)

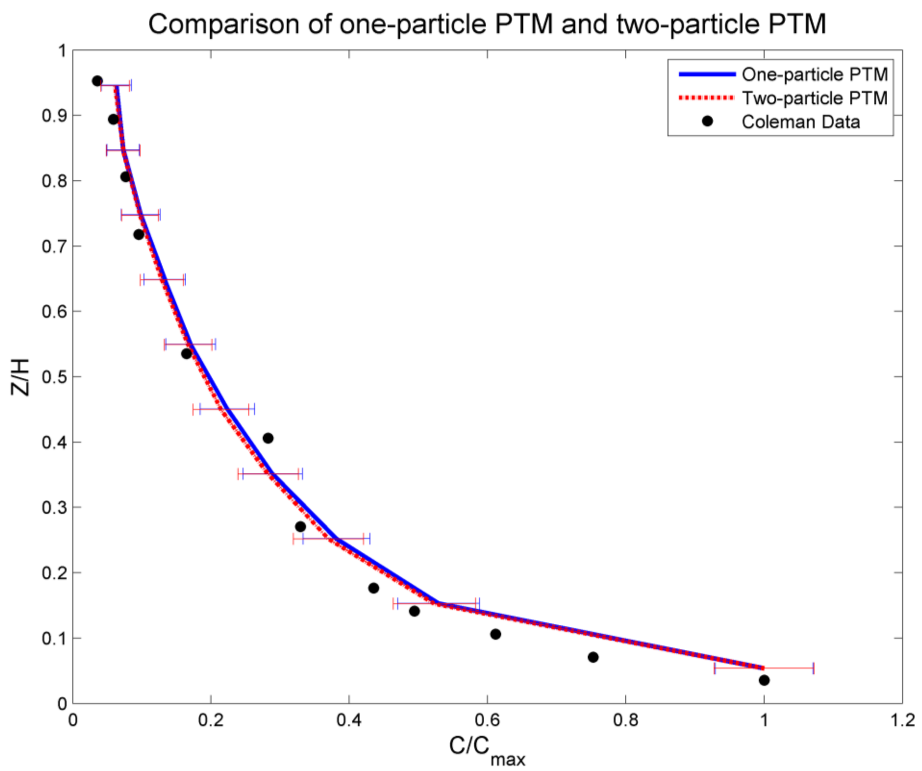

Figure 5.3 Sediment concentrations with on standard deviation by PTMs

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Markovian property

It is hypothesized that movement of sediment particles exhibits the Markovian property. A stochastic process is defined as Markovian as its future state depends primarily on the currently state, not on the previous states. Herein it is proved that the simulation result of concentrations becomes stationary regardless of the initial released location of the sediment particles. Figure 5.4 displays similar results regardless of the initial position of released particles. As such, the particle movement is Markovian. It should be noted that although the initial position is not significant, the particles arrival time to reach a stationary state may be different.

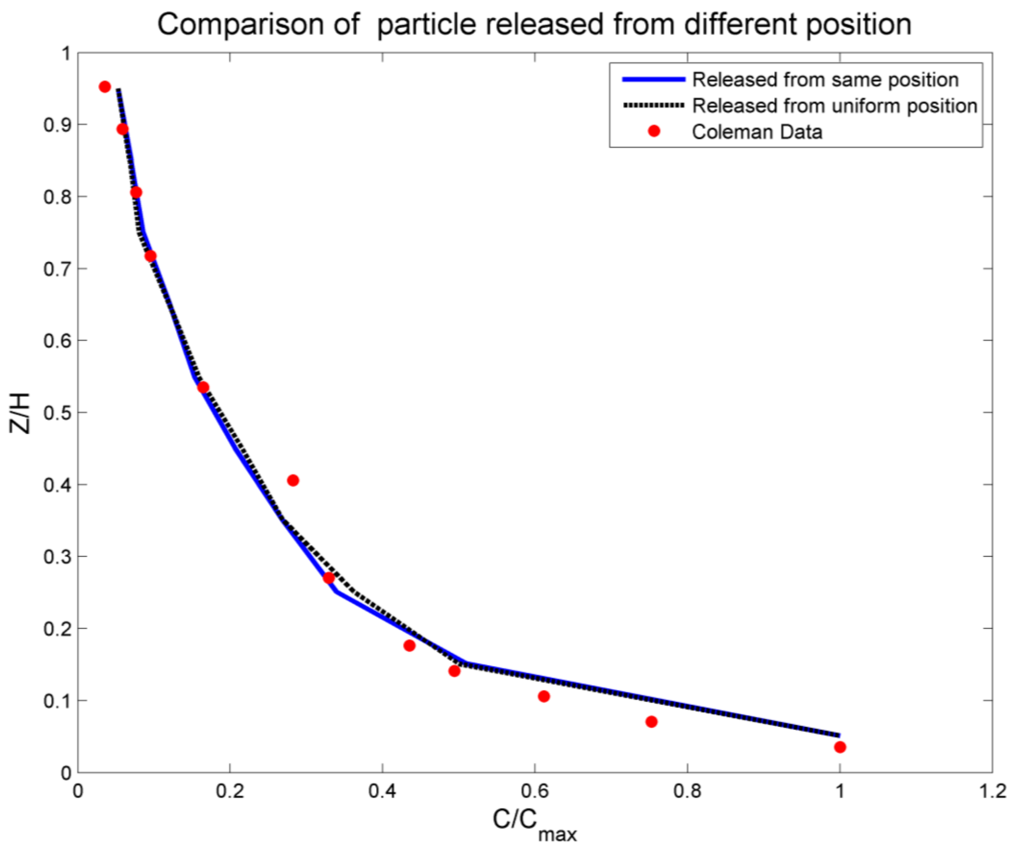

Figure 5.4 Comparison of sediment concentration based on different released locations

Fickian law

After being released for a long time, turbulent eddies are independent of each other

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(i.e. there is no autocorrelation) so that sediment particles diffuse as random process. In our study, turbulent diffusion in analogy to molecular diffusion is based on Fickian law. Particle diffusion can be further classified into subdiffusion, normal diffusion and super-diffusion according to the variance of particle displacement with respect to time based on equation(5.3).

$$\left\langle R^2 \right\rangle \sim t^{\alpha} \tag{5.3}$$

where $\alpha = 1$ leads to normal diffusion, $\alpha < 1$ leads to subdiffusion and $\alpha > 1$ leads to superdiffusion. In this case study, we would like to know whether particle movement is Fickian or not. As shown in Figure 5.5, it can be observed that the variance of particle displacement ($< x^2 + z^2 >$) simulated by the PTMs changes with respect to time. However, the variance of particle distance is not linearly proportional to time. Such particle movement is called anomalous or non-Fickian diffusion. Consequently, sediment particles movement modeled by the PTMs is not the Fickian diffusion. Particles have normal diffusion at the beginning, however, as time increases particles are changed to superdiffusion. The phenomena of re-suspension may lead to anomalous diffusion of particles.

