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A coupled hydrodynamic and particle-tracking model for full-process simulation of nonpoint source pollutants

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Abstract

Nonpoint source (NPS) particulate pollutants are a major source of urban surface pollution. It is essential to better understand and model the dynamic process of NPS pollutants to inform the design of effective strategies for urban stormwater management and pollution control. This work presents a novel coupled hydrodynamic and particle-based model to simulate the full-process dynamics of NPS particulate pollutants from detachment, transport to deposition in urban areas. A particle-based approach is proposed to represent the physical processes of pollutant detachment and deposition. The transport of pollutant particles is simulated using a random-walk particle-tracking model, which can directly trace out the trajectories of individual particles and hence identify the pathways of pollutants. The new coupled hydrodynamic and particle-based stormwater quality model is successfully validated against several analytical and experimental test cases to demonstrate its capability in accurately simulating the full-process dynamics of NPS particulate pollutants in urban areas.

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23 **Key words:**

24 Urban water management; Stormwater quality modelling; Hydrodynamic model; Pollutant
25 wash-off; Particle-tracking; Pollutant transport

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32 **1. Introduction**

33 Today, more than 50% of the world's population are living in urban areas (Bach et al., 2014).
34 By 2040, a further 1.1 million km² areas will be urbanised across the world (Paresi et al., 2016).
35 Urbanisation inevitably increases population density and human activity (e.g. construction,
36 manufacturing and transportation) and grows impervious ground surfaces. This will
37 subsequently create more nonpoint source (NPS) pollutants, such as heavy metals, suspended
38 solids, minerals and nutrients (Arthur et al., 2019). When a storm event occurs, these NPS
39 pollutants will be collected by the rainwater and washed off from the urban surfaces and finally
40 transported to the downstream receiving waters, causing water quality degradation (Tsihrintzis
41 and Hamid, 1997). For example, it is recognised that majority of water body pollution failures
42 in the heavily urbanised Thames river basin are caused by the NPS pollution from road runoff

(DEFRA, 2012). Therefore, effective control of NPS pollutants in the urban runoff is essential for urban water management.

With an emphasis on working with natural processes, Sustainable drainage systems (SuDS), also known as low impact development (LID) or water sensitive urban design (WSUD) in different countries/regions of the world, consist of a series of measures and practices (e.g. swales, rain barrels and artificial wetlands) that are designed and operated to attenuate runoff and mitigate flood risk and meanwhile create other benefits including water quality enhancement through filtration, sorption and biological processes (Ahiablame et al., 2012). To design and implement efficient SuDS to effectively mitigate urban water pollution and improve water quality, it is essential to better understand the full-process dynamics of NPS pollutants during a storm event, defined as detachment from the urban surfaces, transport by the urban runoff and deposition if it occurs (Arthur et al., 2019; Baek et al., 2015; Gilbert and Clausen, 2006; Hong et al., 2016a).

In the last few decades, numerous urban stormwater quality models have been developed and applied to support runoff quality simulations. In most of these models (e.g. Stormwater Management Model (SWMM), Model for Urban Stormwater Improvement Conceptualisation (MUSIC), Soil and Water Assessment Tool (SWAT), wash-off process modelling is a key component implemented to predict runoff quality (Obropta and Kardos, 2007), representing the process of accumulated NPS pollutants being washed off by the runoff during a rainfall event. Pollutant wash-off has been widely estimated using an exponential or event mean concentration (EMC) function. In an exponential function, the amount of pollutants being washed off is assumed to be proportional to the total mass of accumulated pollutants and the runoff rate. The function contains an empirical wash-off coefficient k that has no direct physical meaning (Hong et al., 2016a). The EMC approach relies on estimation of EMC from substantial laboratory or field measurements (Rossman and Huber, 2016). Both methods are

empirical and largely neglect the underlying physics of the wash-off process (Hong et al., 2016a; Sage et al., 2015).

Furthermore, the current practice commonly uses hydrological models to drive wash-off modelling. Whilst they cannot predict the dynamics of runoff and overland flow at a high spatial resolution, these hydrologically based approaches estimate the mass of washed-off pollutants and add it to the nodes (e.g. manholes) of urban drainage systems, neglecting the spatial heterogeneities of urban surfaces and their influences on pollutant distribution and dynamics (Shaw et al., 2006; Rossman and Huber, 2016; Shaw et al., 2009). Therefore, these hydrologically based models are not able to provide the temporal and spatial specificities of pollutant distribution which are useful for better assessment and operation of SuDS.

A few attempts have been made to develop physically based models to predict the wash-off process of NPS pollutants. Shaw et al. (2009, 2006) proposed a physically based model to simulate the process of particulate pollutants detached by raindrops from the urban surfaces, which then travel laterally at the velocity of overland flow until settling back to the ground. However, the model neglected the pollutant detachment caused by the flow stresses and was restricted to one dimension, limiting its wider application in realistic events. Hong et al. (2016a, 2016b) coupled the Hairsine-Rose (H-R) model (Hairsine and Rose, 1992a, 1992b) with the Full Shallow-Water equations for Overland Flow (FullSWOF) model to reproduce the wash-off and transport processes of pollutants on urban surfaces. The coupled model was able to simulate the full process of pollutant dynamics and effectively reflect the spatial heterogeneities of pollutant movements and distribution. However, the model solves the governing equations and predicts the flow and pollutant dynamics on a Eulerian grid-based framework that can only provide the snapshots of pollutant concentration across the simulation domain. But particulate pollutant transport is inherently a Lagrangian process and an Eulerian

model is incapable of entailing particle trajectories to trace out the pathways of pollutants, thus only providing limited value in informing the choice and design of different types of SuDS.

The random walk particle-tracking model (PTM) developed within the Lagrangian framework provides a powerful tool for describing the motions of individual particles in a deterministic Eulerian velocity field (Liang et al., 2007). It has been widely applied in water quality modelling in a range of flow conditions from river (Weitbrecht et al., 2003), estuary (Gomez-Gesteira et al., 1999) to ocean (Olascoaga et al., 2013). Huai et al. (2019) adopted a particle random displacement model to predict the concentration of suspended sediment in an open channel, with a focus on analysing the vertical profile of suspended sediment concentration in a steady vegetated flow. Sämann et al. (2019) recently introduced a PTM based transport model to predict the potential contamination paths of solutes in drainage systems during a pluvial flood event. However, the model considered only point source pollutants and neglected the wash-off process, and so is not applicable to simulate the full-process dynamics of NPS pollutants driven by a rainfall-flooding event in urban areas.

As a summary, most of the existing models for stormwater quality modelling suffer from various restrictions. Further research is still needed to develop alternative numerical approaches to support the modelling of full-process dynamics of NPS pollutants in urban areas during a stormwater event. Given that majority of the NPS pollutants are in the form of particulates or attached to sediments of different sizes (Arthur et al., 2019; Gilbert and Clausen, 2006; Hong et al., 2016a), this work aims to develop and present a new stormwater quality model considers the NPS particulate pollutants directly as particles to simulate their full-process dynamics. The rest of the paper is organised as follow: Section 2 introduces the new model framework, which is tested and validated in Section 3; finally, brief conclusions are drawn in Section 4.

