Different approaches for particle representation in plastic debris transport models

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Different Approaches for Particle Representation in Plastic Debris Transport Models

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ABSTRACT: Knowledge of plastic debris transport mechanism in open waters and its interaction with hydraulic structures (i.e. accumulation and clogging) is of paramount importance for effective waste-removal strategies and sustainable management of plastic debris. To the author's best knowledge, current models for prediction of plastic debris transport assume a highly simplified geometry, while making use of parameterization of the physical processes, therefore pointing out the need for further research. Herein, the effect of shape and buoyancy on the motion of a single particle was studied employing point-particle approach while the background flow is solved using RANS approach. It is observed that the particles with the same amount of plastic mass but different shape and density showed substantially different behaviors, resulting in different trajectories. Since parametrization and point-particle approach were used, even if the particle size is larger than the mesh size, these preliminary results showed that further validation is required for prediction of accurate trajectory by means of resolved-particle approach.

1 INTRODUCTION

Plastic debris of different sizes, shapes, densities, polymer compositions, and mechanical properties have been observed in riverine, estuarine and marine environments, worsening the ecological and aesthetic values of the environment (Derraik, 2002) (Figure 1). Moreover, plastic waste is an important issue for urban flooding (Honingh *et al.*, 2020), especially in those countries that do not have a suitable waste management strategy. Therefore, removal and disposal of plastic debris from the aquatic environment is an urgent issue that needs to be addressed, in line with Goal 14 of United Nations' sustainable development goals.

Figure 1. Plastic waste accumulation upstream of a culvert, Ghana. (Photo courtesy: TUDelft Global Initiative)

It is therefore important to know the trajectories and accumulation zones of plastic waste in order to remove them within the water system, before they reach the ocean. The scientific community - consisting of oceanographers, marine biologists, and hydraulic engineers, has been investigating the behavior of plastic waste, focusing on marine environments and somehow neglecting riverine systems (Al-Zawaidah, Ravazzolo and Friedrich, 2021). To date, main research trends for plastic debris transport can be identified based on geographical locations as (1) marine plastic debris (Van Sebille *et al.*, 2020), (2) riverine/freshwater plastic debris (Horton *et al.*, 2017) and (3) estuarine plastic debris (López *et al.*, 2021). This classification is mostly associated with the differences in transport phenomena in these environments. For instance, the transport processes in estuarine environment is more complex than pure freshwater and saltwater systems, because of stratification of density layers, affecting buoyancy and mixing.

Besides the location, the approaches used in research can be distinguished as: (1) physics-based numerical modelling (Mountford and Morales Maqueda, 2019), (2) stochastic modelling (Maximenko, Hafner and Niiler, 2012), (3) field surveys (Van Emmerik *et al.*, 2019), (4) satellite tracking devices (drifters) (Maximenko, Hafner and Niiler, 2012), (5) laboratory experiments (Waldschläger *et al.*, 2020) and (6) combined methods. Physics-based modelling approaches can be divided into two sub-fields, i.e. (1) Lagrangian transport methods (Wakata and Sugimori, 1989) and (2) Eulerian concentration methods (Mountford and Morales Maqueda, 2019). Regarding stochastic modelling approach, to date the following distinction can be made: (1) transit matrix method (Van Sebille, England and Froyland, 2012) and (2) probability function (Maximenko, Hafner and Niiler, 2012). Laboratory experiments were carried out for the investigation of vertical velocities of plastic particles (Khatmullina and Isachenko, 2017), heteroaggregation of nano- and microplastics and other different particles (Besseling *et al.*, 2017), and water level changes due to plastic debris blockage (Honingh *et al.*, 2020).

In addition to modelling of plastic debris transport, estimation of global plastic mass budget was undertaken by Lebreton *et al.*, (2017) who approached this empirically by means of an inventory of plastic waste input from the urban to the ocean via the rivers based on Mismanaged Plastic Waste (MPW) generation data, rather than using physics-based hydrodynamic and transport models (Neumann, Callies and Matthies, 2014).

Modelling the behavior of plastic waste and particles in the aquatic environment is a difficult task because it requires an understanding of (1) its short- and long-term behavior (physical and chemical degradation, sinking, floating, beaching, washing-off), (2) its interaction with aquatic life (biofouling, biological degradation) and (3) their self-interaction [aggregation (Horton *et al.*, 2017), entanglement]. Moreover, it is also difficult to observe their collective characteristics because plastic debris with different sizes, shapes, densities, polymer compositions and mechanical properties usually coexist in the water system. Complicating factors include the varying entrapment of air and water, that affects buoyancy and inertia.