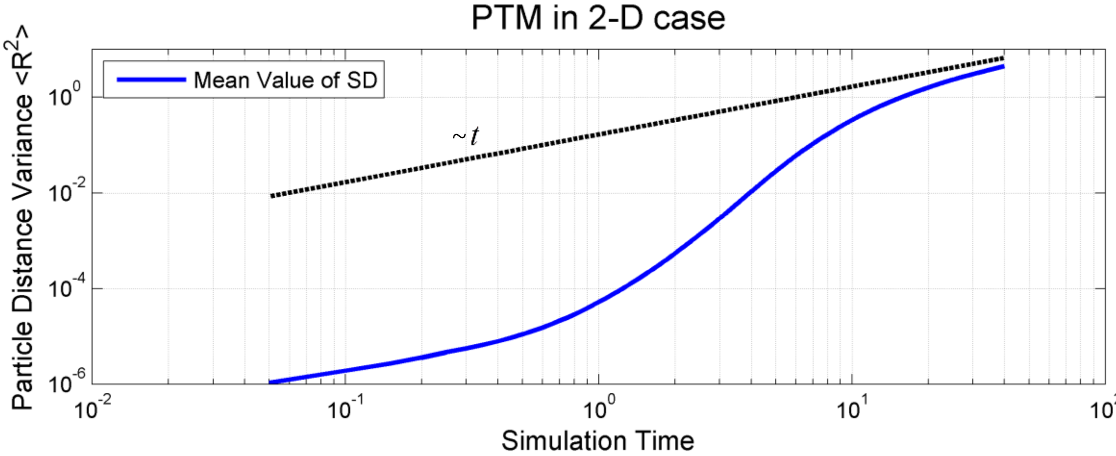

Figure 5.5 The variance of particle distance versus simulation time

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5.3 Case study of particle movement under two-dimensional laminar flow conditions

The aim of this section is to employ the PTM under the laminar flow field. Herein, the particle movement in the lid-driven cavity flow is simulated by PTMs. This flow is the motion of a fluid inside a rectangular cavity flow effect by a constant velocity of one side while the other sides remain at rest. As Figure 5.6, the schematic of cavity is moving with velocity 1 m/s on the upper lid, and the other boundaries remains static because of the no slip condition. The flow is assumed to be incompressible, and the gravity effect is neglected. The governing equation is Navier-Stokes equations which include the continuity equation and momentum equation in x, y direction, as shown below.

Continuity Equation

$$\frac{\partial u}{\partial x}+\frac{\partial v}{\partial y}=0 \tag{5.4}$$

Momentum Equation

$$\begin{cases} u\dfrac{\partial u}{\partial x}+v\dfrac{\partial u}{\partial y}=-\dfrac{1}{\rho}\dfrac{\partial p}{\partial x}+\nu\left(\dfrac{\partial^2 u}{\partial x^2}+\dfrac{\partial^2 u}{\partial y^2}\right) \\ v\dfrac{\partial v}{\partial x}+v\dfrac{\partial v}{\partial y}=-\dfrac{1}{\rho}\dfrac{\partial p}{\partial y}+\nu\left(\dfrac{\partial^2 v}{\partial x^2}+\dfrac{\partial^2 v}{\partial y^2}\right) \end{cases} \tag{5.5}$$

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Table 5.4 presents the conditions in the example. In the initial condition, velocities and averaged pressure are zero. To verify the accuracy of computed flow field, the simulated velocity is compared with Ghia et al. (1982) in the middle of cavity as shown in Figure 5.7. This example aims to simulate particle trajectory and shows that the effect of advection is more significant than diffusion. Since there is no turbulent diffusion but the molecular diffusion in the laminar flow (i.e. there is no difference between the one-particle PTM and two-particle PTM), sediment particles follow the fluid motion almost exactly because of the insignificant degree of molecular diffusion. To model particle trajectory, the PTM as equation(5.1) is utilized based on 2,000 simulations. In particular, the turbulent diffusivity is replaced with molecular diffusivity which can be determined by the Stokes-Einstein equation.

$$D_s = \frac{KT}{6\pi\mu r} \tag{5.6}$$

where K is Boltzmann constant, $1.381 \times 10^{-23} J/K$; T is absolute temperature; μ is kinematic viscosity; and r is radius of a sediment particle.

Environmental conditions	*Value*
Reynolds number	100
Particle diameter (m)	0.00023
Dynamic viscosity (m^2/s)	0.01
Fluid density (kg/m^3)	1
Temperature (^oC)	27

Table 5.4 The environmental conditions under laminar flow

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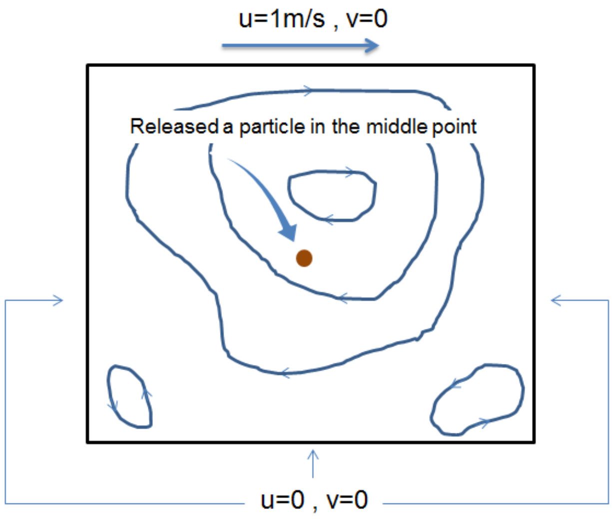

