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LAGRANGIAN NUMERICAL MODELLING OF SUSPENSION AND SALTATION IN THE ATMOSPHERIC BOUNDARY LAYER

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ABSTRACT

This paper introduces a numerical model for two- and three-dimensional numerical simulation of sand drift within the atmospheric boundary layer. The model is based on the Lagrangian, Particle Tracking, model where the flow field is predicted by solving the Navier-Stokes equations for transient, incompressible, viscous flow in a general curvilinear coordinate system.

The two-equation k-ε turbulence model is solved for prediction of the turbulence kinetic energy and its dissipation. Particle trajectories are predicted by solving the equation of motion for each particle with different initial and physical conditions. Due to the statistical description of the turbulence fluctuation and aerodynamics entrainment; identical particles, tracked with the same initial conditions are transported through different trajectories.

The numerical simulation is focused on the threshold condition at which a particle can entrain from rest by wind and the interaction with flow recirculation zones generated around obstacles or buildings located in the flow field. The model is also used to predict the location around an obstacle at which particle deposition may occur.

NOMENCLATURE

ρ Fluid density.
ρ_p Particle density.
D_p Particle diameter.
U_i Instantaneous velocity.
u' Fluctuation velocity.
$\bar{u}$ Mean velocity.
U_{Rel} Fluid-Particle relative velocity.
g Acceleration due to gravity.
C_D Drag coefficient.
Re_p Particle relative Reynolds number.
μ Kinematic viscosity
ϕ Dependent variable.
Γ_ϕ Diffusion coefficient of ϕ.
S_ϕ Source term of ϕ.

INTRODUCTION

Two-phase turbulent dispersed flows are encountered in a wide range of engineering and environmental applications, which are as varied as the dispersion of passive pollutant particles in the atmosphere to combustion systems with dispersing fuel particles. These applications can be categorized into two main categories, natural and technological systems. Natural systems include environmental particulate pollution problems and problems associated with both the atmosphere and hydrosphere. Typical examples of environmental applications are the flow of dust or sand particles and their deposition and re-suspension behaviour. There are a number of two-phase flow systems related to technological applications, such as bubbly flows in pipes, interior particle exhaust pollutant control problems, problems related to fluid spray, the chemical systems involving particle reactants and many others.

Basically, two fundamentally different theoretical approaches are utilised to predict two-phase flows. The Lagrangian, or tracking, approach is that in which individual particles are treated as discrete entities in a flow field and their trajectories are calculated. In the other approach, the so-called Eulerian, or continuum, approach where a cloud of particles is regarded as a continuum, and the appropriate governing equations in the differential form are solved for each phase. The advantages and disadvantages of each of these approaches have been identified by many authors [1-4].

The Eulerian model presented in Alhajraf [5,6] has been successfully employed to simulate the drifting particles, such as sand, snow or dust, around obstacles of different shapes in both two- and three-dimensional domains.

The Lagrangian approach has the advantage of being able to track individual particles in diluted flows, starting from an initial particle sizes, velocity, location and temperature, as they are driven by the continuous fluid phase.

Wind-blown sand is considered to be one form of a multi-phase flow system. In this work a Lagrangian approach based model is presented to simulate the trajectories of sand particles under the action of the wind. This paper discusses the theoretical background of the particle equation of motion followed by the flow field governing equations.

Two trajectory models are employed, the *Deterministic Dispersion Model* (DDM) and the *Stochastic Separated Flow Model* (SSF) to predict individual particle trajectories. These models are implemented and analysed against individual and groups of sand particles that are moved both in suspension and saltation modes over a flat surface. The behaviour of these particles has been investigated as they approach a solid wall perpendicular to the flow direction.

