Lagrangian Particle Tracking: Model Development

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Abstract: The study of micro and nano particle-laden multiphase flow has received much attention due to its occurrence in a wide range of industrial and natural phenomena. Many of these flows are multi-dimensional systems involving strong mass, momentum and energy transfer between carrying fluid and particulate phase. The purpose of the present paper is to survey brief description of Eulerian-Lagrangian modeling of two-phase flow.

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1. Introduction

A two-phase flow is defined as combination of continuous phase, e.g. gas or liquid, and disperse phase, e.g. particles or droplets. They are found in many industrial applications such as cyclone separators, jet mills, deposition in duct or pipe flows (most probably undesired deposition), dust precipitation or coating processes (desired deposition). They also occur in nature, e.g., desert sand storms, pollen in air and dispersion of pollutants. In order to model such a phenomenon, two theoretical approaches are considered, namely the Eulerian-Eulerian (two-fluids) and the Eulerian-Lagrangian approaches. The Eulerian description assumes continuum medium for discrete phase and solve conservative laws for both solid phase and gas phase [1-3]. With the rapid development of computational capabilities, the mixed Eulerian-Lagrangian approach attracted more and more attentions from many researchers. In this approach, the detailed particle motion behavior, which facilitates a better understanding of the physical phenomena, can be revealed by solving the Newtonian motion Equations in Lagrangian coordinate while solving continuity and momentum equations for continuum phase.

In this review we will focus on turbulent Lagrangian description of particle tracking to model two-phase flow and expose development process in modeling such phenomena.

2. Characteristics of Lagrangian description in turbulent flow

Empirical probes have shown that three impacts have to be allowed for, to predict particle dispersion precisely.

2.1 The inertia effect (IE)

The experiments of Wells & Stock [3] and the direct numerical simulations of Squires & Eaton[4] indicate the possibility that the dispersion coefficient for heavy particles exceeds that for fluid particles. Reeks [5] and Pismen & Nir [6] have developed theories which predict that very heavy particles disperse more rapidly, in the long term, than fluid particles.

2.2 The crossing trajectory effect (CTE)

This effect Udine [7], whereby particle dispersion is reduced in the presence of strong body forces due to particles rapidly passing through eddies.

2.3 The continuity effect (CE)

The continuity effect Csanady [1] tells that the dispersion in the direction of the drift velocity exceeds the dispersion in the other two directions. The effect results from the fact that "longitudinal" and "transverse" length scales are different, which is in turn due to continuity equation of fluid motion [8].

3. Particle equation of motion

The surrounding fluid will interact with particles. The Lagrangian approach for the simulation of the disperse phase is based on Newton's equation of motion. To date a number of such forces have been implemented in discrete particle simulations. The reader can refer to [9, 10] for the historical development of such forces. The equation of motion of particles is given by

$$m_p \frac{d\vec{u}^p}{dt} = \sum \vec{F} \tag{1}$$

Here, F is sum of all forces that acting on particles which is represented in Table 1.