Plastic debris models can be differentiated, based on particle size, between (1) nanoplastic (< 100 nm), (2) microplastic (0.1 - 5 mm), (3) mesoplastic (5 - 25 mm) and (4) macroplastic (> 25 mm), although a conventional definition of size is not yet established (Alimi *et al.*, 2018). A discrepancy in the definition of macroplastic size can be seen in Waldschläger *et al.*, 2020, who assumed the macroplastic class for > 5 mm in size. Therefore, this points out the need for a more detailed classification system for plastic waste and particles for better modelling strategies, including relations to flow properties such as buoyancy, response time (Bec, Cencini and Hillerbrand, 2007) and relaxation time.

While most research focused on large-scale plastic accumulation and transport within case studies (Kubota, 1994; Neumann, Callies and Matthies, 2014), a few studies looked at local processes of plastic debris, including vertical distribution of plastic particles (Kooi *et al.*, 2016), rising and settling velocities (Chubarenko *et al.*, 2016) and its wave-induced motion (Alsina, Jongedijk and van Sebille, 2020). Generally, different research methods were applied depending on the physical processes and regions of interest. To the author's best knowledge, current models for prediction of plastic debris transport assume a highly simplified geometry of plastic waste - i.e. spherical, cylindrical shapes, and make use of parametrization of the physical processes, therefore requiring further investigations.

In the current research, the effect of buoyancy and size on the motion of a single particle was studied using the point-particle approach although the considered particle size is larger than the mesh size. The objective of this paper is to demonstrate that the point-particle approach is not sufficiently accurate to predict the trajectory of the large particle compared with the computational mesh size. The preliminary results show that the current point-particle approach necessitates a better parameterization of physical processes, especially in the interaction of particle with the free surface.

1.1 *Numerical Modelling Challenges*

In general, there are two steps in the prediction of plastic debris transport using a numerical model: (1) underlying hydrodynamic model and (2) material transport associated with the flow. Prediction of debris transport can be approached in a detailed manner after the achievement of a flow model that is able to describe velocity, turbulence mixing, diffusion, and dispersion in both horizontal and vertical dimensions.

Generally, the underlying hydrodynamics is simulated solving for the Reynolds equations with turbulence closure models, however, the simulation of particle trajectories is still a difficult task due to the difficulty in particle representation in the numerical model. If the particles are assumed to travel with the flow i.e. negligible inertia, the passive tracer approach is commonly used for particle tracking. With this approach, there exist two techniques for tracing the particles i.e. an Eulerian concentration technique and passive Lagrangian tracking technique, both of which do not consider the particle dynamic and orientation explicitly. However, when inertia and buoyancy become significant, its trajectory should be considered separately from the underlying flow, which leads to a coupling between the particle shape and its net transport. In this case, rotation and orientation of non-spherical particles play an important role in their trajectory via forces such as drag, lift and added-mass. This requires the application of finite-size particle approach in which particles smaller than the resolved length scales can be considered as point masses, i.e. the so-called point-particle method, neglecting the presence of particle in the continuous fluid in the evaluation of the equations of motion, thereby accounting for the particle dynamics. Another difficulty with this method is the lack of force coefficients for asymmetrical and irregular shapes.

Lastly, it should be mentioned that plastic items of significant dimension should not be modelled as point particles because of their specific dynamics, which otherwise would result in non-physical behaviors. Hence, a method that accounts for variation of hydrodynamic forces around the plastic item should be applied, including particle orientation, particle-particle interaction and interactions with banks and structures. However, the computational resources limit the numbers and detailed representation of the particles in the computational domain since this method requires a high resolution for the hydrodynamics as well and might go beyond the RANS approach, with techniques such as LES, DES or even DNS.

2 METHODOLOGY

In order to model the accumulation process of plastic debris at a hydraulic structure or waste-collection device, a proper representation of particles is necessary to simulate the physical behavior of particle-particle interaction, jointly with the structure. This research is divided into three stages visualized in Figure 2: (1) identifying the forces acting on the particle and their influences on the particle trajectory using point-particle approach, (2) comparison of results using resolved-particle approach, and (3) modelling accumulation process by considering particle-particle interaction and particle-structure interaction.