PARTICLE EQUATION OF MOTION

The Lagrangian approach considers individual particles, which are tracked as they are driven by the flow of the continuous phase. The particle trajectory can be determined by solving its equation of motion, which can be deduced from Newton's Second Law. The particle equation of motion was first derived by Basset, Boussinesq and Oseen, and is commonly known as the B-B-O equation, Shirolkar [4]:

$$m\frac{d\bar{U}_p}{dt}=\sum F \qquad (1)$$

where the right hand side consist of the summation of all forces exerted on the particle along its trajectory. These summed forces are conventionally separated into the effects of drag, body forces, lift force, pressure, Basset force, virtual mass force and other forces (e.g. particle-particle collision, Saffman force and wall interactions):

$$m\frac{d\bar{U}_p}{dt}=F_D+F_g+F_L+F_{pressure}+F_B+F_V+F_{ohters} \qquad (2)$$

Separation of the total sum of forces given by the above equation is not always valid, as there can be non-linear interactions between the various forces. Such interactions are not well understood but are typically small enough to be neglected for many flow applications. Moreover, under normal atmospheric conditions and due to the large difference between air and sand particles densities ($\rho << \rho_p$), Equation (2) can be simplified to include only drag and gravity terms, [1,3,8,9]:

$$\frac{d\bar{U}_p}{dt}=\frac{U_i-U_p}{\tau_p}+g \qquad (3)$$

where $U_i=\bar{U}+u'$ is the instantaneous air velocity, and τ_p is the particle relaxation time:

$$\tau_p=\frac{4\,\rho_p\,D_p^2}{3\,\mu\,C_D\,\mathrm{Re}_p} \qquad (4)$$

The drag coefficient C_D depends on the relative Reynolds number between the air and particle phases:

$$C_D=\frac{24}{\mathrm{Re}_p}\,(1+0.15\,\mathrm{Re}_p^{0.687}) \qquad (5)$$

where:

$$\mathrm{Re}_p=\frac{\rho\,|U_{rel}|\,D_p}{\mu} \qquad (6)$$

The particle trajectory is then computed by integrating Equation (3) with respect to time:

$$\frac{dX_p}{dt}=U_p \qquad (7)$$

The fluctuating component of the instantaneous velocity u' is calculated based on the turbulence kinetic energy k by assuming that the turbulent flow is homogenous and isotropic.

FLOW FIELD SIMULATION

The governing equations for the continuous flow field (air) are derived from time-averaged dependent variables under the framework of Eulerian coordinates. The turbulent shear stresses are modelled using the eddy viscosity assumption based on the well-known two-equation turbulence model, kinetic energy equation k and its dissipation rate ε. For unsteady, incompressible and viscose flow, the conservation equations can be expressed in a general form as.

$$\underbrace{\frac{\partial(\rho\phi_i)}{\partial t}}_{\text{Rate of change in }\phi}+\underbrace{\frac{\partial}{\partial x_j}(\rho u_j\,\phi_i)}_{\text{Convection term}}=\underbrace{\frac{\partial}{\partial x_j}\left[\Gamma_\phi\frac{\partial\phi_i}{\partial x_j}\right]}_{\text{Diffusion term}}+\underbrace{S_\phi}_{\text{Source term}}$$

where ϕ represents the dependent variables that are required to be expressed such as u, v, w, k and ε. Thus, following the different expression of ϕ, it is possible to form continuity, momentum and turbulence model equations by substituting the variable ϕ, the diffusion coefficient Γ_ϕ and the source term S_ϕ. Detailed expressions for each dependent variable are presented in Table 1.

The above equations are discretised and solved using the finite volume method based CFD code SOFIE, [10,11].

LAGRANGIAN PARTICLE TRACKING MODELS

Equations (3), (4) and (7), are most commonly used in Lagrangian models to track individual particle trajectories. The solution of Equation (4), accounting for the effect of fluid velocity fluctuation due to the turbulent eddies, requires the full time history of turbulent flow. Such information requires solution of the instantaneous governing equations, the Navier-Stokes equations, in an Eulerian reference frame. Thus, different techniques that involve random sampling of the fluctuating velocity components have been developed, [1,2,4,8,2]. Two conventional particle tracking models are employed to simulate the particle trajectories based on how the instantaneous flow velocity is calculated.

