Contents lists available at ScienceDirect

International Communications in Heat and Mass Transfer

journal homepage: www.elsevier.com/locate/ichmt

Transport of pollutant particles in a reservoir due to diurnal temperature variation[☆]

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article info abstract

Available online 1 March 2014

Keywords: Natural convection Particle transport Reservoir Diurnal thermal forcing Computational Fluid Dynamics Discrete Phase Model

This study is concerned with particle transport in a reservoir model subject to diurnal temperature variation at the water surface. A Computational Fluid Dynamics (CFD) code coupled with a Discrete Phase Model (DPM) is adopted to examine the particle transport in the reservoir. The particle deposition and dispersion as well as the concentration of particles in various regions of the water body are examined. The present study demonstrates the importance of buoyancy-driven flows for particle deposition and dispersion in reservoirs. © 2014 Elsevier Ltd. All rights reserved.

1. Introduction

The presence of pollutants or nutrients in reservoirs or lakes may have a negative impact on the quality of the stored water. One of the potential severe consequences is the bloom of cyanobacteria in the storages. Not only does the bloom disrupt the normal ecosystem of the water body, but also the microcystin released from the cyanobacteria is a threat to drinking water quality and thus a threat to public health. Understanding the deposition and dispersion behaviour of pollutant or nutrient particles is essential for water quality management. In general particles suspended in a fluid are transported by the flow, either passively, in which case the particles simply follow the flow and have no other interaction, or actively, in which case the particles may have a degree of self-determination, for example their buoyancy, and may interact with the flow. One such flow is the buoyancy-driven flow resulting from temperature gradients (e.g. [\[1](#page--1-0)–3]).

In natural water bodies the pollutant or nutrient particles are usually introduced in the near-shore region, either from local runoff or stream inflow. Previous studies have demonstrated that the buoyancy-driven flows resulting from diurnal thermal forcing (e.g. [\[1](#page--1-0)–4]) provide an important transport mechanism in the near-shore region of reservoirs. These studies [\[1](#page--1-0)–4] have reported a distinct instability in the form of plunging plumes from the surface during the cooling phase. During the radiation heating phase, the re-emission of residual radiation from the bottom may also generate rising plumes. In addition, the presence

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of a sloping bottom in the near-shore region results in a lateral temperature gradient with warmer water in the shallow part during the heating phase and cooler water during the cooling phase. This generates a circulation out along the surface during heating, or a plunging flow along the slope during cooling [\[1,5,6\].](#page--1-0)

Numerical studies of particle transport in fluids have been reported extensively. Among these investigations, Guha [\[7\]](#page--1-0) reviewed the particle transport mechanisms in laminar and turbulent flow regimes respectively under both the Eulerian–Eulerian and Eulerian–Lagrangian frameworks. Studies of particle motion induced by natural convection have also been reported. For instance, Akbar et al. [\[8\]](#page--1-0) numerically examined particle deposition and dispersion in fluids within a square cavity under natural convection. Puragliesi et al. [\[9\]](#page--1-0) and Pallares and Grau [\[10\]](#page--1-0) discussed the effect of particle properties on their motion in fluid flows under different configurations. Direct comparisons of the particle deposition rates were carried out with different particle relaxation times which characterise the particle sizes and densities [\[9,10\].](#page--1-0) Although most of the existing studies have addressed the extent to which both the fluid flows and the particle properties affect the particle transport in fluids, few studies have quantified the dependency of the particle deposition and dispersion on the induced fluid flows under natural convection.

In the present study, the particle transport in a reservoir model under a cycling temperature imposed at the water surface is numerically simulated using the finite volume CFD code ANSYS FLUENT 13 coupled with a built-in Discrete Phase Model (DPM) under the Eulerian–Lagrangian framework. The purpose of this study is to quantify the dependency of the particle transport, including their deposition and dispersion behaviour, on particle properties and the diurnal thermal forcing.

[☆] Communicated by W.J. Minkowycz.

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2. Numerical details and tests

2.1. Fluid flow model formulation

A two-dimensional (2D) reservoir model (refer to Fig. 1) is considered here. The model consists of a region with a sloped bottom and the other adjacent deep region of a uniform depth. In Fig. 1, L and L_1 are the total length of the reservoir model and the length of the section with a uniform depth respectively; *H* is the maximum water depth; and S is the inclination of the sloped bottom. The dimensions shown in Fig. 1 are all normalised by the maximum water depth. The tip of the model is cut off at $x = 0.16$ in order to avoid a singularity in the numerical model, and an extra vertical wall is added at that location.