2. Model description

The proposed stormwater quality model couples together three modelling components to respectively represent the ambient flow hydrodynamics, pollutant wash-off and transport processes. The overall modelling framework is illustrated in Fig. 1, in which the hydrodynamic model is coupled to the other two components and also provides a grid/mesh for particle initiation and flow fields as necessary for the following pollutant wash-off and transport modelling. The wash-off process modelling is achieved using a new particle-based approach to implement the H-R model for predicting particles being washed off from the urban surfaces. The new particle-based wash-off model is then coupled with a random walk PTM to trace out the individual transport trajectories of suspended particles and thus identify the pathways of NPS particulate pollutants.

Fig. 1 The new coupled stormwater quality modelling framework.

2.1 Hydrodynamic modelling

To predict the flow fields for particle tracking in the coupled stormwater quality modelling framework as already shown in Fig. 1, the High-Performance Integrated hydrodynamic Modelling System (HiPIMS) (Liang and Smith, 2015) is adopted in this work. HiPIMS solves the full two-dimensional (2D) SWEs using a Godunov-type shock-capturing numerical scheme and is implemented on multiple GPUs for substantially improved computational efficiency and further technical details can be found in Xia et al. (2019). In this study, the GPU-accelerated HiPIMS provides the required spatially and temporally varying flow information to drive the pollutant wash-off and transport modelling components that are run on CPUs.

2.2 Wash-off modelling

Initially, the H-R model was coupled with a finite volume SWE model to simulate the dynamic process of pollutants on urban surfaces (Hong et al., 2016a). Since a Lagrangian particle-tracking model (Section 2.3) is developed and used for pollutant transport in this study, the H-R model is accordingly implemented using a particle approach to describe the pollutant wash-off process, which will be introduced in detail in the following sub-sections. Fig. 2. illustrates the overfall particle-based framework for wash-off process modelling. In each time step, the updated distribution of particles following the transport process modelling is transferred to mass concentration for the subsequent wash-off estimation, i.e. quantifying the concentrations of suspended and deposited pollutants. The updated mass concentration is then transferred back to particle form for a new round of transport process modelling using a particle-tracking model.

Fig. 2 The particle-based framework for wash-off process modelling.

2.2.1 Governing equations

In the proposed particle-based H-R model, the computational domain is firstly decomposed into a uniform grid, which is taken to be identical to the computational grid created for hydrodynamic modelling. The NPS pollutants are represented by particles of a single-class size that are evenly distributed in the grid cells. During a simulation, these particles may be either suspended in the flow or deposited on the ground surface. As demonstrated in Fig. 3, deposited particles may be detached from the ground by rainfall impact or shear flow stress to become suspended in the flow; meanwhile, the suspended particles may deposit back to the ground surface if certain flow conditions are met, forming a deposition layer from which particles can be re-detached again. It is noted that the model is proposed to be applied in urban areas where impervious surfaces predominantly exist and therefore pollutant infiltration is not considered in this work.

Fig. 3 The particle-based Hairsine-Rose model for pollutant wash-off.

As illustrated in Fig. 3, the particle-based mass balance equations may be written as:

$$\frac{\partial M_s}{\partial t} = e + r - d \quad (1)$$

$$\frac{dM_d}{dt} = d - e - r \quad (2)$$

where M_s and M_d are the mass concentrations (kg/m^2) of the suspended and deposited particles, respectively; t is the time (s); e is the rainfall-driven detachment rate ($\text{kg m}^{-2} \text{s}^{-1}$); r denotes the flow-driven detachment rate ($\text{kg m}^{-2} \text{s}^{-1}$); d is the deposition rate of particles ($\text{kg m}^{-2} \text{s}^{-1}$).

The rainfall-driven particle detachment rate e is related to the rainfall intensity, available particles on the ground surface and mass threshold, and it may be estimated using the following formula:

$$e = \frac{a_d P M_d}{m^*} \quad (3)$$

where a_d is a coefficient representing the detachability of particles (kg/m^3); P is the rainfall intensity (m/s); m^* is the threshold of the particle mass concentration required to shield the

177 original particles from further detachment (kg/m^2) The particle detachability coefficient a_d
 178 may be calculated using (Proffitt et al., 1991):

$$179 \quad a_d = \begin{cases} a_{d_0}, & h \leq h_0 \\ a_{d_0} \left(\frac{h_0}{h}\right)^b, & h > h_0 \end{cases} \quad (4)$$

180 in which a_{d_0} is the initial detachability coefficient (kg/m^3); h is the water depth (m); h_0 is the
 181 threshold of water depth (m) to define the particle detachability, estimated using the following
 182 formula as suggested by Mutchler and Hansen (1970):

$$183 \quad h_0 = 0.33D_R \quad (5)$$

184 where D_R is the mean raindrop size (m).

185 According to Heng et al. (2011), the amount of particles required to shield the original
 186 particles from further detachment is analogous to a_d . Once the mass of particles on the ground
 187 surface exceeds m^* , the deposited particles M_d should be equal to m^* and the threshold value
 188 m^* may be calculated by:

$$189 \quad m^* = \begin{cases} m_0^*, & h \leq h_0 \\ m_0^* \left(\frac{h_0}{h}\right)^b, & h > h_0 \end{cases} \quad (6)$$

190 where m_0^* is the initial fixed threshold of mass concentration; b is a positive constant (Heng et
 191 al., 2011). Accordingly, Eq. (3) can be rewritten as:

$$192 \quad e = \begin{cases} \frac{a_d P M_d}{m^*}, & M_d \leq m^* \\ a_d P, & M_d > m^* \end{cases} \quad (7)$$

193 The flow-driven detachment rate r is related to the changing rate of potential energy of the
 194 particulate sediment and may be calculated using (Hong et al., 2016a):

$$r = \frac{\Omega_e}{\frac{\rho_s - \rho_w}{\rho_s} gh} \quad (8)$$

where Ω_e is the effective stream power (W/m^2); ρ_s and ρ_w are the densities (kg/m^3) of the particulate sediment and water, respectively; $g = 9.81 \text{ m/s}^2$ is the acceleration due to gravity. The effective stream power Ω_e is defined as follows (Hong et al., 2016a):

$$\Omega_e = F(\Omega - \Omega_0) \quad (9)$$

where F is the effective fraction of excess stream power; Ω represents the total stream power (W/m^2), and Ω_0 is the threshold of stream power (W/m^2) below which no entrainment will occur. Ω is calculate by (Hong et al., 2016a):

$$\Omega = \rho_w g S_f q \quad (10)$$

where S_f is the friction slope calculated using the Manning equation and q is the water flux or unit-width discharge (m^2/s).