Table 1: Formulation of the general transport equation variables

Equation	ϕ	Γ_ϕ	S_ϕ
Continuity	1	0	0
x-Momentum	U	Γ_u	$-\frac{\partial P}{\partial x}+S_u$
y-Momentum	V	Γ_v	$-\frac{\partial P}{\partial y}+S_v$
z-Momentum	W	Γ_w	$-\frac{\partial P}{\partial z}+S_w$
Kinetic energy	k	μ_T / σ_k	$\tau_{ij}\frac{\partial U_i}{\partial X_j}-\varepsilon$
Kinetic energy dissipation	ε	$\mu_T / \sigma_\varepsilon$	$C_{1,\varepsilon}\frac{\varepsilon}{k}\left(\tau_{ij}\frac{\partial U_i}{\partial X_j}\right)-C_{2,\varepsilon}\rho\frac{\varepsilon}{k}$

Deterministic Dispersion Model (DDM)

The DDM is the simplest way of solving the particle equation of motion since the effect of the fluctuating velocity components on the fluid velocity is not included. Particle suspension relies on velocity fluctuations; therefore, this model is only useful when studying saltating particles. Once the mean flow velocity is calculated for the continuous phase, the particle equation of motion can be directly solved for particle velocity and location. Since only the particle convective velocity, u_p^c, is included, particles with the same initial conditions and physical properties will follow identical trajectories.

The turbulent dispersion effect could be included by estimating the dispersive component of the particle velocity, which can be obtained from the gradient diffusion approximation [4] such that:

$$u_p = u_p^c + u_p^d \tag{9}$$

where

$$u_p^d = -\Gamma_p \frac{1}{\bar{n}_p}\frac{\partial \bar{n}_p}{\partial x} \tag{10}$$

is the dispersive component of the particle velocity, $\bar{n}_p$ is the particle density number, $\Gamma_p = \mu_p^t / \sigma_p^t$ is the particle diffusivity and μ_p^t and σ_p^t are the turbulent particle viscosity and turbulent particle Schmidt number respectively. The turbulent particle viscosity is related to the fluid turbulent viscosity by the following expression:

$$\mu_p^t = \frac{\mu_t}{1+\tau_p / \tau_{fL}} \tag{11}$$

where τ_p is the particle relaxation time, and τ_{fL} is the Lagrangian fluid timescale, which will be discussed in the following section.

Stochastic Separated Flow Model (SSF)

This model involves the instantaneous fluid velocity instead of the mean velocity used in DDM. The key problem in this model is to determine:

1. The fluctuating component of the fluid velocity along the particle trajectory.
2. The integration time step over which the fluid properties can be assumed to be locally constant.

The particle is assumed to interact with a series of turbulent eddies as it moves along the flow field. Thus, turbulence information is required to evaluate the velocity fluctuation components, eddy lifetime and eddy length scale. Eddy lifetime and length scale can be estimated from the local turbulent kinetic energy k and the rate of kinetic energy dissipation ε along the particle trajectory.

Different assumptions are made in order to simplify the nature of the turbulent particle dispersion. Some frequently used assumptions are as follows:

1. Assuming that the statistical properties of the turbulent quantities are independent of space, the turbulent flow can be referred to as homogenous.
2. The turbulence is called isotropic if its statistical features show no preference for any direction.

Therefore, based on these assumptions, the turbulent kinetic energy contained in an eddy is given by

$$k = \frac{1}{2}\left(u'^2 + v'^2 + w'^2\right) = \frac{3}{2}u'^2 \tag{12}$$

Since the fluid velocity fluctuation component is assumed to be the same in all directions, the standard deviation is given by:

$$\sigma = \sqrt{\frac{2k}{3}} \tag{13}$$

Assuming that the local turbulent properties are constant over each time step, each turbulence eddy is characterised by a constant velocity fluctuation, timescale (eddy lifetime) and length scale (eddy size).