Forces	Expression	Reference s
Drag	$\vec{F}_{Drag} = \frac{\pi d_p^2}{8} \rho_f C_D \left \vec{u} - \vec{u}_p \right (\vec{u} - \vec{u}_p), m_p = \frac{\pi}{6} \rho_p d_p^3, C_D = \frac{24}{\text{Re}_p} (1.0 + 0.15 \text{Re}^{0.687}), \text{Re}_p = \frac{\rho_f \left \vec{u} - \vec{u}_p \right d_p}{\mu}$	[9]
Gravity	$\vec{F}_{Gravity} = m_p \vec{g}$	
Saffman	$\vec{F}_{seffman} = 1.61d_p^2 (\mu \rho_f)^{1/2} \times \vec{\omega} ^{-1/2} [(\vec{u} \cdot \vec{u}_p) \times \vec{\omega}], \vec{\omega} = \nabla \times \vec{u}$	[11]
Magnus	$\vec{F}_{magnus} = \frac{\pi}{8} \frac{d_p^2}{d_p^2} \rho_f \left[(\frac{1}{2} \nabla \times \vec{u} - \nabla \times \vec{u}_p) \times (\vec{u} - \vec{u}_p) \right]$	[12]
Virtual mass force	$\vec{F}_{VM} = C_{Vm} \rho_f V_p \frac{d(\vec{u} - \vec{u}_p)}{dt} / 2, C_{Vm} = 2.1 - 0.132 / (0.12 + A_c^2), A_c = (\vec{u} - \vec{u}_p)^2 / (d_p d(\vec{u} - \vec{u}_p)/dt)$	[13]
Basset history	$\vec{\mathbf{F}}_{Basset} = \frac{3}{2} d_p^2 \sqrt{\pi \rho_f \mu} \left[\int_0^t \frac{d(\vec{\mathbf{u}} - \vec{\mathbf{u}}_p)}{dt} (t - t')^{-1/2} dt' + \frac{(\vec{\mathbf{u}} - \vec{u}_p)_0}{\sqrt{t}} \right], (\vec{\mathbf{u}} - \vec{u}_p)_0 = initial \ velocity \ difference$	[14]
Brownia n	$\vec{F}_{Brownian} = m_{p}\vec{G}\sqrt{\frac{\pi S_{o}}{\Delta t}}, So = \frac{216\nu k_{Boltzman}T}{\pi^{2}\rho_{f}d_{p}^{5}S^{2}C_{c}}, C_{c} = 1 + \frac{2\lambda}{d_{p}}(1.257 + 0.4e^{-1.1d_{p}/2\lambda}), \lambda = \nu(\frac{\pi M_{G}}{2RT_{f}})^{1}$	[15]
Turbo- phoresis	$\vec{\mathbf{F}}_{Turbo} = -\frac{1}{2} \rho_p \frac{\pi d_p^3}{6} \frac{\partial u_r}{\partial r}$	[16]
Thermo -	$\vec{F}_{Themno} = -f \ \frac{C_T \upsilon}{T} \nabla^2 T \ , \ f = \frac{3\pi\mu d_p}{C_c} \ , \ C_T = \frac{2.34(k_{Boltzman}/k_p + 2.18Kn)C_c}{(1+3.42Kn)(1+2k_{Boltzman}/k_p + 4.36Kn)}$	[17, 18]
phoresis		
-	Acting forces on particles	ef eenien

The difference between the velocity of carrying fluid and of a particle moving in the carrying fluid causes the Drag force. The effect of gravity force on particle motion should be included, in the case where the free-fall velocity of particles and the velocity of carrying fluid are the same order of magnitude. The non-uniformity of the profile of averaged velocity of carrier fluid results in Saffman lifts force [11]. The Magnus force is due to the particle rotation. During particle motion in a fluid, particles of complex shape (a spherical) always rotate. The spherical particles will also rotate in a flow with a no uniform velocity profile. The added mass or virtual mass force is the inertia added to a particle because an accelerating or decelerating body must move some volume of surrounding fluid as it moves through it. The Basset history term is the drag caused by unsteady motion of the particle in a viscous medium. If the size of particle suspended in a fluid is very small, the motion of the particle affected by discrete nature of molecular motion of the fluid which is called the Brownian force. Turbo-phoresis force arises because of the non-uniformity of the profile of fluctuation velocity of carrier fluid. Thermophoresis force arises as a result of the nonuniformity of the temperature profile of carrier fluid.

4. Fluid-phase flow model

The conservation equations for the fluid flow are given by (in tensorial notation):

$$(\rho_{f}\phi)_{,i} + (\rho_{f}U_{i}\phi)_{,i} = (\Gamma\phi_{,i})_{,i} + S_{\phi} + S_{\phi p}$$
(2)

Where, ρ_f is the gas density, U_i are the Reynoldsaveraged velocity components, and Γ is an effective transport coefficient. The source terms S_{ϕ} and $S_{\phi p}$ are arisen from the transport equation and presence of particles, respectively. The k(energy contained in velocity fluctuations)– ε (rate of transfer of kinetic fluctuation energy to heat by viscous friction) model is widely used for the simulation of turbulent fluid flows in practical applications. Error! Reference source not found. and Table 2. Summary of terms in the general equation for the different variables that describe the fluid phase in Cartesian flowdemonstrate the different variables and source terms that describe the fluid phase; respectively. The direct influence of the dispersed phase on the continuous phase is usually taken into account by formulating appropriate source terms for all quantities under consideration. In the situation which mass loading of particles is low, the influence of particles on their carrier phase is negligible. Thus, the source terms that appear in the conservative equations as a result of particles are zero. In many situations, the mass loading particle to fluid ratio is too large to allow one to be satisfied with the one-way approach discussed in the previous subsection. In the Euler-Lagrange approach the interaction between both phases requires an iterative solution procedure, which is usually called two-way coupling. The discrete form of Reynolds Stress Model equations and their relevant source terms were presented by Gouesbet and Berlemont[9] and Lain et al[10]. In addition to two-way coupling simulation, four way coupling simulation accounts for inter-particle collisions which was considered by many researchers [10, 19-23].