The rate of particle deposition d is determined by the settling velocity and available particles in the flow (i.e. suspended particles):

$$d = v_s * \frac{M_s}{h} \quad (11)$$

where v_s is the settling velocity (m/s) of the suspended particles, which is estimated using the following equation as suggested by Cheng (1997):

$$v_s = \frac{\left(\sqrt{25 + 1.2d_*^2} - 5 \right)^{1.5} \nu}{d} \quad (12)$$

where d is the particle diameter (m); ν denotes the kinematic viscosity (m^2/s); and d_* is given by:

$$d_* = \left(\frac{\theta g}{v^2} \right)^{\frac{1}{3}} d \quad (13)$$

with:

$$\theta = \frac{(\rho_s - \rho_w)}{\rho_w} \quad (14)$$

2.2.2 Time step

According to Heng et al. (2011), the allowable time step of the H-R model for soil erosion and sediment dynamics should be restricted by the following condition:

$$\Delta t \leq \frac{h_{min}}{v_s + f(t)} \quad (15)$$

where $f(t)$ is the infiltration rate of the soil. For impervious surfaces, zero infiltration rate applies, and the allowable time step may be accordingly adapted to be:

$$\Delta t \leq \frac{h_{min}}{v_s} \quad (16)$$

However, the calculation of e , r and d in the H-R model is supported by the flow information predicted by HiPIMS which is output at a prescribed time interval. This output time interval is commonly much larger than Δt as defined by Eq. (16) and may subsequently cause numerical instability. To relax the restriction on the time step of the wash-off modelling, an implicit numerical scheme is adopted and implemented so that the HiPIMS output time interval can be used as the time step for wash-off calculation and the following transport process modelling.

The implicit time-marching scheme for the governing equations (1-2) are given as follows:

$$M_s^{n+1} = M_s^n + \Delta t \left(\frac{a_d P M_d^{n+1}}{m^*} + \frac{\Omega_e}{\frac{\rho_s - \rho_w}{\rho_s} g h^n} - v_s * \frac{M_s^{n+1}}{h^n} \right) \quad (17)$$

$$M_d^{n+1} = M_d^n + \Delta t \left(v_s * \frac{M_s^{n+1}}{h^n} - \frac{a_d P M_d^{n+1}}{m^*} - \frac{\Omega_e}{\frac{\rho_s - \rho_w}{\rho_s} g h^n} \right) \quad (18)$$

Herein, we re-arrange Eq. (18) and then substitute it into Eq. (17) to derive new time-marching formulae for M_s^{n+1} and M_d^{n+1} that can be implemented explicitly:

$$M_s^{n+1} = \frac{\omega h^n M_s^n + (\omega - 1) h M_d^n + \Delta t h^n \frac{\Omega_e}{\frac{\rho_s - \rho_w}{\rho_s} g h^n}}{\omega h^n + \Delta t v_s} \quad (19)$$

$$M_d^{n+1} = \frac{h^n M_d^n + \Delta t M_s^{n+1} v_s - \Delta t h^n \frac{\Omega_e}{\frac{\rho_s - \rho_w}{\rho_s} g h^n}}{\omega h} \quad (20)$$

$$\omega = 1 + \frac{a_d}{m^*} P \Delta t \quad (21)$$

where the relevant parameters can be evaluated according to Eq. (4-14).

2.2.3 Representing mass concentration using particles in the particle-based approach

For a particle-based model as the one developed in this work, it is necessary to represent the mass concentration using particles distributed in a cell for the following transport process modelling. Since the total number of particles in an arbitrary cell is fixed in a single time step during wash-off modelling (which is consistent with the mass balance equations (Eq. (1-2)), it is only necessary to calculate the number of suspended particles and the number of deposited particles can be simply obtained by subtracting the number of suspended particles from the total number of particles. The mass concentration of suspended pollutants updated in Eq. (19) is transferred to the number of suspended particles in the cell under consideration using the following scheme:

$$P_s^i = \frac{M_s^{n+1}}{m_p} S^i \quad (22)$$

250 where P_s^i is the ‘number’ of suspended particles in cell i , which is returned directly as a real
251 number; m_p is the mass of a single particle (kg); S^i is the area (m²) of cell i .

252 The real number P_s^i calculated in Eq. (22) is then rounded to become an integer (N_s^i) to
253 specify the final number of suspended particles in cell i :

$$254 \quad N_s^i = \lfloor P_s^i \rfloor \quad (23)$$

255 Apparently, small mass error exists in this round-off process, which must be properly avoided.

256 Herein, de is introduced to define the remaining decimal error between P_s^i and N_s^i :

$$257 \quad de = P_s^i - N_s^i \quad (24)$$

258 where de is obviously always smaller than ‘1’. To eliminate the mass error during a simulation,
259 de is added up across the grid cells in sequence. When the accumulated error becomes equal
260 to or larger than ‘1’, a suspended particle is created and placed in the current cell. The
261 subsequent remaining error will then be added to the next cell and the procedure continues until
262 all of the cells in the domain are swept through. This final decimal error will be neglected. It
263 should be noted that this procedure is implemented to largely ensure mass conservation and
264 will not create any major disturbance to the numerical solution as the mass of a particle is
265 always very small.

266 Now, the number of suspended particles in cell i is updated for the next step of transport
267 process modelling and the difference between the updated (N_s^{n+1}) and the existing (N_s^n)
268 particle numbers can be readily sought:

$$269 \quad \Delta N_s^i = N_s^{n+1} - N_s^n \quad (25)$$

270 If $\Delta N_s^i > 0$, it indicates ΔN_s^i deposited particles are disturbed and become suspended from the
 271 ground surface, which will be randomly distributed inside cell i . On the other hand, if $\Delta N_s^i <$
 272 0 , ΔN_s^i currently suspended particles are randomly selected and become deposited.

273 2.3 Particle transport modelling

274 The suspended particles updated in the last section will be moved and transported by the urban
 275 surface runoff induced by rainfall using a particle-tracking model as introduced in this section.

276 2.3.1 Governing equations

277 Since the particulate pollutants are small and their presence will not impose any accountable
 278 feedback to the ambient flow hydrodynamics in a macro-scale simulation, the pollutant
 279 particles are assumed to immediately react to and move according to the flow velocity at the
 280 location where the particle is located. In a 2D simulation domain as considered in this work,
 281 the semi-discretised governing equations for the particle-tracking model are given by:

$$282 \quad x(t + \Delta t) = x(t) + u(x, y, t) \cdot \Delta t + \sqrt{2D_{xx}\Delta t} \cdot \Lambda \quad (26)$$

$$283 \quad y(t + \Delta t) = y(t) + v(x, y, t) \cdot \Delta t + \sqrt{2D_{yy}\Delta t} \cdot \Lambda \quad (27)$$

284 in which (x, y) is the position of the particle in the phase space, u and v are the depth-average
 285 flow velocity predicted by the hydrodynamic model as briefly introduced in Section 2.1. The
 286 random walk terms are also included to account for the diffusion effect, with D_{xx} and D_{yy}
 287 respectively denoting the longitudinal and transverse diffusion coefficients (m^2/s) and Λ being
 288 a random number that conforms to a normal distribution with a 0 mean and standard deviation
 289 (Follett et al., 2016; Huai et al., 2019). Herein, Λ is generated by a random number generator
 290 in the numerical solution.