The velocity fluctuation used in each eddy is determined by random sampling over a Gaussian Probability Density Function (PDF), which has a mean of zero and unity variance, and is given by:

$$u' = \xi\sqrt{\frac{2k}{3}} \tag{14}$$

where ξ is the Gaussian random variable.

Thus, for each time step u' is randomly sampled and its corresponding PDF assumed to be a Gaussian form. For an isotropic assumption, the variance of the fluctuating velocity can be estimated from the local turbulent kinetic energy;

therefore, the mathematical expression for the PDF of the fluctuating velocity in isotropic flows is given by:

$$P(u') = \frac{1}{\sqrt{2\pi}\sqrt{\frac{2k}{3}}} e^{\left[-\frac{3u'^2}{4k}\right]} \quad (15)$$

Under the non-isotropic flow assumption, for each coordinate direction, independent fluctuating velocities are randomly sampled using the above PDF expression at every time step.

The local turbulence properties determine whether or not a given particle remains in an eddy. The particle may stay in an eddy for the whole eddy lifetime and then follow the turbulence properties of another eddy, or it may have enough momentum to cross the eddy boundaries to become involved with another eddy. This is commonly known as the *Crossing Trajectory Effect*. In order to account for the crossing trajectory effect, the time interaction between the particle and an eddy should be determined properly. Thus, it should be the minimum of either the eddy lifetime or the time required for the particle to cross the eddy, which is known as the residence time.

Both eddy and residence timescales are dependent on the eddy length scale. Thus many authors have used different expressions to determine the eddy time and length scales whilst using the same expression for the residence timescale [4]. The expression generally applied to the residence time scale, also known as the eddy transit time, is

$$\tau_r = -\tau_p \ln\left(1 - \frac{l_e}{\tau_p \left|\vec{U} - \vec{U}_p\right|}\right) \quad (16)$$

where:

$$l_e = \frac{C_\mu^{3/4} k^{3/2}}{\varepsilon} \quad (17)$$

Therefore, the particle is assumed to interact with an eddy as long as both the integration time step and the relative distance of interaction satisfy the following criteria:

$$\Delta t = Min[\tau_{fL}, \tau_r] \quad (18)$$

and

$$\left|\Delta \vec{X}\right| \le l_e \quad (19)$$

where the fluid-particle relative velocity during the eddy-particle interaction time is approximated by its value at the beginning of the interaction. It is important to note that the expression of the residence timescale has no solution when $l_e > \tau_p \left|\vec{U} - \vec{U}_p\right|$, and in this case, the particle is assumed to be trapped by the eddy, and the interaction time will be the eddy lifetime.

Knowledge of the particle-eddy interaction time and the randomly sampled fluctuating velocity allow Equations (3) and (7) to be solved for the particle's new position and velocity. At each new position, a new fluctuating velocity is sampled from a new PDF generated on the basis of the new local turbulent properties. Thus, the movement of the particle can be tracked throughout the flow domain until the full particle trajectory is finished.

This is the basis of the SSF model, which is based on the eddy lifetime concept. Unlike the DDM, particles with the same physical properties and initial conditions will not have identical trajectories. Rather, these will change as a result of the local fluctuating velocity component in the SSF model.

PARTICLE THRESHOLD CONDITION

When the wind strength increases, the aerodynamic forces applied on the particle surface will approach the particle's body forces but act in the opposite direction. The result of these forces is the sum of many forces that may have a significant effect on the movement of the particle, as shown in equation (2). A particle threshold value is the value at which the particle resisting force is equal to the forces applied by the flow field on it [13]. For a loose, dry and spherical particle, the threshold velocity was related by Bagnold and lately modified by others, to the particle size and density:

$$U^* = A\left(\frac{\rho_p\, g\, D_p}{\rho}\right)^{1/2} \quad (20)$$

where A is the dimensionless threshold velocity. According to Bagnold [13], A equals 0.11 for quartz particles with 0.25 mm in diameter and density of $2000\, kg/m^3$. Under these conditions, the particle threshold velocity is 0.22 m/s at which a distinction between deposition and erosion can be classified.