In real-life situations, pollutant or nutrient particles usually enter reservoirs through sidearms (corresponding to the sloped-bottom region) and are carried around within the water bodies by various processes. In this study, particle dispersion by natural convection in the near-shore region is investigated. In the numerical model, the endwall and bottom are assumed rigid and no-slip and the water surface is assumed to be stress-free. In order to simulate the effect of the diurnal temperature variation, a sinusoidal function of temperature is specified at the water surface as follows:

$$
T(t) = T_0 + \frac{\Delta T}{2} \sin(2\pi t/P) \quad \text{at } y = 0 \tag{1}
$$

where $T(t)$ is the instantaneous surface temperature at the time instant t; P is the period of the thermal forcing cycle; T_0 is the initial temperature; and ΔT is the difference between the maximum and minimum temperatures over one thermal forcing cycle. This thermal forcing excludes heating by solar radiation, and thus is relevant to periods of no or low solar insolation. Apart from the water surface, all the other surfaces including the extra vertical wall at the tip, the deep-end wall and the sloped and flat bottoms are assumed adiabatic. The water body within the computational domain is initially stationary with a uniform temperature T_0 .

The flow in the reservoir model is assumed to be laminar and twodimensional within the parameter ranges considered here (see more details about the flow parameters in [Section 2.3](#page--1-0)). The fluid flow motion and temperature change within the reservoir model are governed by the usual Navier–Stokes and energy equations with Boussinesq assumption [\[11\]:](#page--1-0)

$$
u_x + v_y = 0 \tag{2-1}
$$

$$
u_t + uu_x + vu_y = -\rho_0^{-1} p_x + \nu \nabla^2 u \tag{2-2}
$$

$$
v_t + uv_x + vv_y = -\rho_0^{-1} p_y + \nu \nabla^2 v + g\beta (T - T_0)
$$
 (2-3)

$$
T_t + uT_x + vT_y = \kappa \nabla^2 T \tag{2-4}
$$

where *u* and *v* are the velocity components in horizontal and vertical directions respectively, T the temperature, ρ_0 the density at the reference temperature T_0 , p the pressure, g the acceleration due to gravity, ν the kinematic viscosity, β the thermal expansion coefficient, and κ the thermal diffusivity.

2.2. Particle model formulation

Particles are injected at a specific location of interest within the tip region, as shown in Fig. 1. The quantity of the injected particles is measured by the volume fraction, which is the ratio of the total volume of the particles to the total volume of the surrounding flow domain (referred to as volume fraction of particles hereinafter). The close vicinity of the tip region is excluded from the particle injection because this region is dominated by conduction with an extremely weak flow and thus particles injected there are unlikely to be carried around by the flow [\[5,12\]](#page--1-0). Any particles injected into this region will only be affected by pure gravitational settling and therefore are of little interest. To avoid the start-up effect of the diurnal flow, the particles are injected at the beginning of the third diurnal cycles after the fluid flow has reached a quasi-steady state. The injection of particles is once only and the specific locations of the injected particles are subject to a random distribution. The initial particle distribution is shown in Fig. 1, which appears to be approximately uniform but is randomly distributed across the region of injection. All the injected particles have the same initial temperature, the same density, the same diameter, and a zero initial velocity. The particles are assumed to be insoluble and chemically non-reactive in the present numerical model and take on the temperature of the surrounding fluid at each location.

In the present DPM, a 'reflect' wall boundary condition for particles is assumed at the water surface. A particle impacting the surface will bounce back immediately, and the standard reflection rule is followed to determine the direction of the particle motion after bouncing. It is assumed that the fluid surface tension is sufficiently large for this to occur (refer to [\[13\]\)](#page--1-0). The bouncing process is assumed to have no influence on any internal property of the particle. Apart from the water surface, all the other walls of the model have a 'trap' wall boundary condition, which means that any particle reaching the wall will be deposited and removed from the flow domain, and thus will not be involved in subsequent calculations.

The particle motion is determined by the motion of fluid flows, buoyancy and other minor forces applicable to the particles. A oneway coupling method is adopted in the present numerical model and therefore, the motion of the particles does not affect the flow. This is deemed appropriate for the very low volume fraction of particles considered in this model. Particle tracking is based on the Lagrangian framework and adopts Newton's second law of motion in the DPM. The governing equation for particle motion is given below [\[8\]:](#page--1-0)

$$
\frac{du_p}{dt} = \frac{u_f - u_p}{\tau} + \left(1 - \frac{\rho_0}{\rho_p}\right)g + F_a
$$
\n(3)

Fig. 1. Schematic of the numerical model (not to scale).

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