291 2.3.2 Numerical scheme

The governing equations (26-27) are divided into two parts to account respectively for particle advection and diffusion and handled separately in the adopted numerical solution scheme. For particle advection, a second-order Runge-Kutta (RK) integration method is used to update the particle positions to the next time step. Taking the x -direction Eq. (26) as an example, the RK integration scheme may be expressed as:

$$x(t + \Delta t) = x(t) + \frac{\Delta t}{2} (K_1 + K_2) \quad (28)$$

where K_1 and K_2 are the Runge-Kutta coefficients defined as follows:

$$K_1 = u(x(t), y(t), t), \quad K_2 = u(x(t + \Delta t), y(t + \Delta t), t) \quad (29)$$

The advection part of the y -direction Eq. (27) is solved similarly.

It should be noted that the flow velocity fields output from HiPIMS are grid-based, i.e. u and v are only discretely available at the centre of each of the grid cells. A bilinear interpolation scheme is therefore implemented to obtain the flow velocities at the specific position where the particle under consideration is located (which can be anywhere within a cell) and support the above particle advection calculation.

Finally, for each of the particles, the random walk diffusion terms, $\sqrt{2D_{xx}\Delta t} \cdot \Lambda$ and $\sqrt{2D_{yy}\Delta t} \cdot \Lambda$, are calculated and the resulting particle displacements are directly added to $x(t + \Delta t)$ and $y(t + \Delta t)$ updated by the above Runge-Kutta advection step to obtain the final particle position for this time step.

3. Results and discussion

In this section, the new coupled hydrodynamic and particle-tracking model for stormwater quality modelling is validated by simulating four test cases.

3.1 Solute advection and diffusion in a uniform flow field

The first test case considers the advection and diffusion of a solute cloud in a steady uniform flow (Zhang et al., 2015), aiming to validate the particle-tracking model for pollutant transport. In an $800 \text{ m} \times 200 \text{ m}$ frictionless channel with a horizontal bed, a solute cloud moves from upstream to downstream, driven by a steady flow with $h = 1 \text{ m}$, $u = 1 \text{ m/s}$, $v = 0 \text{ m/s}$. The analytical solution of the solute concentration (c) for this idealised case is provided as:

$$c(x, y, t) = \frac{c_0/h}{4\pi t \sqrt{D_{xx}D_{yy}}} e^{\left(-\frac{(x-x_0-ut)^2}{4D_{xx}t} - \frac{(y-y_0)^2}{4D_{yy}t}\right)} \quad (30)$$

with $c_0 = 233.06$, $D_{xx} = 1.02 \text{ m}^2/\text{s}$ and $D_{yy} = 0.094 \text{ m}^2/\text{s}$ as adopted in Zhang et al. (2015). At the start of the simulation, the peak concentration is located at $(x_0, y_0) = (0, 100)$. The simulation starts at $t = 60 \text{ s}$ and the initial contours of the solute concentration as defined by Eq. (30) is shown in Fig. 4. Transmissive conditions are imposed in all four lateral domain boundaries. Simulation is run until $t = 600 \text{ s}$ with 480,000 particles while each particle represents $4.86 \times 10^{-4} \text{ kg}$ of mass.

Fig. 4 Schematic of the solute cloud test at the initial time.

Fig. 5 compares the analytical solution with the numerical prediction in terms of concentration profile at different output times. As expected, the solute cloud is driven by the steady flow and transported from upstream to downstream, accompanied by the diffusion of the concentration as time increases. The numerical prediction agrees satisfactorily with the analytical solution, and both of the transport and diffusion processes are well captured by the particle-tracking transport model.

Fig. 5 Comparison between the predicted concentration profile and analytical solution.

In order to visualize the movement of particles, positions of all particles at different output times are presented in Fig. 6 and particles are plotted in different colours according to the particle density in the corresponding cell containing them. Contours of the analytical concentration are also plotted in the figure for comparison. Since the solute concentration is relevant to the particle density in a cell, the consistency between the particle density and the analytical concentration field (as reflected by the contour lines) confirms again the capacity of the current particle-tracking transport model in accurately simulating the transport of a concentration field with diffusion.

Fig. 6 Particle clouds and analytical concentration contours at different output times.

One of the main advantages of the adopted particle-based approach is its capability to trace out an individual particle's trajectory to effectively depict its source, pathway and final destination. Fig. 7 provides the trajectories of four sample particles in the simulation domain during the 600 s of simulation, plotted at a 5 s time interval. This clearly shows each of the individual particles being driven from their initial location to downstream during the simulation. The diffusion effect imposed by the random walk algorithm on the particle dynamics is evident as all of the particles are drifted back and forth in the y -direction in addition to being predominantly transported by the unidirectional flow from upstream to downstream.

Fig. 7 Trajectories of the four selected sample particles.

Fig. 8 Relative errors of the simulation results against the number of particles being used.

Further simulations are carried out to investigate the convergence of the simulation results against the number of particles being used to represent the concentration field, ranging from 1,000 to 1,000,000. To quantitatively compare the numerical and analytical results, the relative errors are calculated and presented in Fig. 8. Apparently, the simulation errors decrease with the increasing number of particles being used, which effectively indicates the convergence of the simulation results. Converged simulation results are achieved from using 250,000 particles and further increase of the particle number will no longer substantially improve the simulation accuracy. When 1 million particles are used, there is still about 5% of relative simulation error, which may be due to numerical diffusion and also the inherent error created by the normal distribution based random number generation algorithm in the C++ library (to generate the random numbers in the modelling approaches as introduced in Section 2) and cannot be entirely eliminated.

3.2 Pollutant wash-off and transport in a uniform flow field

Based on the previous test case as considered in Section 3.1, two more tests are designed herein with different initial conditions to validate the detachment and deposition modules of the proposed particle-based wash-off model. All simulations are run for 600 s with 250,000 particles.

3.2.1 Particle deposition during the transport process

In this test, all of particles are assumed to be initially suspended in the shallow flow, i.e. no pollutant particle is found on the ground surface at the start, which may be mathematically expressed as:

$$M_d^0 = 0 \quad (31)$$

$$M_s^0 = h \frac{c_0/h}{240\pi\sqrt{D_{xx}D_{yy}}} e^{\left(-\frac{(x-x_0-60u)^2}{240D_{xx}} - \frac{(y-y_0)^2}{240D_{yy}}\right)} \quad (32)$$

When the simulation starts, particles are assumed to deposit at a constant settling velocity (v_s) of 0.01 m/s and no particle is allowed to re-suspend from the ground surface, i.e. the rainfall intensity (P) and effective fraction of excess stream power (F) are both assumed to be 0 to ensure zero particle detachment rates. Based on these assumptions, the analytical solution of the concentration field is derived and given by:

$$c(x, y, t) = e^{-0.01t + \ln\left(\frac{c_0}{240\pi\sqrt{D_{xx}D_{yy}}} \times e^{-\frac{(x-x_0-t-60)^2}{240D_{xx}} - \frac{(y-y_0)^2}{240D_{yy}}}\right)} \quad (33)$$

Fig. 9 illustrates the predicted concentration profiles output at every 100 s. As the time passes, the pollutant concentration in the flow decreases due to deposition, which is accurately captured by the model. The predicted profiles compare excellently well with the analytical solutions. This effectively confirms the model's performance in predicting particle deposition.