	φ	Γ	S_{ϕ}
Continuity	1	0	0
X-Momentum	U	$\mu + \mu_t$	$\frac{\partial}{\partial x} \left(\Gamma \frac{\partial U}{\partial x} \right) + \frac{\partial}{\partial y} \left(\Gamma \frac{\partial V}{\partial x} \right) + \frac{\partial}{\partial z} \left(\Gamma \frac{\partial W}{\partial x} \right) - \frac{\partial P}{\partial x} + \rho g_x$
Y-Momentum	V	$\mu + \mu_t$	$\frac{\partial}{\partial x} \left(\Gamma \frac{\partial U}{\partial y} \right) + \frac{\partial}{\partial y} \left(\Gamma \frac{\partial V}{\partial y} \right) + \frac{\partial}{\partial z} \left(\Gamma \frac{\partial W}{\partial y} \right) - \frac{\partial P}{\partial y} + \rho g_y$
Z-Momentum	W	$\mu + \mu_t$	$\frac{\partial}{\partial x} \left(\Gamma \frac{\partial U}{\partial z} \right) + \frac{\partial}{\partial y} \left(\Gamma \frac{\partial V}{\partial z} \right) + \frac{\partial}{\partial z} \left(\Gamma \frac{\partial W}{\partial z} \right) - \frac{\partial P}{\partial z} + \rho g_z$
Turbulent Kinetic Energy	k	$\mu + \frac{\mu_t}{\sigma_k}$	$G_k - \rho \varepsilon$
Viscous Dissipation Rate	ε	$\mu + \frac{\mu_t}{\sigma_{\varepsilon}}$	$\frac{\varepsilon}{k} (C_1 G_k - C_2 \rho \varepsilon)$
Production of Turbulent Kinetic Energy	G_k	$G_{k} = \mu_{t} \begin{cases} 2 \left[(\frac{\partial U}{\partial y} \\ (\frac{\partial U}{\partial y} \\) \end{cases} \right] \end{cases}$	$\frac{U}{x}^{2} + \left(\frac{\partial V}{\partial y}\right)^{2} + \left(\frac{\partial W}{\partial z}\right)^{2} \Big] + \frac{\partial V}{\partial x}^{2} + \left(\frac{\partial U}{\partial z} + \frac{\partial W}{\partial x}\right)^{2} + \left(\frac{\partial V}{\partial z} + \frac{\partial W}{\partial y}\right)^{2} \Big]$
Eddy Viscosity	μ_t	$\mu_t = \rho c_\mu \frac{k^2}{\varepsilon}$	

Table 2. Summary of terms in the general equation for the different variables that describe the fluid phase in Cartesian flow

	ϕ	$S_{\phi p}$	Reference
Continuity	1	0	
X-Momentum	U	$S_{Up} = -\sum_{k=1}^{N^{p}} [m_{k} N_{K} \Delta t_{L} \times \sum_{n=1}^{N^{T}} \{ \frac{u_{p})_{k}^{n+1} - u_{p} }{\Delta t_{L}} - g_{x} (1 - \frac{\rho_{f}}{\rho_{p}}) \}]$	[9, 20-22, 24, 25]
Y-Momentum	V	$S_{Vp} = -\sum_{k=1}^{N^{p}} [m_{k} N_{k} \Delta t_{L} \times \sum_{n=1}^{N^{T}} \{ \frac{v_{p} p_{k}^{n+1} - v_{p} p_{k}^{n}}{\Delta t_{L}} - g_{y} (1 - \frac{\rho_{f}}{\rho_{p}}) \}]$	
Z-Momentum	W	$S_{Wp} = -\sum_{k=1}^{N^{p}} [m_{k} N_{k} \Delta t_{L} \times \sum_{n=1}^{N^{T}} \{\frac{w_{p}}{k} p_{k}^{n+1} - w_{p} p_{k}^{n} - g_{z} (1 - \frac{\rho_{f}}{\rho_{p}})\}]$	
Turbulent Kinetic Energy	k	$S_{kp} = \overline{u_i^p S}_{ui} - U_i \overline{S}_{ui} = \overline{u^p S}_{Up} + \overline{v^p S}_{Vp} + \overline{w^p S}_{Wp} - (U \overline{S}_{Up} + V \overline{S}_{Vp} + W \overline{S}_{wp})$	
Viscous Dissipation Rate	ε	$S_{\varepsilon p} = C_3 \frac{\varepsilon}{k} S_k$	
Constants		$C_1 = 1.44; \ C_2 = 1.44; \ C_3 = 1.87; \ C_\mu = 0.09; \ \sigma_k = 1.0; \ \sigma_\varepsilon = 1.3$	
Table 3.Fluid phase	e sou	rce terms in Cartesian flow	