In the present work, surface erosion is simulated by spreading uniformly sized particles over a surface. The particles are then injected from rest into the flow field, with initial vertical and horizontal velocities, when the surface shear velocity reaches a value greater than the particle threshold velocity. Then Lagrangian calculations of the particle trajectory will start and continue until either the particle leaves the computational domain or is captured by a flow zone in which the flow shear velocity dropped to a value below threshold velocity.

RESULTS AND DISCUSION

Lagrangian models, DDM and SSF, were implemented to simulate trajectories of sand particles over a flat sand surface and around a solid wall perpendicular to the flow direction. Details of there implementation can be found in Alhajraf [5].

Two case studies were covered in this section. The aim was to examine the Lagrangian models against flow fields comprising of a mixture of air and sand particles. First, different modes of particle movement such as suspension and saltation were considered for flow passing over a flat bed covered by loose, spherical shaped particles.

Then, a solid wall was placed perpendicular to the flow direction to emphasis the effect of the recirculation eddies generated around the wall on the particle trajectories.

The two dimensional flow field domain was specified as a flat surface of 100 m long and 5 m high. The computational domain consisted of 100 x 50 grid points in the axial and vertical directions respectively. The grid distribution in the axial direction was uniform with resolution of 1.0 m and in the vertical direction it was non-uniform with higher resolution close to the surface. This arrangement ensures sufficient resolution in the flow boundary layer near the surface.

The inlet velocity was set according to the atmospheric log-law profile with a friction velocity of 0.374 m/s and a surface roughness of 1.0e-4 m. The surface was divided into erodible and non-erodible patches. Particles were patched over a 5 m long erodible section starting at 5 m downstream from the domain inlet boundary (Figure 1), where the flow field became fully developed. A maximum of 10,000 particles was enabled to be entrained from the patch surface into the flow field whenever the threshold conditions were satisfied. It was assumed that when a particle hit the bed surface, it rebounded into the flow field until it left the computational domain or was captured by an eddy. Rebound velocity is controlled by a coefficient of restitution, particles will stick on the surface when the coefficient of restitution is set to zero, and rebound with the same vertical and horizontal velocities when its value equals 1.0.

In the first case, a single particle was set to inject under given conditions in which the horizontal friction velocity attached to the erodible surface exceeded the particle threshold velocity. Figure 2 shows the trajectories of a particle of a 0.25 mm diameter injected vertically at lift-off velocities of 1.0, 1.5 and 2.0 m/s respectively with coefficient of restitution set to zero. The span of the trajectory increased with the increase in the lift-off velocity, while all trajectories followed a path of a similar shape.

For a constant lift-off velocity of 0.5 m/s, the trajectories of particles with different diameters are shown in Figure 3, which shows that smaller particles have a longer trajectory span than larger particles.

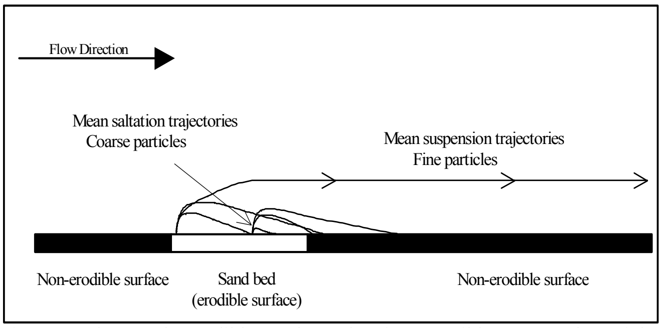

Figure1: The patch erodible surface showing possible types of particle movements.