Figure 5.6 The initial conditions of cavity problem

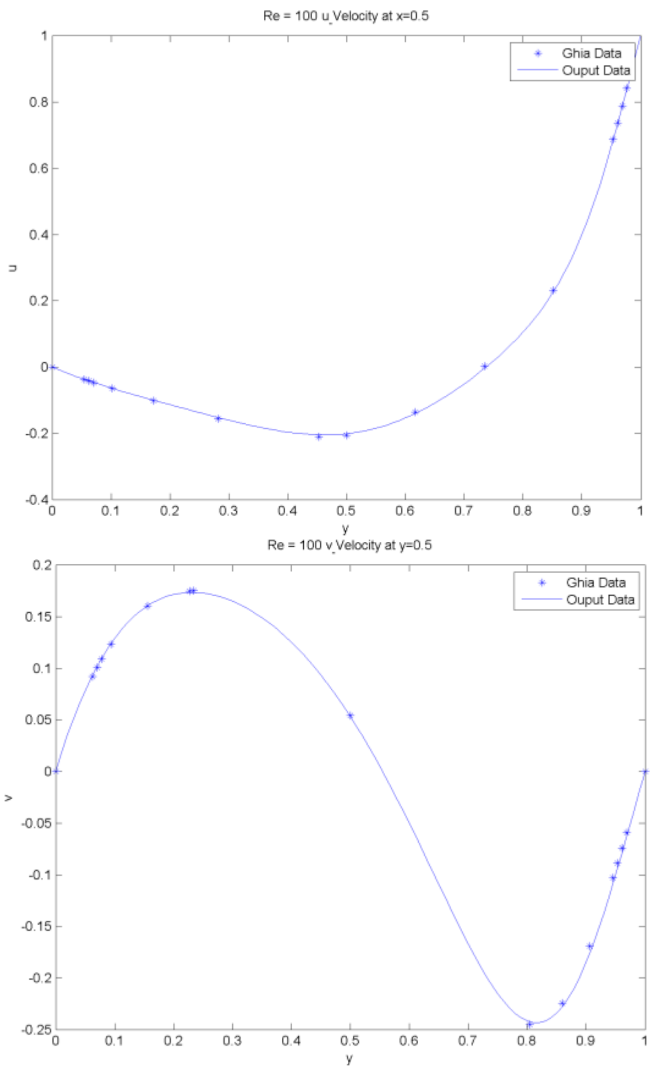

Figure 5.7 Validating flow field to Ghia et al. (1982) data

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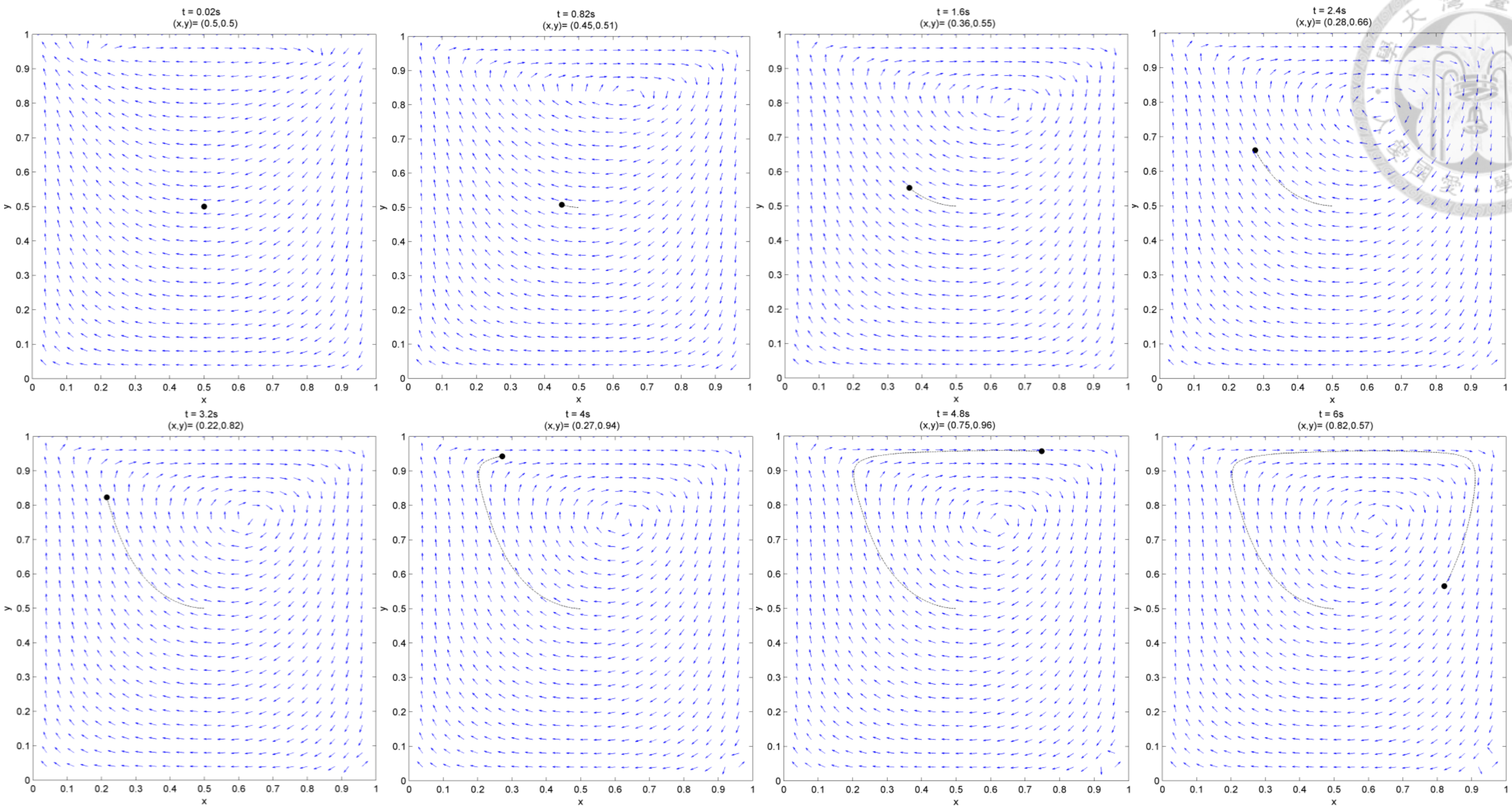