Fig. 9 Particle deposition test: numerical and analytical concentration profiles at different output times.

3.2.2 Particle detachment during the transport process

In this test, all of particles are initially attached to the ground surface, i.e. no pollutant particle is found in the shallow flow at the start, which may be mathematically described as:

$$M_d^0 = \frac{c_0/h}{240\pi\sqrt{D_{xx}D_{yy}}} e^{\left(-\frac{(x-x_0-60u)^2}{240D_{xx}} - \frac{(y-y_0)^2}{240D_{yy}}\right)} \quad (34)$$

$$M_s^0 = 0 \quad (35)$$

When the simulation starts, particles are assumed to be detached from the ground surface at a constant detachment rate of 0.01 and no particle will deposit back to the ground surface (i.e. $v_s = 0$). To maintain the constant detachment rate, m_0^* is taken to be equal to the concentration of deposited particles, and P , a_{d0} , b , F and D_R are set to be 0.01, 1, 1, 0 and 10, respectively. Based on these assumptions, the analytical solution of the concentration field is given by:

$$c(x, y, t) = e^{-0.01t + \ln\left(\frac{c_0}{240\pi\sqrt{D_{xx}D_{yy}}} \times e^{-\frac{(x-x_0-t-60)^2}{240D_{xx}} - \frac{(y-y_0)^2}{240D_{yy}}}\right)} \quad (36)$$

The numerical and analytical concentration profiles on the ground surface are shown in Fig. 10 at different output times. The pollutant concentration at the initial location decreases with time as the pollutant particles detached from the ground surface are transported to the downstream. Excellent agreement between the numerical prediction and analytical solution validates the particle detachment module of the wash-off model.

Fig. 10 Particle detachment test: numerical and analytical concentration profiles at different output times.

3.3 Pollutant wash-off and transport on urban road surfaces

In this section, the new coupled hydrodynamic and particle-based stormwater quality model is further validated by reproducing the wash-off experiments reported by Egodawatta et al. (2007). The experiments were designed to investigate pollutant wash-off process using simulated rainfall on three urban road surfaces in the Gold Coast Region, Queensland State, Australia. All three sites are located in the typical urban residential areas with different slopes. Each of the sites were demarcated into even plot surfaces of 3 m² (2 m × 1.5 m). The initial pollutant loads on the road surfaces were determined by collecting samples using a vacuum cleaner from the most downstream plot at each of the sites. The road names, slopes and initial pollutant loads of all of the three experimental sites are summarised in Table 1.

Table 1 Basic information about each of the experiment sites from Egodawatta et al. (2007).

Site	Slope of the road (%)	Pollutant mass on the 3 m ² experiment sites (g)
Lauder Ct.	10	9.3
Gumbeel Ct.	7.2	32.6

During the experiments, a rainfall simulator was used to produce different rainfall intensities and apply over different plots in each of the road sites, starting from the second most downstream plot and moving upstream in sequence. The runoff samples were collected using a catch tray and a vacuum system at the downstream end of each of these plots at a given time period. The fraction wash-off (F) was then defined as the weight ratio between the cumulative washed-off pollutants and the initial pollutant load. Here in this work, the experiments conducted with rainfall intensities of 40 mm/h, 65 mm/h, 86 mm/h, 115 mm/h and 133 mm/h are considered and simulated to provide representative results. It should be noted that 310 μm median particle size is applied in all of the three sites in this study since our numerical experiments show that the use of slightly different particle size between 305 μm and 310 μm (values extracted from the original median particle size gradation curve) has little impact on the final results.

Given the relatively small plot area and predominant convective dynamics of the rainfall-induced surface flow in these experiments, the diffusion effect in the pollutant transport process is negligible. With respect to other key model parameters in wash-off modelling, Hong et al. (2016a) suggested that their values could be selected from the test ranges suggested in the previous soil erosion studies (Beuselinck et al., 2002; Heng et al., 2011; Jomaa et al., 2010; Proffitt et al., 1991). Hong et al. (2019) also indicated that simulation results were not sensitive to the choices of parameters b , F and Ω_0 . Therefore, these parameters directly take the median values of the suggested test ranges as shown in Table 2. However, two more parameters, i.e. a_{d_0} and m_0^* , are still needed to be specified. According to the Hong et al. (2019, 2016a), a_{d_0} may be selected from a range between 1500 and 4500 kg/m^3 but careful calibration is needed to decide an appropriate value in relation to rainfall intensity. Heng et al. (2011) suggested a

range of values for m_0^* in the context of soil erosion with infiltration effect, which is not directly applicable to the current study that is focused more on impervious urban surfaces.

Table 2 Recommended values for model parameters.

Symbol	Units	Range	Value
b	-	0.8—2	1
F	-	0.01—0.03	0.02
Ω_0	W/m ²	0.15—0.35	0.25
D_R	mm		2

Fig. 11. Changes of model parameters a_{d_0} and m_0^* against the rainfall intensity.

To calibrate the wash-off model and find the best-fitted values for a_{d_0} and m_0^* , the Nash-Sutcliffe efficiency (NSE) coefficient and root-mean-square deviation (RMSD) are calculated by comparing the numerical simulation results with observations. The best-fitted a_{d_0} and m_0^* selected following a series of numerical experiments are listed in Table 3 and also plotted in Fig. 11 against the rainfall intensity. It is evident that the best-fitted values of a_{d_0} are consistent across the three road sites and only varies slightly for the same rainfall intensity. But a_{d_0} is found to be more sensitive to rainfall intensity and its values decrease as the rainfall intensity

increases. These conclusions are generally consistent with those reposted in the previous study (Hong et al., 2019) where a_{d_0} was recommended to take the value of 3625.3 kg/m³ for light rain, 1523.7 kg/m³ for moderate rain and 1641.9 kg/m³ for heavy rain. For m_0^* , it is trivial to tell that its values vary across a small range between 0.12 kg/m² and 0.05 kg/m² and generally decrease with the increasing rainfall intensity except for Gumbeel Ct. where m_0^* has a smaller value corresponding to the 40 mm/h rain than 65 mm/h and 86 mm/h. Compared with the similar m_0^* values on Lauder Ct. and Piccadilly Pl., the corresponding values on Gumbeel Ct. are greater. This may be explained by the different initial pollutant loads on the three roads and the initial pollutant mass on Gumbeel Ct. was almost 3 times greater than other two sites, as shown in Table 1. Therefore, the value of m_0^* may be also related to the initial pollutant load and further investigation will be needed in further research.

Table 3 The best-fitted values for a_{d_0} and m_0^* .

Rainfall intensity (mm/h)	Lauder Ct.		Gumbeel Ct.		Piccadilly Pl.	
	a_{d_0}	m_0^*	a_{d_0}	m_0^*	a_{d_0}	m_0^*
	(kg/m ³)	(kg/m ²)	(kg/m ³)	(kg/m ²)	(kg/m ³)	(kg/m ²)
40	3800	0.09	3200	0.1	3500	0.09
65	2300	0.08	2100	0.12	2200	0.09
86	1600	0.08	1600	0.12	1600	0.09
115	1600	0.06	1500	0.09	1600	0.08
133	1500	0.06	1500	0.06	1500	0.05

Fig. 12 Comparing the numerical results with measurements and empirical estimations obtained for different rainfall intensities on Lauder Ct.