5. Lagrangian modeling

A common feature of most Lagrangian methods used to date is the decomposition of the driving fluid velocity into the mean and the fluctuating parts. The mean fluid velocity field results from the continuous phase computation and is interpolated at particle locations. Then, a Lagrangian model gives the fluctuating component. In order to develop stochastic models for the generation of fluctuations, one typically uses, together with particle parameters (such as τ_p), a few quantities derived from the fluid variables, like the Eulerian length scale L_E or the Lagrangian time scale T_L . The modeling of fluid fluctuation velocity is complicated, because of two effects that cause the fluid element and particle trajectories to differ: first, particle inertia that induces a relative

instantaneous motion of particles with regard to their fluid neighborhood, and second, mean particle drift due to gravity.

5.1 Eddy Interaction Model

Hutchinson et al [26]considered particles which have one-directional radial motion in a turbulent pipe flow. Their well-known model is called eddy life time model. The model uses a stochastic approach to predict the characteristic of discrete phase. The adequate characteristic of the eddy interaction model lies in its simplicity and the fact that the only statistics required by the model are representative length, time and velocity scales, whereas, in the autocorrelation models (will discuss in the next section), the forms of either the temporal (Lagrangian) or the spatial (Eulerian) velocity auto-correlation functions (or both of these) are required. In single eddy interaction model (SEIM) each of a number of individual particles is tracked through a series of interactions with fluid eddies whose length, "lifetime" and velocity can all be random variables. Their model modified by some researchers to account for various particles dispersion [27-29].

The effective eddy interaction time interval t_i in which the velocities are kept constants are set to the minimum of the integral eddy life time T_e and the time scale for the crossing of the eddies t_c in order to account for the turbulence structure of the carrier phase as well as for the crossing trajectory effect[29]which is given by

$$t_c = -\tau_r \ln(1 - \frac{L_e}{\tau_r \left| \vec{u} - \vec{u}_p \right|})$$
(3)

In this approach[30, 31]as shown in Figure, at the start of the interaction time between fluid and particle (t = 0), the particle will be assumed to be sitting at the center of the eddy with velocity of U_{p0} . During the interaction of eddy and non-fluid particle, instantaneous fluid velocity of eddy is remained constant in space and time within the eddy and is given by

$$u = U + u' \tag{4}$$

Where u is the instantaneous eddy velocity, U is the mean velocity and u 'is the fluctuating velocity which is given by

$$u' = \gamma_i \sqrt{\frac{2k}{3}} \tag{5}$$

Where γ_i is the zero mean unit variance Gaussian random vector.

With proceed of time both the eddy and the non-fluid particle have moved in space. The eddy moves with its instantaneous fluid velocity while the non-fluid particle movement is governed by the Newtonian equation of motion (Eq. (1)). The non-fluid particle remains under the influence of that eddy until the interaction time exceeds the eddy lifetime (T_e), or distance between the center of eddy and non-fluid particle ($d(t_1)$) exceeds the eddy length L_e . So in this approach interaction time is given by

$$t_i = \min(T_e, t_c) \tag{6}$$

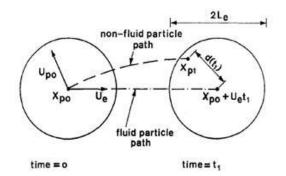


Figure 1. Eddy interaction model (from[30, 31])

Inertia and crossing trajectory and continuity effects have not been considered in original EIM. Some modifications have been taken to account by Graham[30, 31] to amend these deficiencies. The drawbacks of the method are twofold: a resulting velocity correlation coefficient is linear (rather than exponential) and the velocity record for a fluid particle is discontinuous (rather than continuous).