Figure 5.8 One of realizations of sediment particle released from original at time 0.02, 0.82, 1.6, 2.4, 3.2, 4, 4.8, 6s, respectively

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5.4 Case study of particle movement under fully developed uniform channel flow

In this section, particle movement under fully developed turbulent flow condition is simulated. Detailed channel flow field with large eddy simulation (LES) was provided by Chou (in press). In order to model the turbulent flow, there are two main issues. Firstly, the governing equation is a nonlinear equation. And secondly, it is difficult to simulate multiple scaled eddies due to numerical constraints. The basic concept of LES is that simulating the large scale turbulence with numerical analysis directly but modeling the effect of small scale turbulence on large scale turbulence by a sub-grid scale model such as the Smagorinsky model. In other words, the LES simulates turbulence by dividing turbulence into large scale and small scale eddies by means of low-pass filtering. Figure 5.9 presents the data of mean flow velocity, turbulent kinematic energy and turbulent viscosity via LES. With these data, the sediment diffusion coefficient with the Schmidt number proposed by Adsi et al. (2011) can be quantified.

Table 5.5 presents the CFD simulated flow conditions and sediment particle properties. The Rouse number is 0.465 and thus the particle is considered to be suspended particle. Based on equation(4.34) by Absi et al. (2011) via the proposed Schmidt number, the sediment diffusivity can be determined as Figure 5.10, as the TKE and turbulent viscosity are supplied. As in Figure 5.10, unlike the Rouse diffusion formula, it can be observed that sediment particles have diffusion near the water surface based on Absi et al. (2011). In this case study, 1,000 particles are presented and released at the top of surface. Figure 5.11 is the ensemble mean trajectory of sediment particles based on 5,000 simulations. As Figure 5.12, ensemble mean of longitudinal and vertical

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velocity with respect to time is presented. It can be observed that the ensemble mean position of the particles in the vertical direction is very near the bed at the end of time.

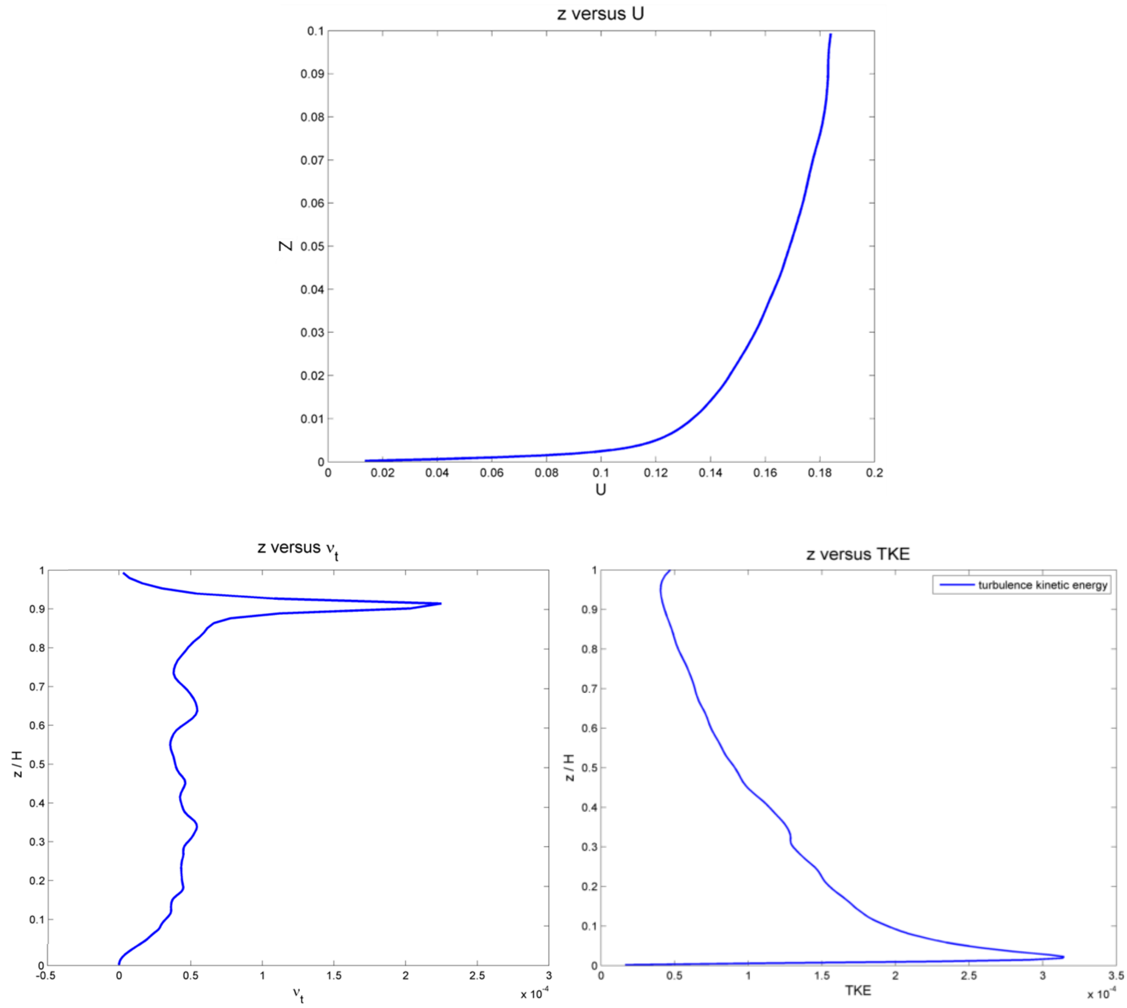

Figure 5.9 The flow conditions of mean velocity (m/s), turbulent viscosity (m^2/s) and TKE (turbulent kinetic energy (m^2/s^2))