Five identical particles were injected using the same initial conditions and different numerical models DDM, and SSF, as shown in Figure 4. As mentioned above, DDM leads to identical particle trajectories for particles with the same physical and initial conditions. As shown in Figure 4a, all five particles followed the same path and appeared as a single trajectory. In SSF, Figure 4b shows that when the effect of the flow field fluctuating velocity is involved, the particle trajectories were not identical even for the same physical and initial conditions.

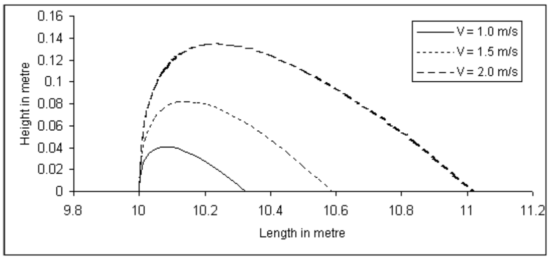

Figure 2: Single particle injected vertically into the flow field with a different initial vertical velocity.

Due to the turbulent eddies, the particles may or may not follow the mean flow field. If the particle response time is greater than the eddy lifetime, then the particle will move with no turbulence effects on it, as shown in Figure 4b for the SSF model using a 0.1 mm particle diameter.

Figure 5 shows particle trajectories for particles with different sizes. Using the DDM model, small particles were suspended in the flow and move for a long distance before striking the surface. Heavier particles saltated (bounced) on the surface with a definite saltation trajectory span. When the turbulent effect was involved in the trajectory calculation using the SSF model, the saltated particle followed the turbulent eddy whenever the eddy lifetime exceeded the particle's response time, and it responded to the force of gravity if the eddy lifetime became lower than its response time.

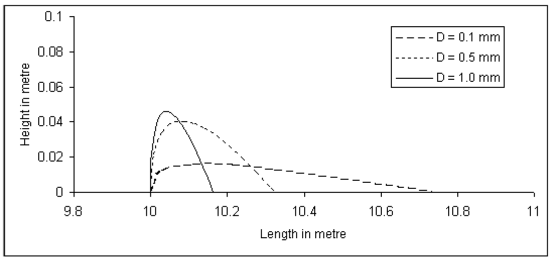

Figure 3: Single particle injected vertically into the flow field with a different initial diameter.

Figure 6 shows a comparison between the saltation trajectories using the SSF model when turbulent eddies have influenced the particle trajectory. The figure shows the randomness of the trajectories of a sample of 100 particles injected from identical initial conditions using two different particle sizes. Figure 6a shows that the trajectories of smaller particle were affected by the turbulent eddies, and moved in non-smooth saltation trajectories. For the heavier particles (Figure 6b), the saltation trajectories were clearly defined, showing no influence of turbulence on the particle trajectory.

Ten thousand particles were patched on the erodible surface defined in the flat surface (Figure 7). When the particle threshold condition is satisfied, the flow will start to entrain particles from the surface. Particles start with some lift-off velocity and then move with the flow field according to the forces applied on the individual particle. A high particle concentration is found near the surface, which illustrates how the majority of particles move close to the surface in saltation mode, with only a few of them being suspended in the flow for some longer time and distance.

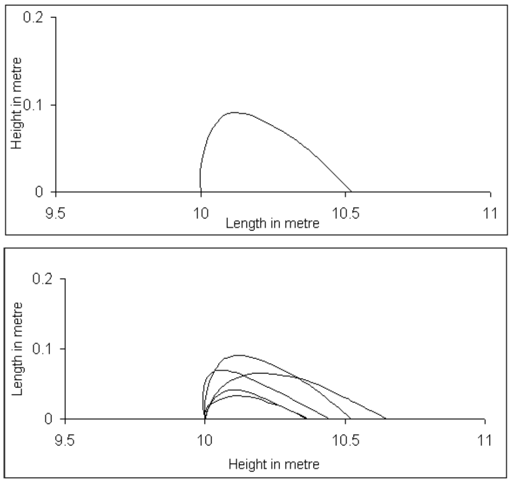

Figure 4: A group of particles injected vertically into the flow field with identical initial conditions. a. DDM model and b. SSF model.