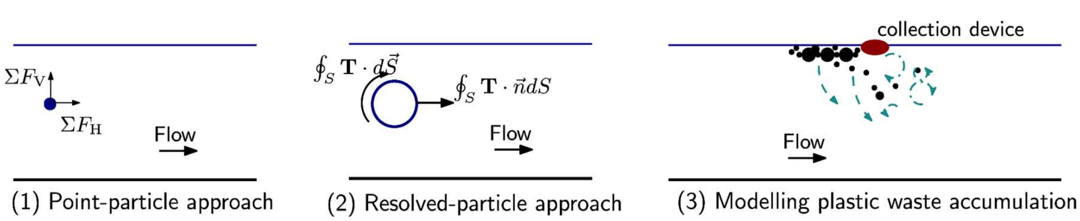

Figure 2. Three stages of modelling plastic waste accumulation at the collection device. F_V and F_H denote the horizontal and vertical forces acting on the particle due to fluid, respectively. $\mathbf{T}$ denotes the traction force acting on the surface of the volume particle and dS is the differential area. $\vec{n}$ is the unit normal vector pointing outward.

In stage 1, the influence of fluid forces such as pressure gradient, virtual mass, lift and buoyancy on the particle dynamics will be studied using the point-particle approach. This approach is only valid for particles smaller than the computational mesh size. Therefore, in stage 2 similar studies will be extended using resolved-particle approach to validate the observations from stage 1. In resolved-particle approach, a particle which is larger than mesh size, needs to be discretized and imposed appropriate boundary conditions on its interface with ambient fluid. After evaluating the insights from previous stages, the accumulation process of plastic items at the hydraulic structure will be studied, incorporating the interaction between particles themselves, and fluid-particle.

As a first step, this paper investigates the trajectory of the particle and its dependence on buoyancy, drag and added-mass (or virtual-mass) forces, using point-particle method, i.e. without resolving the particle. Reynolds-Averaged Navier-Stokes equations with realizable k-ε closure model were applied for solving fluid continuum with particle equations for discrete particles.

The numerical model simulated a channel with dimension 5.0 m × 0.2 m × 0.4 m and it is referenced to a typical laboratory flume. In each case, the particle is released at (0.002, 0.08, 0.02) m of the flume coordinate, i.e. about half of the water depth, while accounting for buoyancy, virtual-mass and lift force in the particle equation. The computational mesh size is 0.015 mm for *x*, *y* and *z*-dimensions, aiming for $y^+ = 100$. The velocity profile of the simulated flow was found in agreement with the theoretical profile.

A description of the simulations is summarized in Table 1. The *Point* case aimed to simulate a 1 liter plastic bottle as a compact situation, and its mass is assumed 20 g. Therefore, the diameter of the solid spherical particle that would have the same mass of the bottle is 15.12 mm. In the *Empty* case, the bottle is filled with air but the same amount of plastic is kept to compare the behavior. Finally, the *Half-filled* case is simulated for the bottle half filled with water and half with air. Due to water mass inside the bottle, the density changes significantly, but the diameter remains the same as in *Empty* case. These three cases simulate different configurations of plastic bottles in the river channel. It should be noted that, in all of simulations, the particle shape is assumed to be a sphere and density of PET is 1380 kg/m^3.

Here the restitution coefficient, i.e. the ratio of relative velocity of the particles after collision to before collision, was assumed 1 for the interaction between the particle and the bottom, and 0.2 for the particle and the free surface.

Table 1. Three cases of simulations for the same amount of plastic.

ID	Description	Density (kg/m^3)	Diameter (mm)
Point	compacted bottle.	1380.00	15.12
Empty	bottle filled with air.	20.92	62.30
Half-filled	bottle filled with water and air, each half.	513.78	62.30

3 RESULTS AND DISCUSSION

The trajectories of the particle for the three simulations are shown in Figure 3. The point particle condensed from the 1 liter plastic bottle shows a sinking behavior while the particles filled with air and water float. Once the point particle hits the bottom of the flume, it bounces until the equilibrium condition is found. This is not the case for floating particles where the behavior is mainly dependent on the restitution parameter, which needs an additional study on the interaction between free surface and rising particles. The same holds for the particle-turbulence interaction. This knowledge may be important for accumulation processes near the hydraulic structure where some particles remain trapped, while others can pass underneath it.