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Environmental conditions	*Value*
Flow depth (m)	0.1
Friction Reynolds number	820
Reynolds number	16110
Karman coefficient	0.41
Shear velocity (m/s)	0.0082
Particle specific gravity	1.025
Particle diameter (m)	0.00023
particle volume concentration	0.046%

Table 5.5 The CFD and sediment environmental conditions

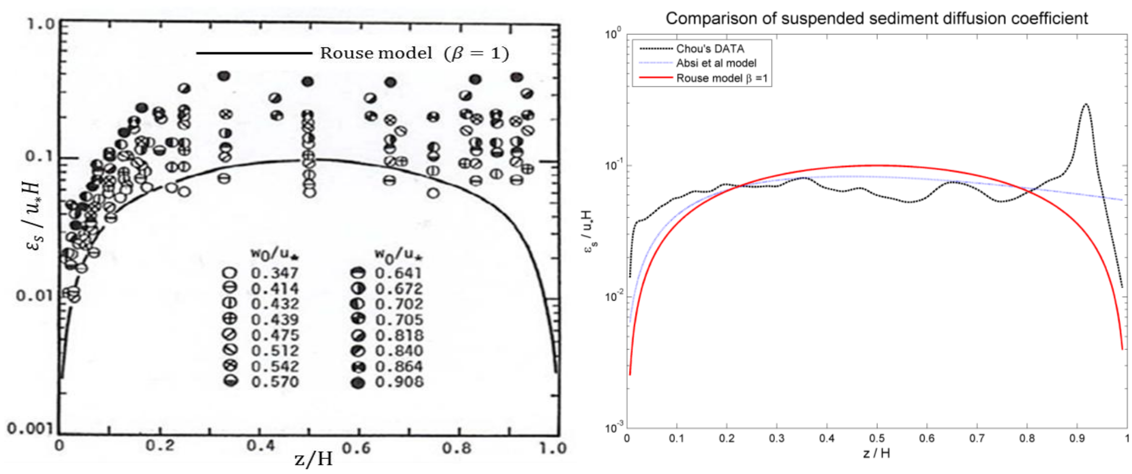

Figure 5.10 Comparison of Rouse model, Absi et al.(2011) model and the computed turbulent diffusivity

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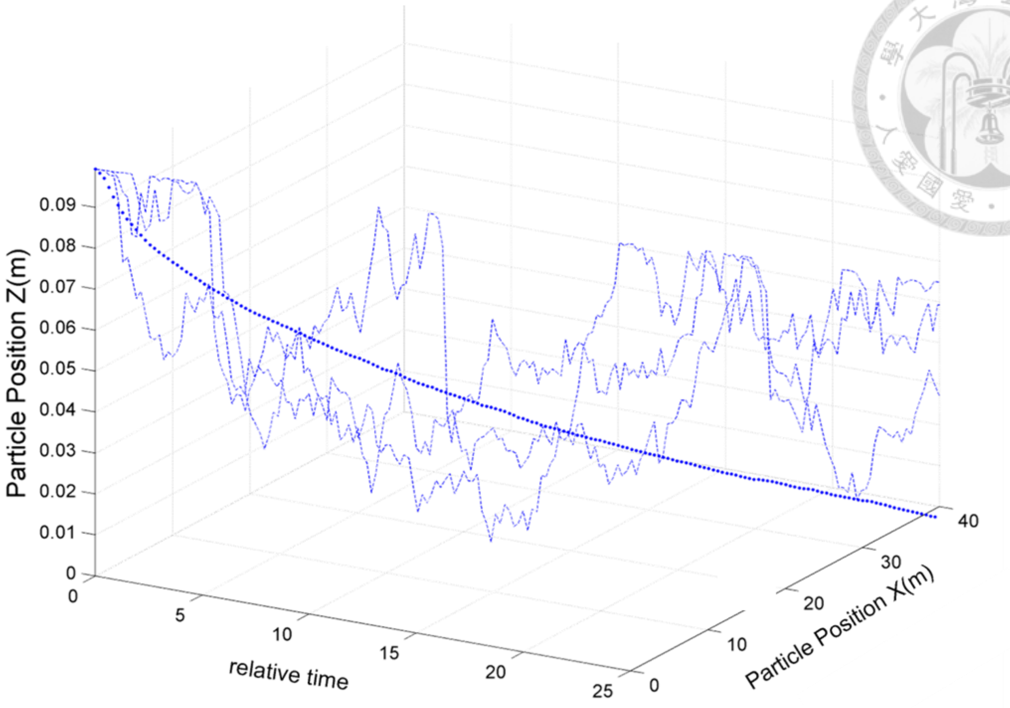

Figure 5.11 Ensemble mean of sediment particle trajectories (bold dot line) in 2-D flow