The experiments are reproduced using the proposed particle-based stormwater quality model with the parameters as suggested in Tables 2 and 3. The results are plotted in Figs. 12-14, respectively for the three road sites, and compared with measurements of wash-off fraction (F) and also the results obtained from the empirical equations as proposed by Egodawatta et al. (2007). All of the simulation results achieve an acceptable level of agreement with the measured data, indicating that the proposed model is capable of simulating the full-process of pollutant dynamics on urban surfaces after calibration. In particular for the results as shown in Fig. 13(c, e) and Fig. 14(b, c), the returned values of NSE generally show an increasing trend with increasing rainfall intensity. This may indicate that the proposed model performs better on heavy rains, which may be due to the adoption of median particle size to represent the whole range of pollutant particles. The light rains may not be efficient in detaching the sediments represented uniformly as a whole using the median particle size. But in reality, the light rains may still be able to efficiently detach the smaller sediments which are not well represented by the model (i.e. sediments smaller than the median particle size). This may subsequently lead to less accurate predictions as observed. Additionally, the model seems to overpredict the pollutants being washed off for short-duration rainfall events but underpredict for long-duration

events on Gumbeel Ct., relative to the other two sites. But the predictions follow the same trends as the results from the empirical equations, i.e. the observations from the Gumbeel Ct. experiment do not agree as well with the equation results in comparison with the other two sites, indicating abnormality in experimental measurements.

The runtimes for the five simulations for Lauder Ct., conducted on a Dell Latitude laptop with a 4-core Intel i7-8650U CPU, are listed in Table 4, together with the event times. In all of the simulations, a grid with 200 x 150 cells is adopted and 9×10^4 particles are used to represent the initial pollutant load. Given the small simulation site, the computational time is considered to be high and further improvement in computational efficiency is needed for large-scale applications, which may be achieved through implementation of the entire coupled modelling framework on GPUs.

Table 4 Computational time for Lauder Ct.

Rainfall intensity (mm/h)	Lauder Ct.	
	Computational Time (min)	Event Time (min)
40	15	35
65	13	30
86	11	25
115	10	25
133	8	20

Fig. 13 Comparing the numerical results with measurements and empirical estimations obtained for different rainfall intensities on Gumbeel Ct.

Fig. 14 Comparing the numerical results with measurements and empirical estimations obtained for different rainfall intensities on Piccadilly Pl.

In addition to the model parameters as mentioned before, the performance of the proposed stormwater quality model may be also sensitive to other model settings, including e.g. grid resolution and the number of particles being used to represent the pollutant loads. Herein, more simulations are run to first test the convergence of simulation results against the number of particles. Two typical rainfall intensities, 40 mm/h and 133 mm/h, are selected and simulations are run on all three road sites with the number of particles increasing from 0.1×10^4 to

12×10^4 . NSE and RMSE calculated against the wash-off fraction are used to assess model performance and the results are presented in Fig. 15 and Fig. 16 respectively for the two different rainfall intensities. Clearly, the numerical results appear to converge as the number of particles increases and the simulation accuracy can no longer be further improved when the number of particles moves beyond 3×10^4 .

Fig. 15 Convergence test against the number of particles used to represent the initial pollutant loads on the three road sites using 40 mm/h rainfall input.

To evaluate the sensitivity of the simulation results to the grid resolution, i.e. the number of grid cells used to distribute pollutant particles during the wash-off process, further simulations are conducted on the Piccadilly Pl. site using an example rainfall input of 133 mm/h. Based on the results from the above convergence test against the number particles, 3×10^4 particles are used and the number of grid cells varies from 12 to 12×10^4 . Fig. 17 shows the simulation results and it is clear that the results start to converge from 7,500 cells.

Fig. 16 Convergence test against the number of particles used to represent the initial pollutant loads on the three road sites using 133 mm/h rainfall input.

Fig. 17. Convergence test against the number of grid cells used to distribute pollutant particles.

3.4 Pollutant wash-off and transport in a V-shaped catchment

Finally, the new coupled model is applied to an idealised V-shaped catchment to further validate its capability in predicting runoff-driven pollutant dynamics on more complex topographies involving SuDS features. As shown in Fig. 18, the two hillsides have a topography chosen to be the same as the Lauder Ct. considered previously in section 3.3 and are connected to a channel with a slope of 0.1 in the middle which is installed with a container of 0.5 m $\times$ 0.2 m $\times$ 0.3 m to represent a detention pond and a 0.5 m $\times$ 0.2 m infiltration area to mimic a vegetated swale (represented by an infiltration rate of 3.61×10^{-6} m/s and a Manning

coefficient of $0.1 \text{ m/s}^{1/3}$). A load of 9.3 g pollutants is uniformly distributed on the surface of each of the hillsides, but no pollutants are initially placed in the channel. Constant and uniform rainfall of 133 mm/h continuously falls on the whole catchment for 1200 s (i.e. 20 mins) from the beginning. All boundaries are closed, except for the downstream channel outlet where open boundary conditions are imposed. A uniform grid of 0.01 m resolution is used to discretise the domain for the simulation.

Fig. 18 Schematic of the V-shaped catchment with SuDS features.

Fig. 19(a) presents the hydrographs of water depth predicted by HiPIMS at the locations before (L1), inside (L2) and at the end of the detention pond (L3), inside (L4) and at the end of the swale (L5). The flow is intercepted by the pond and develops a larger water depth (L2) compared with the depths at other locations. The pond reaches its maximum capability after 449s; from then the water depth inside the pond (L2) stops growing and becomes steady. The water depths at the downstream locations (L3, L4, L5) show a small rise in sequence to reflect the release of water from the pond, as illustrated in Fig. 19(b). The difference of water depth between L3 and L4 indicates that the effect of higher bed friction (Manning coefficient) and infiltration in the swale has been correctly captured, which effectively reduces the overland flow at the downstream. Since the experimental settings for Lauder Ct are adopted in this test, the simulation results in terms of wash-off fraction should be consistent with the experimental measurements and this is confirmed in Fig. 20.

Fig. 19 Water depth hydrographs at different locations in the channel during the rainfall event: (a) Water depths at all five locations; (b) Water depths at four locations without L2.

Fig. 20 Comparing the predicted wash-off fraction with the measurements.

Fig. 21 Initial particle distribution at the hillsides.