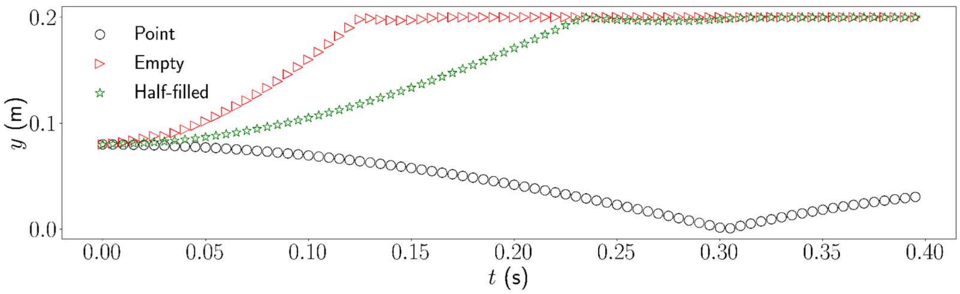

Figure 3. Vertical position of the particle for three cases.

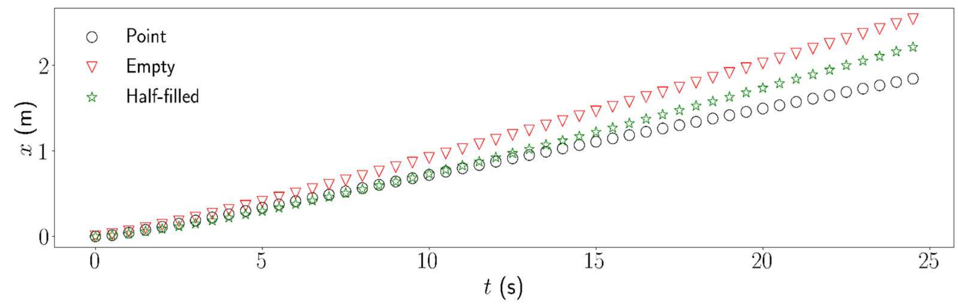

Figure 4. Horizontal trajectory of the particle for three cases in Table 1.

Figure 4 depicts the streamwise displacement of the particle for all three cases. The empty bottle was the fastest among the tested scenarios and the point particle (which is dense and small), located near the bottom moves slower than the half-filled bottle. In fact, the particle kinematics is the result of the interplay between drag, added-mass (both affected by particle size), and buoyancy caused by density differences. Moreover, the velocity gradient of the ambient flow can also play an important role in particle kinematics such as lift force contribution. However since parametrization was used for the lift force, added-mass and drag force in this research, variation of fluid forces on the particle surface were not accounted for.

It should be noted that in this preliminary study the validation for the particle trajectory was not conducted although the flow field in the numerical flume was observed as the fully developed flow. However, the bouncing behavior in the sinking case of the point particle was found qualitatively similar to the experimental case (Gondret, Lance and Petit, 2002).

4 CONCLUSIONS

In this research, some examples were provided for the effect of shape and buoyancy on the motion of a particle using point-particle approach, even if particle size is larger than computational mesh size. RANS equations were solved for the flow field with realizable k-ε closure model. The small and dense point particle showed a sinking trajectory with a bouncing behavior during its initial impact with the bottom. The empty and half-filled bottles showed a raising trajectory, however they do not show such a bouncing behavior since a restitution coefficient of 0.2 was used. This pointed out that further investigations for a better understanding of rising particle and free surface interaction are needed, important to model the accumulation process.

These preliminary results show that particles with the same amount of plastic, but different shapes show totally different particle trajectory because of the change in density. This kind of complexity can also be expected in real-life situation where a variety of plastic waste debris exists in the riverine system, exposed to many environmental factors. In fact, for the application to plastic waste whose size is around 20 cm, the particle trajectory should be simulated using resolved-particle approach where the particle occupies the computational mesh explicitly, without any physical parameterization of drag force, lift force and virtual mass coefficients. With this approach, one can include the variations of the turbulent flow field around the particle, leading to more accurate calculation of forces acting on the particle surface.

These preliminary results showed that further validation is required for prediction of accurate trajectory by means of resolved-particle approach. Hence, within this research, the resolved-particle approach will be applied for particle representation in the hydrodynamic model where large flow structure is also solved, thereby considering some scales of turbulent fluctuation. It is expected that the results from resolved-particle approach will be compared with the current point-particle approach for large particles.

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