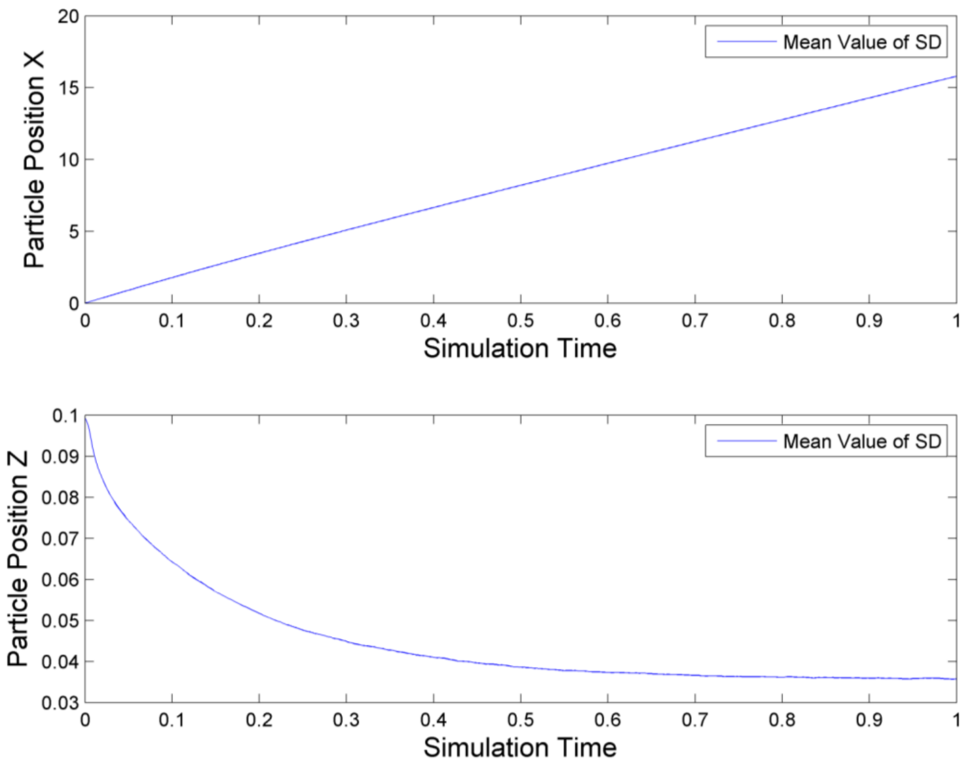

Figure 5.12 Ensemble mean of sediment particles position in x, z-direction versus simulation time

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Particle entrainment is subject to flow intensity and the mean flow velocity is shown in Figure 5.9. Based on the re-suspension criteria equation(4.38), whether a particle will be entrained or not is determined by the turbulent perturbations. Apparently, the fluctuating velocity in the vertical direction is not strong enough to bring the sediment up. In Figure 5.13, the ensemble variance of particle position in the longitudinal direction is increasing with respect to time; the behavior of diffusion may cause this phenomenon. By the trajectory of sediment particles, the sediment concentration can be estimated. In this case, to examine the sediment concentration along the vertical direction, the water depth is divided into 10 segments. The sediment concentration can be regarded as the number of sediment particles in the grid. Figure 5.14 shows the sediment concentration profile and concentration fluctuations in this case study. The uncertainty of sediment particles movement may cause concentration fluctuations. In Figure 5.15, it shows one of the realizations of sediment clouds. As we can see, sediment particles may re-suspend owing to turbulent eddies.

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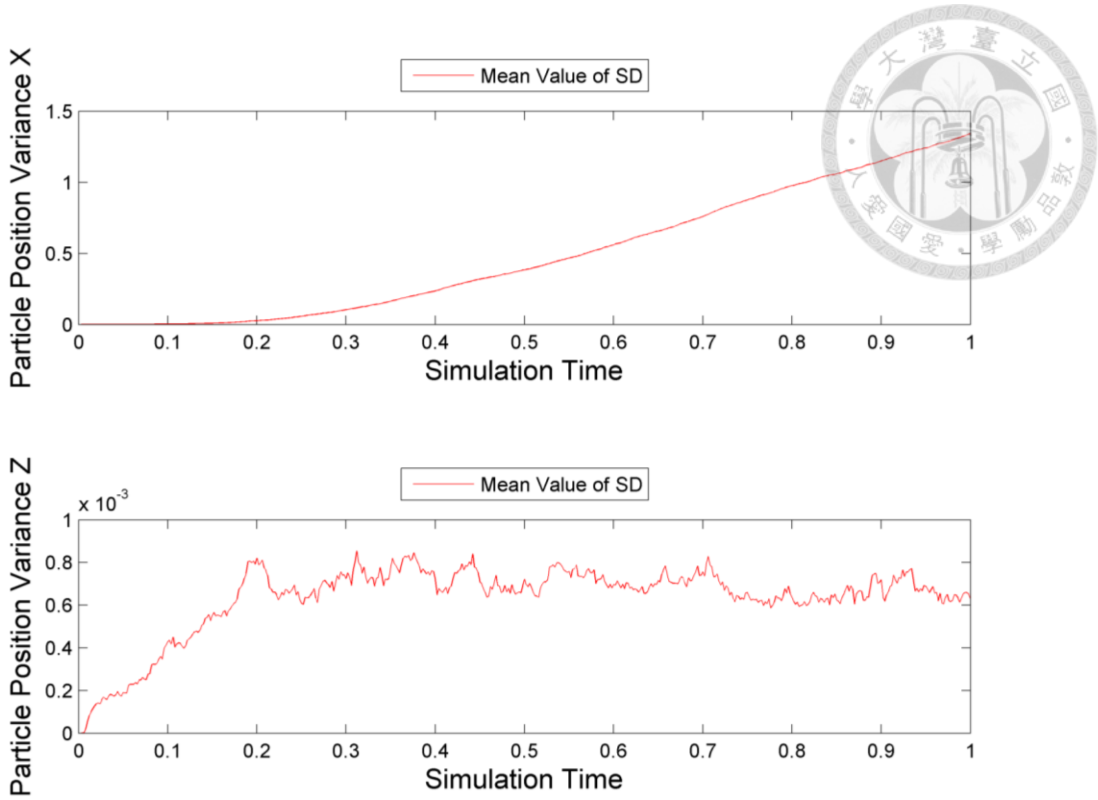

Figure 5.13 Ensemble variance of sediment particles position in x, z-direction versus simulation time