To identify the sources of pollutants in the pond and the infiltration area, the initial distribution of particles in the hillsides is divided into five regions marked in different colours, as illustrated in Fig. 21, in which the location of the detention pond and the swale are also indicated. Fig. 22 represents the particles located inside the detention pond and swale at different output times. Apparently, due to its location, the detention pond only captures

pollutants from regions 1 & 2, i.e. only red and blue particles are detected inside the spot, during the whole rainfall event. The pollutants flow into the swale come from region 3 and 4 at the beginning. As time increases, pollutant particles from region 1 & 2 (red and blue particles) start to ‘leak’ from the pond and travel to the swale. Since region 5 is downstream of both SuDS features, the pollutants from this region are not captured by either of the features. To quantify the composition of pollutant particles in the two SuDS features, percentages of particles from different regions are calculated and plotted in Fig. 23 for (a) the detention pond and (b) the swale. As confirmed in Fig. 23(a), the pond only captures particles from regions 1 & 2 and the number of particles increases until approx. $t = 10$ min to reach the pond’s maximum capability. After that, a small amount of pollutants starts to ‘leak’ from the pond and move downstream to reach the swale area, which is reflected in the particle composition plot in Fig. 23(b) for the swale. For the swale, the number of particles (from regions 3 & 4) in the area reaches its peak at the very earlier stage and starts to decrease afterwards. Since vegetation interception and pollutant infiltration are not considered in the current model, the swale only slows down the flow and also the movement of the particles but cannot intercepts any pollutants. Therefore, the total amount of pollutants containing in the area are also smaller than those in the pond at the corresponding moments. As a whole, the simulation results are as expected and successful simulation of this test case demonstrates that the proposed modelling framework can effectively identify the source and trace out the pathways of pollutants passing any specific location. Such information will be very useful for the planning and design site-specific controlling measures, i.e. SuDS, to more effectively manage urban surface pollutants.

Fig. 22 Snapshots of particles located at the two SuDS features at different output times.

Fig. 23 Particle composition at the two SuDS features during the rainfall event: (a) Detention pond; (b) Swale.

4. Conclusions

In this study, a new coupled hydrodynamic and particle-based water quality model is developed to simulate the full-process dynamics of NPS particulate pollutants induced by rainfall in urban areas, from pollutant detachment, transport to deposition. Based on a particle-based approach, the model can effectively represent the physical processes of pollutant wash-off and transport and trace out the trajectories or fates of individual particles to identify the pathways of NPS

pollutants. To our best knowledge, this is the first time such a coupled modelling strategy is reported to simulate the full-process dynamics of NPS pollutants in urban areas.

The new coupled model is successfully validated by simulating idealised and experimental test cases with satisfactory results obtained, in comparison with analytical solutions or experiment measurements. The current model is based on a coupled hydrodynamic and particle-based modelling approach which can better depict the hydrodynamics of the rainfall generated overland flow comparing with the traditional hydrological or simplified hydraulic models. The use of the particle-based methods can effectively represent the Lagrangian dynamics of the pollutant particles and trace out the trajectories of individual particles, which can be subsequently used to derive the pathways of pollutants.

Whilst potentially providing a useful tool to improve the planning and design practice of nature-based solutions (e.g. SuDS) to achieve multiple benefits in urban water management, the current model still has a number of limitations that will benefit from further developments in the future. Firstly, a single class size based on the median particle diameter is used to represent pollutant loads in the model. The simulation results from the experiment test cases indicate that this may not be adequate to accurately depict the pollutant dynamics driven by low-intensity rainfall and this is consistent with the conclusions reported by Hong et al. (2016a). Secondly, further theoretical research is still needed to better understand the behaviours of certain model parameters, e.g. a_{d_0} and m_0^* , for different applications. Furthermore, the model needs further improvement on computational efficiency, e.g. through implementing the entire coupled modelling system on high-performance GPUs, for simulations involving large number of particles over a large domain. Finally, the current NPS modelling system does not include modelling components to explicitly simulate different types of SuDS. Immediate future work will be to develop and couple compatible modelling strategies for different types of SuDS to support the planning and design of SuDS and assess their operation performance in practice.

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638 **References**

- 639 Ahiablame, L.M., Engel, B.A., Chaubey, I., 2012. Effectiveness of low impact development
640 practices: Literature review and suggestions for future research. *Water. Air. Soil Pollut.*
641 223, 4253–4273. <https://doi.org/10.1007/s11270-012-1189-2>
- 642 Arthur, S., Krivtsov, V., Allen, D., 2019. Blue-green infrastructure – perspectives on water
643 quality benefits, C780b.
- 644 Bach, P.M., Rauch, W., Mikkelsen, P.S., McCarthy, D.T., Deletic, A., 2014. A critical review
645 of integrated urban water modelling - Urban drainage and beyond. *Environ. Model.*
646 *Softw.* <https://doi.org/10.1016/j.envsoft.2013.12.018>
- 647 Baek, S.S., Choi, D.H., Jung, J.W., Lee, H.J., Lee, H., Yoon, K.S., Cho, K.H., 2015.
648 Optimizing low impact development (LID) for stormwater runoff treatment in urban
649 area, Korea: Experimental and modeling approach. *Water Res.* 86, 122–131.
650 <https://doi.org/10.1016/j.watres.2015.08.038>
- 651 Beuselinck, L., Hairsine, P.B., Govers, G., Poesen, J., 2002. Evaluating a single-class net
652 deposition equation in overland flow conditions. *Water Resour. Res.* 38, 15-1-15–10.
653 <https://doi.org/10.1029/2001wr000248>
- 654 Cheng, N.-S., 1997. Simplified settling velocity formula for sediment particles. *J. Hydraul.*
655 *Eng.* 123, 728–731. [https://doi.org/https://doi.org/10.1061/\(ASCE\)0733-](https://doi.org/https://doi.org/10.1061/(ASCE)0733-9429(1997)123:8(728))
656 [9429\(1997\)123:8\(728\)](https://doi.org/https://doi.org/10.1061/(ASCE)0733-9429(1997)123:8(728))
- 657 DEFRA, 2012. Tackling water pollution from the urban environment: Consultation on a

strategy to address diffuse water pollution from the built environment 26.

Egodawatta, P., Thomas, E., Goonetilleke, A., 2007. Mathematical interpretation of pollutant wash-off from urban road surfaces using simulated rainfall. *Water Res.* 41, 3025–3031. <https://doi.org/10.1016/j.watres.2007.03.037>

Follett, E., Chamecki, M., Nepf, H., 2016. Evaluation of a random displacement model for predicting particle escape from canopies using a simple eddy diffusivity model. *Agric. For. Meteorol.* 224, 40–48. <https://doi.org/10.1016/j.agrformet.2016.04.004>

Gilbert, J.K., Clausen, J.C., 2006. Stormwater runoff quality and quantity from asphalt, paver, and crushed stone driveways in Connecticut. *Water Res.* 40, 826–832. <https://doi.org/10.1016/j.watres.2005.12.006>

Gomez-Gesteira, M., Montero, P., Prego, R., Taboada, J.J., Leitao, P., Ruiz-Villarreal, M., Neves, R., Perez-Villar, V., 1999. A two-dimensional particle tracking model for pollution dispersion in A Coruna and Vigo Rias (NW Spain). *Oceanol. Acta* 22, 167–177. [https://doi.org/10.1016/S0399-1784\(99\)80043-7](https://doi.org/10.1016/S0399-1784(99)80043-7)

Hairsine, P.B., Rose, C.W., 1992a. Modeling water erosion due to overland flow using physical principles: 2. Rill flow. *Water Resour. Res.* 28, 245–250. <https://doi.org/10.1029/91WR02381>

Hairsine, P.B., Rose, C.W., 1992b. Modeling water erosion due to overland flow using physical principles: 1. Sheet flow. *Water Resour. Res.* 28, 237–243. <https://doi.org/10.1029/91WR02380>

Heng, B.C.P., Sander, G.C., Armstrong, A., Quinton, J.N., Chandler, J.H., Scott, C.F., 2011. Modeling the dynamics of soil erosion and size-selective sediment transport over nonuniform topography in flume-scale experiments. *Water Resour. Res.* 47.