5.1.1 Eddy scale determination

As discussed earlier, to predict Particle motions in eddy interaction models three parameters are therefore determined: (i) eddy velocity, (ii) eddy lifetime and (iii) eddy length. Wang [32]have shown that the choice of eddy lifetime distribution in the eddy interaction model determines the form of the Lagrangian fluid velocity auto-correlation function.

Eddy scales used by Hutchinson and James et al[33]were obtained from empirical correlations using Laufer [34]pipe flow data. Gosman & Ioannides [27]assumed that the eddy length and lifetime are equal to the dissipation scales, given by

$$T_{e} = \sqrt{3/2} C_{\mu}^{3/4} \frac{k}{\varepsilon}, \quad L_{e} = C_{\mu}^{3/4} \frac{k^{3/2}}{\varepsilon}$$
(7)

Where k and \mathcal{E} is the turbulence kinetic energy and its rate of dissipation, respectively and $C_{\mu} = 0.09$. Eddy scales in the near-wall turbulence studied by Kallio&Reeks[35]where determined from laws of similarity at the wall. Milojevic[29]proposed the following eddy length and time scales which is given by

$$T_e = C_T \frac{k}{\varepsilon}, \quad L_e = \sqrt{\frac{2}{3}} C_T \frac{k^{3/2}}{\varepsilon}$$
(8)

Typically a value of C_T is in the range of 0.2 to 0.96.

Call & Kennedy[36] accounted for anisotropic turbulence by the use of a Reynolds stress turbulence model for the primary flow, thereby allowing for different eddy velocities in different coordinate directions. Graham & James[31]investigated the performance of different eddy interaction models with random length and time scales.

5.2 Auto-correlation method

In analyzing turbulent two phase flow we almost deal with Lagrangian fluid velocity autocorrelation and Eulerian fluid velocity autocorrelation functions. These two functions represent correlations between fluctuations of velocity of carrier phase and have the following general form, respectively:

$$R_{L}(t,\tau) = \frac{\left\langle u_{f}(t)u_{f}(t+\tau)\right\rangle}{\left\langle u_{f}^{2}(t)\right\rangle}$$
(9)

$$R_{E}(x,t) = \frac{\left\langle u_{f}(x_{0},t_{0})u_{f}(x_{0}+x,t_{0}+t)\right\rangle}{\left\langle u_{f}^{2}(x_{0},t_{0})\right\rangle}$$
(10)

Where $u_f(t)$ and $u_f(t+\tau)$ are the fluid velocity at

time t and $t + \tau$, respectively and angled brackets indicate ensemble averaging over many such particles. Lagrangian velocity coloration function is one of the most important statistics of turbulent flows.

 R_L should satisfy some requirements as following requirements:

I.
$$\tau \to 0 \Rightarrow R_L \to 1, \ \tau \to \infty \Rightarrow R_L \to 0$$

II.
$$(dR_L/d\tau)_{\tau=0} = 0, \ (d^2R_L/d\tau^2)_{\tau=0} < 0$$

Desjonqueres et al [37] proposed a Lagrangian method in which a correlation matrix is used in random process, which simulates the Lagrangian time correlations along the particle path. In the one dimensional formulation we have the following procedure in order to generate fluctuation velocities ([9, 38 and 39]):

Consider U' as the fluctuating velocity in the different time steps as follow

$$\mathbf{U}' = [u'_{x}(0), u'_{x}(\Delta t), \dots, u'_{x}(i\,\Delta t), \dots, u'_{x}(n\,\Delta t)] \quad (11)$$

Define uncorrelated zero mean and unit variance Gaussian vector U' and Y have the following relationship

$$\mathbf{U}' = BY \tag{12}$$

There is a symmetric, positive-definite matrix A which has the following relationship with B as follow:

$$A = BB^{T} \tag{13}$$

Where, B^{T} is the transpose matrix of B.