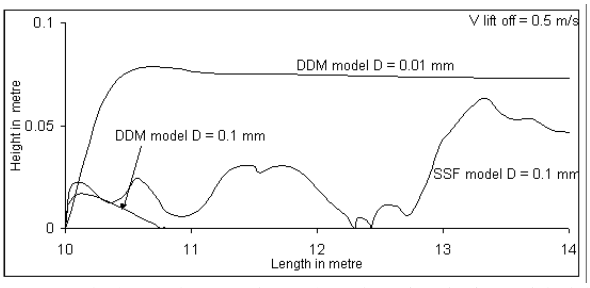

Figure 5: Saltation and suspension trajectories of a single particle injected vertically into the flow field with different particle sizes using the DDM and SSF models.

A 2.0 m high solid wall was placed in the computational domain perpendicular to the flow direction. It was presumed that this would result in two recirculation regions, one in front of the wall and the other behind it. Particles entering either of these regions were expected to settle and accumulate as a result of the reduction in the flow momentum.

The behaviour of individual particles entering these recirculation zones was examined using the SSF model. Initially, particles were patched over a 5 m length and were distributed uniformly upstream from the wall in a manner similar to that in the flat surface example.

For SSF simulation, 10 representative parcels of particles were injected from each location where the threshold conditions was satisfied. This number of parcels is much lower than the statistically significant number of particles required from a single location. Since a qualitative idea of where and when most of the particles could be captured was all that was required, and realising that a long computational time is required to inject a statistically significant number of particles, this low number of representatives was chosen.

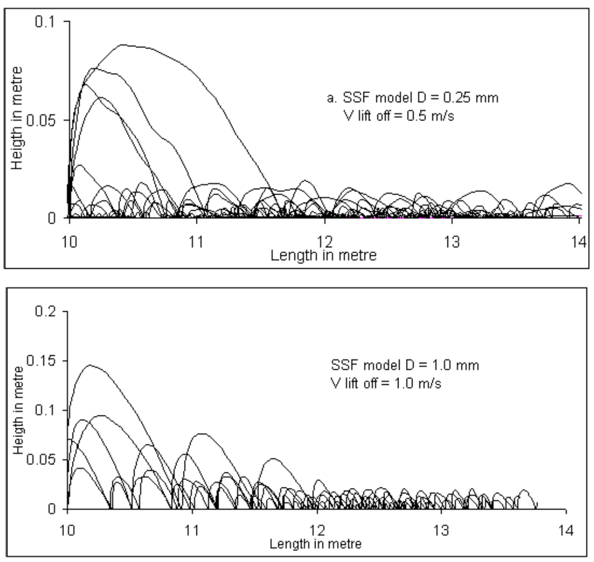

Figure 6: a group of particles injected vertically into the flow field with identical initial conditions using the SSF model

Figure 8 shows the drifting of the particles at different time steps. When particles reached the front recirculation zone, most particles were captured when the reverse flow met the incoming flow and the flow friction velocity dropped to values below the particle threshold value.

CONCLUSION

Different Lagrangian, particle trajectory numerical models were implemented and analysed. The advantages and disadvantages of these models were clarified through several test cases. These models were employed to simulate an individual and group of particle trajectories as they are driven by the flow field under the influence of both drag and gravitational forces. The different particle transport modes, such as suspension and saltation, were investigated. Under identical physical and initial conditions, SSF showed more realistic results with randomly sampled velocity fluctuation.

Although the Eulerian approach mentioned elsewhere is considered as the most practical and efficient approach to numerically simulate the drifting phenomena, the Lagrangian approach shows a potential ability to provide detailed information on individual particle behaviour in more complicated flow fields as long as the flow regime can be considered as a dilute flow. In dense flow systems, the theory behind these models is considered impractical and a more complicated particle equation of motion is essential, which should take into account the ignored forces, such as particle-particle collision and Magnus forces.