681 <https://doi.org/10.1029/2010WR009375>

682 Hong, Y., Bonhomme, C., Le, M.H., Chebbo, G., 2016a. A new approach of monitoring and
683 physically-based modelling to investigate urban wash-off process on a road catchment
684 near Paris. *Water Res.* 102, 96–108. <https://doi.org/10.1016/j.watres.2016.06.027>

685 Hong, Y., Bonhomme, C., Le, M.H., Chebbo, G., 2016b. New insights into the urban washoff
686 process with detailed physical modelling. *Sci. Total Environ.* 573, 924–936.
687 <https://doi.org/10.1016/j.scitotenv.2016.08.193>

688 Hong, Y., Liao, Q., Bonhomme, C., Chebbo, G., 2019. Physically-based urban stormwater
689 quality modelling: An efficient approach for calibration and sensitivity analysis. *J.*
690 *Environ. Manage.* 246, 462–471. <https://doi.org/10.1016/j.jenvman.2019.06.003>

691 Huai, W., Yang, L., Wang, W.J., Guo, Y., Wang, T., Cheng, Y. guang, 2019. Predicting the
692 vertical low suspended sediment concentration in vegetated flow using a random
693 displacement model. *J. Hydrol.* 578. <https://doi.org/10.1016/j.jhydrol.2019.124101>

694 Jomaa, S., Barry, D.A., Brovelli, A., Sander, G.C., Parlange, J.Y., Heng, B.C.P., Tromp-van
695 Meerveld, H.J., 2010. Effect of raindrop splash and transversal width on soil erosion:
696 Laboratory flume experiments and analysis with the Hairsine-Rose model. *J. Hydrol.*
697 395, 117–132. <https://doi.org/10.1016/j.jhydrol.2010.10.021>

698 Liang, Q., Smith, L.S., 2015. A High-Performance Integrated hydrodynamic Modelling
699 System for urban flood simulations. *J. Hydroinformatics* 17, 518–533.
700 <https://doi.org/10.2166/hydro.2015.029>

701 Liang, Q., Taylor, P.H., Borthwick, A.G.L., 2007. Particle mixing and reactive front motion
702 in unsteady open shallow flow - Modelled using singular value decomposition. *Comput.*
703 *Fluids* 36, 248–258. <https://doi.org/10.1016/j.compfluid.2006.01.018>

704 Mutchler, C.K., Hansen, L.M., 1970. Splash of a waterdrop at terminal velocity. *Science*
705 (80-.). 169, 1311–1312. <https://doi.org/10.1126/science.169.3952.1311>

706 Obropta, C.C., Kardos, J.S., 2007. Review of Urban Stormwater Quality Models:
707 Deterministic, Stochastic, and Hybrid Approaches1. *JAWRA J. Am. Water Resour.*
708 *Assoc.* 43, 1508–1523. <https://doi.org/10.1111/j.1752-1688.2007.00124.x>

709 Olascoaga, M.J., Beron-Vera, F.J., Haller, G., Triñanes, J., Iskandarani, M., Coelho, E.F.,
710 Haus, B.K., Huntley, H.S., Jacobs, G., Kirwan, A.D., Lipphardt, B.L., Özgökmen, T.M.,
711 H. M. Reniers, A.J., Valle-Levinson, A., 2013. Drifter motion in the Gulf of Mexico
712 constrained by altimetric Lagrangian coherent structures. *Geophys. Res. Lett.* 40, 6171–
713 6175. <https://doi.org/10.1002/2013GL058624>

714 Paresi, M., Melchiorri, M., Siragusa, A., Kemper, T., 2016. Atlas of the Human Planet.
715 Mapping Human Presence on Earth with the Global Human Settlement Layer.
716 <https://doi.org/10.2788/889483>

717 Proffitt, A.P.B., Rose, C.W., Hairsine, P.B., 1991. Rainfall Detachment and Deposition:
718 Experiments with Low Slopes and Significant Water Depths. *Soil Sci. Soc. Am. J.* 55,
719 325. <https://doi.org/10.2136/sssaj1991.03615995005500020004x>

720 Rossman, L.A., Huber, W.C., 2016. Storm Water Management Model Reference Manual
721 Volume III – Water Quality. United States Environ. Prot. Agency III, 235.
722 <https://doi.org/EPA/600/R-15/162> |

723 Sage, J., Bonhomme, C., Al Ali, S., Gromaire, M.C., 2015. Performance assessment of a
724 commonly used “accumulation and wash-off” model from long-term continuous road
725 runoff turbidity measurements. *Water Res.* 78, 47–59.
726 <https://doi.org/10.1016/j.watres.2015.03.030>

727 Sämann, R., Graf, T., Neuweiler, I., 2019. Modeling of contaminant transport during an
 728 urban pluvial flood event – The importance of surface flow. *J. Hydrol.* 568, 301–310.
 729 <https://doi.org/10.1016/j.jhydrol.2018.10.002>

730 Shaw, S.B., Parlange, J.Y., Lebowitz, M., Todd Walter, M., 2009. Accounting for surface
 731 roughness in a physically-based urban wash-off model. *J. Hydrol.* 367, 79–85.
 732 <https://doi.org/10.1016/j.jhydrol.2009.01.004>

733 Shaw, S.B., Walter, M.T., Steenhuis, T.S., 2006. A physical model of particulate wash-off
 734 from rough impervious surfaces. *J. Hydrol.* 327, 618–626.
 735 <https://doi.org/10.1016/j.jhydrol.2006.01.024>

736 Tsihrintzis, V.A., Hamid, R., 1997. Modeling and management of urban stormwater runoff
 737 quality: A review. *Water Resour. Manag.* <https://doi.org/10.1023/a:1007903817943>

738 Weitbrecht, V., Uijttewaal, W., Jirka, G.H., 2003. 2-D Particle Tracking to Determine
 739 Transport Characteristics in Rivers with Dead Zones. *Shallow flows* 1–8.

740 Xia, X., Liang, Q., Ming, X., 2019. A full-scale fluvial flood modelling framework based on
 741 a high-performance integrated hydrodynamic modelling system (HiPIMS). *Adv. Water*
 742 *Resour.* 132. <https://doi.org/10.1016/j.advwatres.2019.103392>

743 Zhang, L., Liang, Q., Wang, Y., Yin, J., 2015. A robust coupled model for solute transport
 744 driven by severe flow conditions. *J. Hydro-Environment Res.* 9, 49–60.
 745 <https://doi.org/10.1016/j.jher.2014.04.005>

746