Element of matrix A obtain simply by Frenkiel [40] family of the correlation as follow

$$a_{ij} = \exp(\frac{-|j-i|\Delta t}{(m^2+1)\tau_L})\cos(\frac{m|j-i|\Delta t}{(m^2+1)\tau_L})$$
(14)

where m is the loop parameter and m = 1 is a recommended value[9]. In the final step we use Cholesky factorization in order to B obtain from A.

5.3 Lagrangian temporal construction Model

Lu et al [41] proposed a Lagrangian model which represents satisfactory results in compared to experimental results. In their model, at time t, the particle and a corresponding fluid point start out from the same position X_S (Figure 2). After one time step, they arrive at X_f and X_P , respectively, and the distance between them is Δs . The relative coordinate system O- $\Xi\Omega\Theta$ is chosen such that its original point, O, is located at the position X_f , and the Θ -axis passes through the position X_P ([41-43]).

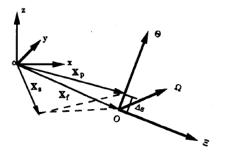


Figure 2. The locations of the particle and a fluid particle (from[42])

With the aid of time series analysis, the normalized fluctuating component in the location of particle in the *i*-direction of relative coordinate system O- $\Xi\Omega\Theta$ is obtained by (no summation convention is used):

$$W_{i}(X_{P}) = a_{i}b_{i}W_{i}(X_{S}) + \Psi_{i} \quad (i = 1, 2, 3)$$
(15)

Where

$$W_i = \frac{u_i}{\sqrt{u_i^2}}$$
 (*i* = 1, 2, 3) (16)

In Eq. (15), Ψ_i are mean zero, $\sqrt{1-(a_ib_i)^2}$ variance Gaussian random numbers and a_i , b_i are

Lagrangian auto-correlation and Eulerian spatial velocity correlations functions, respectively which they for example pick from the Frenkeil [40]family of auto-correlations as follow

$$a_i = \exp(\frac{-\Delta t}{\tau_i^L}), \ b_i = \exp(\frac{-\Delta s}{2\Lambda_i})\cos(\frac{\Delta s}{2\Lambda_i}), \ (i = 1, (17))$$

Where are Λ_i the length scales and τ_i^L are the Lagrangian time scales.

5.4 Kraichnan Fourier modes

Kraichnan [44]suggested a simple method for generating a random field which resembles a pseudo-isotropic turbulence. In this approach fluctuation velocities are obtained as below

$$\vec{u}(\vec{X}_{p},t) = \sqrt{\frac{2}{N}} \left\{ \sum_{n=1}^{N} \vec{u}_{1}(\vec{k}_{n}) \cdot \cos(\vec{k}_{n}, \vec{X}_{p} + \omega_{n}t) \right\}$$
(1)

Where

$$\vec{u}_1(\vec{k}_n) = \vec{\zeta}_n \times \vec{k}_n, \ \vec{u}_2(\vec{k}_n) = \vec{\xi}_n \times \vec{k}_n$$
(19)

And

$$\overrightarrow{k_n} \cdot \overrightarrow{u_1(k_n)} = \overrightarrow{k_n} \cdot \overrightarrow{u_2(k_n)} = 0$$
(20)

Satisfy the incompressibility condition. The components of vectors $\vec{\xi_n}$, $\vec{\zeta_n}$ and the values of frequency ω_n , were picked independently from a three or two dimensional Gaussian distribution with a standard deviation of unity. Each component of $\vec{k_n}$, is a Gaussian random number with a standard deviation that depends on energy spectrum [44]. Here, N is the number of terms in the series that usually is considered as 100.

Some modifications were taken to account for anisotropy effects [21, 22 and 45].

5.5 Models based on the Langevin equation

A following stochastic differential equation has been proposed to model the behavior of fluid velocities

$$\frac{du_i}{dt} = -\frac{u_i - U_i}{T_L} + (\frac{2u_i^2}{T_L})^{1/2} \psi_i(t)$$
(21)

Here, $\psi_i(t)$ is the Wiener process (white noise); it is a stochastic process of zero mean, $\langle \psi_i(t) \rangle = 0$, a variance equal to the time interval $\langle (\psi_i(t))^2 \rangle = dt$. The above is the Langevin equation first proposed to model the Brownian motion; in that context, it represents the equation of motion of a small particle in surrounding fluid [46, 47]. Some models presented by Pozorski & Minier

[46] which account for main three effects in Lagrangian simulation, i.e. IE, CTE and CE.

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