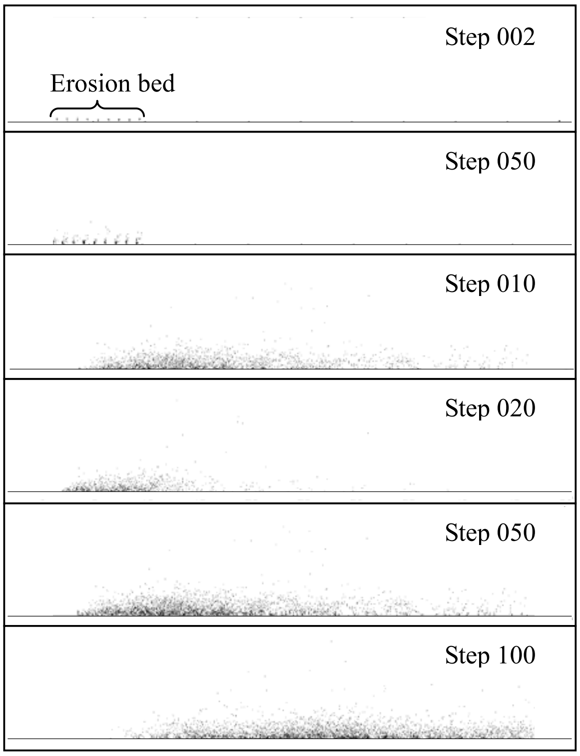

Figure 7: Ten thousand particles eroded from a sand bed placed just downstream the inlet domain. Figures show different steps of the Lagrangian calculations using the SSF model over a flat surface.

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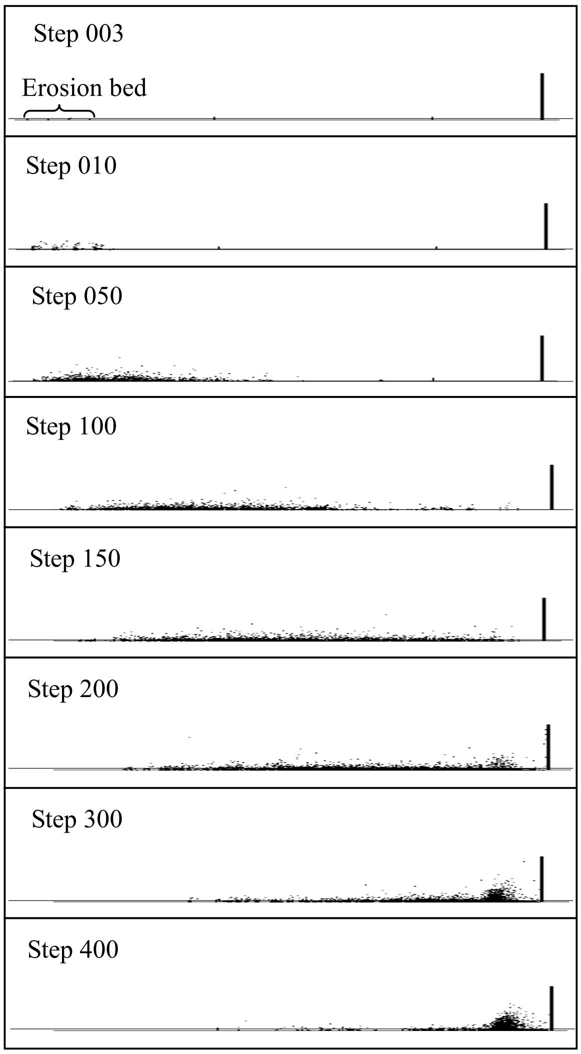

Figure 8: Ten thousand particles injected upstream of a solid wall placed perpendicular to the flow direction. Figures show different steps of the Lagrangian calculations using the SSF model around solid wall.