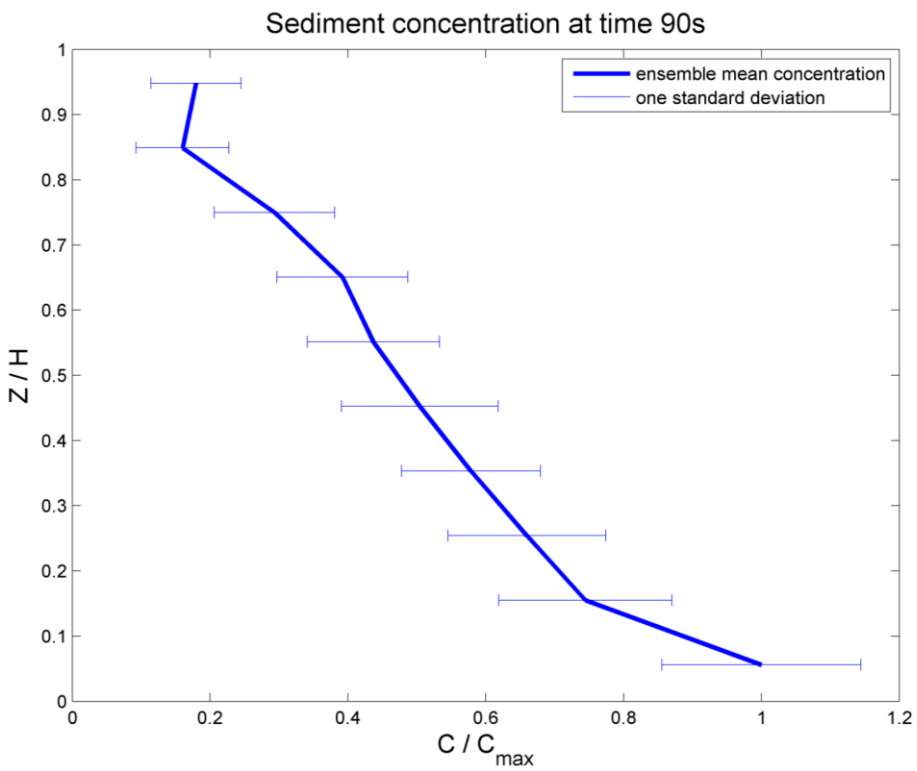

Figure 5.14 Ensemble sediment concentration

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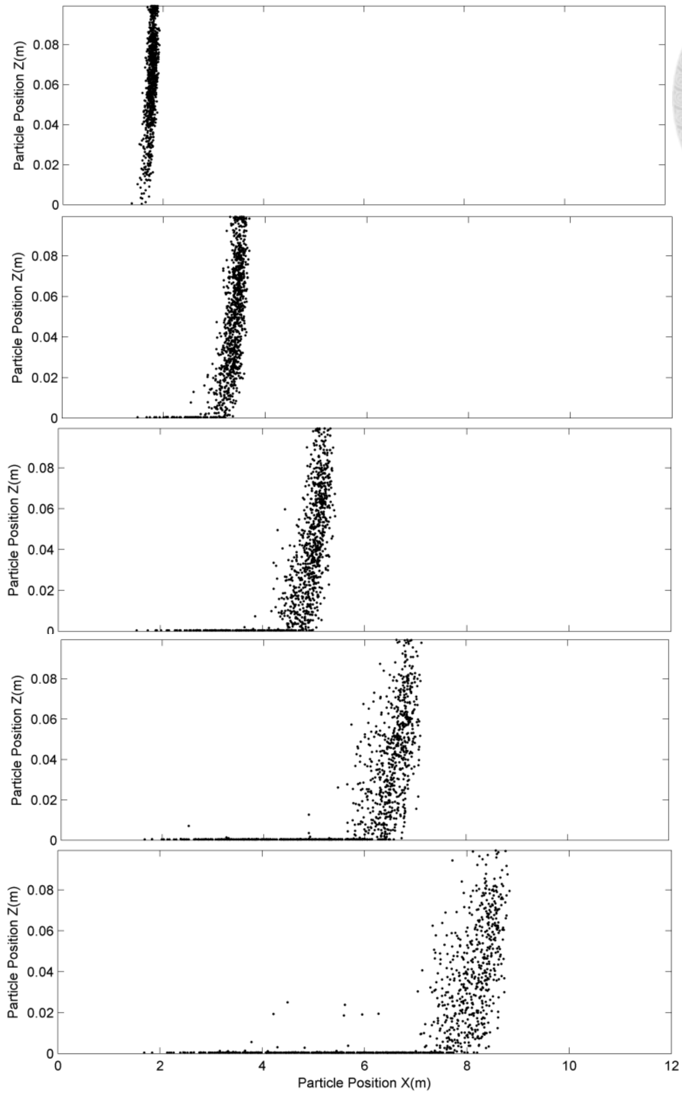

Figure 5.15 Sediment particle cloud in this channel flow

5.5 Summary and Conclusions

This chapter presents simulation results of particle trajectories under three different flow conditions. The first case study is to examine results from the PTMs' against the experimental data. In the first case study, the sediment particles' ensemble means of velocities and concentrations are validated against the suspended sediment particles. The PTMs are suggested to employ suspended particles because the ADE is the prototype of the PTMs. Thus, the PTMs are usually used to describe suspended

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particles.

The Markovian property of the PTMs is validated in the first case study. In this hypothesis, the initial position of particles is not significant, but may be affected by the arrival time of sediment particles. The other hypothesis is that particle movement is demonstrated to be Fickian, which is referred to when the variance of particle displacement is linearly proportional to time. However, the variance of particles displacement and time are not a linear proportion as the result. Re-suspended sediment particles may cause particle movement to be anomalous diffusion. In this case study, particles diffuse in superdiffusion as a result of re-suspension. Turbulent flow exhibits multiple scales, particles may be brought by any scales of turbulences. This behavior is called Levy flight (Shlesinger et al., 1987).

Besides, there is a comparison of the two-particle and one-particle PTMs under Coleman experimental conditions. First, it can be seen that the difference between these two models lies in concentration fluctuations, as described in the ensemble variance of concentrations. One of the reasons may be attributed to large eddies. Multiple scaled eddies exist in turbulent flows; as such, sediment particles may be in the influence region of large eddies. Hence, sediment particles would have similar random motion behaviors. To describe the impact of large eddies, parameter β is introduced to the two-particle PTM in equation(4.10). According to Spivakovskaya and Heemink (2006), the parameter β lies in the region between 0 and 1. Herein, the parameter β is assumed to be a constant.

In addition to validate against experimental data, the purpose of the first case study is to demonstrate the diverse concentration fluctuations. In the two-particle PTM, which takes the space correlation of the turbulence into account, the variance of sediment concentrations is higher than that of one-particle PTM. This may be resulted from the

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concern about spatial correlations of the turbulence which variegates the trajectories of sediment particles. Moreover, the closer to the bed, the higher the variation of sediment particle trajectories. This phenomenon is on account of the mechanism of re-suspension and gravity forces. Gravity forces lead particles to settling at the bed while the re-suspension mechanism affects particle motions near the bed; therefore, the trajectories near the bed are uncertain.

In the second case study under laminar flow conditions, the molecular diffusion instead of the turbulent diffusion plays a significant role. Main flow dominates the motions of particles; namely, a sediment particle almost follows flow direction in the laminar flow with a minor diffusion effect.

Our last case study is to simulate particle movement in turbulent flows. Sediment transport becomes more unpredictable due to the complex behavior of turbulence. In this thesis, forces exerted on sediment particle movement can be categorized into deterministic forces and stochastic force (e.g. turbulent fluctuations). This is described as the well-known Langevin equation. By means of Dr. Chou's turbulent flow data, we can simulate the movement of sediment particles and sediment concentrations using PTMs.

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Chapter 6 Summary and Recommendations

6.1 Summary and Conclusions

Transport of sediment particles has been of environmental significance recently especially for suspended sediment. Water quality is one of the significant issues for sediment transport, as it is related to sediment concentrations. There are many approaches available to estimate sediment concentrations such as the advection-diffusion equation or empirical formulas. In this thesis, a state-of-the-art method, the SD-PTM, is employed. This research focuses on the characteristics of individual sediment particles such as the settling velocity and spatially correlated turbulent effect instead of assemblage of sediment particles. Random movement of sediment particles caused by turbulence is considered as well. In chapter 3, some basic stochastic theories are introduced. With the assumption of Random Walk, turbulent diffusion is analogous to molecular diffusion. In mathematics, the Wiener process that describes the stochastic characteristics of Brownian motion is defined. Development of PTMs is detailed in chapter 4. The Markovian property and the Fickian law are also presented in chapter 5. The hypotheses proposed in chapter 1 is verified using the SD-PTMs. Critical hydraulic parameters are defined in chapter 4, and example simulations are presented. In our models, we do not employ the diffusion formula proposed by Rouse, as turbulent diffusivity on the water surface is not exactly zero in reality. Rather, the formula suggested by Absi et al. (2011) is applied here. To examine the model, the proposed PTMs are also validated against experimental data such as data of Muste et al. (2009) and Coleman (1986) for particle velocity and sediment concentrations, respectively. After validation, the PTMs are applied to various flow conditions such as cavity problem and fully developed uniform turbulent channel flows.

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6.2 Recommendations for Future Research

In order to address particle random movement attributed to spatial turbulent correlation in turbulent flows, the two-particle PTM is employed. However, the parameter β is not easy to be determined. The parameter β might need an experimental investigation or CFD validation. Moreover, for the suspended particles, the lag time between sediment particles and fluid particles caused by the drag force may exist. As to the mechanism of re-suspension, if we can consider the bed load motion, a better criterion of re-suspension should be obtained. More effort to refine the PTMs for sediment transport in open channel flows is desirable.

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APPENDIX

NOTATION

The following symbols are used in this study:

Chapter 3

$c(x,t)$ = concentration

D = diffusion coefficient

$f(X_t,t)$ = the function of drift term

$g(X_t,t)$ = the function of diffusion term

$\dot{W}_t$ = Gaussian White noise process

E[ ] = expected value

X_n, $X(\tau)$ = random variable

$\mathcal{N}(0,1)$ = standard normal distribution with a zero mean and a unit standard deviation

λ = mean drift term

μ = diffusion coefficient

Chapter 4

c = concentration changing with time and space

$\overline{U}$, $\overline{V}$, $\overline{W}$ = the direction of x, y and z mean flow velocities, respectively

w_s = particle settling velocity

ε_x, ε_y, ε_z = the sediment diffusion coefficient in x, y and z direction

$A(x,t)$ = the deterministic forces

$B(x,t)$ = the random forces

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dB_t / dt = Gaussian White noise

dB_t = the Wiener process

$f\left(x,t|x_0,t_0\right)$ = the conditional probability density function for x at time t, from the initial position x_0 at time t_0

β = the diffusion effect which can be chosen between 0 to 1;

B = the standard Brownian motion as same as single particle model

B' = a correlated Brownian motion independent of B

$\sqrt{1-\beta^2}B(t)$ = the diffusion due to molecular diffusion and small scale turbulence

$\beta B'(t)$ = the diffusion due to large scale turbulence

$f(r)$ = a correlated coefficient related to distance between particles

I_2 = identity matrix

$\overline{u}$ = mean velocity

u' = velocity fluctuations caused by turbulent eddies

κ = von Karman constant

l = Prandtl's mixing length

ν = kinematic viscosity

δ_s = the high of laminar sublayer

k_s = roughnees high

w_{s_0} = the settling velocity of sediment particle at zero concentration

w_s = the settling velocity of sediment particle at concentration S_v

k = the coefficient of experimental investigation, Cai (1956) gives a value 0.75 for k by considering the force conservation

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D_{gr} = the effective sediment particle diameter which is defined as $d\left(\frac{g(S-1)}{\nu^2}\right)^{\frac{1}{3}}$

d = sediment particle diameter

g = gravity acceleration

S = specific gravity

ε_m = the momentum exchange coefficient

ε_z = the diffusion coefficient

$\sqrt{\overline{w'^2}}$ = turbulent intensity

β_d = the proportion of the sediment diffusion coefficient to the momentum diffusion coefficient

Sc_t = Schmidt number

ν_t = eddy viscosity or the diffusivity of momentum

St = Stokes number

τ_p = the particle timescale

τ_t = the integral turbulence timescale or large eddy's turnover time

ρ_f and ρ_s = the density of fluid and solid, respectively

α_0 = a coefficient for two-equation ($k-\varepsilon$ model) which is defined as α / C_μ

Chapter 5

$\bar{U}$ and $\bar{W}$ = mean flow velocities in longitudinal and vertical direction

w_s = particle settling velocity

ΔB_t = independent Gaussian distribution

$\Delta B_t'$ = the dependent Gaussian distribution

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X_{n+1} = the particle position in the x-direction at time t_{n+1}

X_n = the particle position in the x-direction at time t_n

Z_{n+1} = the particle position in the z-direction at time t_{n+1}

Z_n = the particle position in the z-direction at time t_n

ε_x and ε_z = the turbulent diffusion coefficient in the x, z direction, respectively

j = 1, 2 for distinguishing the paired particles in two-particle PTM

h = water depth

$\langle R^2 \rangle$ = the variance of particle displacement

K = Boltzmann constant, $1.381 \times 10^{-23} J/K$

T = absolute temperature

μ = kinematic viscosity

r = radius of a sediment particle

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