Significance of buoyancy in turbulence closure for computational fluid dynamics modelling of ultraviolet disinfection in maturation ponds

(Role of buoyancy for ultraviolet disinfection in maturation ponds)

N.W. Dahl[1,*], P.L. Woodfield[1], B.A.F. Simpson[1], C.J. Lemckert[2], H.M. Stratton[3]

[1] School of Engineering, Griffith University, Gold Coast, Queensland, Australia

[2] Faculty of Arts and Design, University of Canberra, ACT, Australia

[3] School of Natural Sciences, Griffith University, Nathan Campus, 170 Kessels Road, Nathan, Queensland, 4111, Australia

* Corresponding Author. Building G09, Room 1.02, Griffith School of Engineering, Gold Coast Campus, Griffith University, QLD, 4222, Australia.

E-mail Address: nicholas.dahl@griffithuni.edu.au (N.W. Dahl), p.woodfield@griffith.edu.au (P.L. Woodfield), ben.simpson@griffith.edu.au (B.A.F. Simpson), charles.lemckert@canberra.edu.au (C.J. Lemckert), h.stratton@griffith.edu.au (H.M. Stratton).

Abstract

Buoyancy-driven turbulent dispersion in a maturation pond is studied by a combination of field measurements and computational fluid dynamics. Modelling flow in maturation ponds requires turbulent closure models because of the large physical size and the need to model on diurnal time scales. Simulation results are shown to be more sensitive to the inclusion of a buoyancy production term appearing in the turbulent transport equations than to the model choice. Comparisons with experimental thermal profiles show that without this term, thermal mixing is over predicted. When including the term, stratification occurs but thermal mixing is under predicted in the lower water column. In terms of pond performance, the effect of this term is to

cause increased surface die-off of *Escherichia coli* during sunlight hours due to the generation of stratification. It is recommended that future modelling consider and implement this term.

Keywords: buoyancy production term; *E. coli*; inactivation; kinetic modelling

Introduction

Maturation ponds have the purpose of pathogen disinfection and are important for the treatment of wastewater. Disinfection is predominantly sunlight driven by various mechanisms which are mostly dependent on the ultraviolet (UV) spectrum (Davies-Colley et al., 2000; Maïga et al., 2009a,b; Bolton et al., 2010; Fisher et al., 2011; Kadir and Nelson, 2014; Nguyen et al., 2014, 2015; Silverman et al., 2015; Maraccini et al., 2016; Silverman and Nelson, 2016).

Early modelling techniques to evaluate disinfection simplified the internal pond hydraulics. This was done by assuming certain flow regimes and empirically evaluating die-off kinetics for microbial disinfection by either using plug flow (Sarikaya and Saatci, 1987), completely stirred tank reactor (CSTR) flow (Marais, 1974; Sarikaya and Saatci, 1987; Mayo, 1995; Von Sperling, 1999, 2005) or dispersed flow (Wehner and Wilhelm, 1956; Polprasert and Bhattarai, 1985; Sarikaya and Saatci, 1987; Sarikaya et al., 1987; Qin et al., 1991; Herrera and Castillo, 2000; Von Sperling, 1999, 2005; Bracho et al., 2006). These simple equations are particularly useful for quick estimations but suffer from inherent shortcomings that disallow the transient and spatial effects from sunlight disinfection. Moreover, changes in internal hydrodynamics have been reported to be significantly important (Dahl et al., 2017b).

Computational fluid dynamics (CFD) modelling of hydrodynamic flows and the implementation of disinfection models to maturation ponds have been developing (Wood et al., 1995, 1998; Shilton and Harrison, 2003; Shilton and Mara, 2005; Sweeney et al., 2005; Abbas et al., 2006; Shilton et al., 2008; Badrot-Nico et al., 2009; Alvarado et al., 2012a,b; Dahl et al., 2017b) in parallel with the continual improvements to sunlight kinetic rate models (e.g. Nelson and co-workers). However, the application of the sunlight disinfection models to CFD modelling of maturation ponds has been slower in being implemented. The majority of workers modelling disinfection in maturation ponds have employed constant first order decay rates (e.g. Shilton and Harrison, 2003; Shilton and Mara, 2005; Abbas et al., 2006; Badrot-Nico et al., 2009) while Dahl et al. (2017b) solely modelled disinfection via transient sunlight methods. Important CFD studies have also been done in other types of waste stabilisation ponds (Salter et al., 2000; Baléo et al., 2001; Vega et al., 2003; Sah et al., 2011; Passos et al., 2014), aquatic ponds (Peterson et al., 2000), UV chemical reactors (Wols et al., 2015; Xu et al., 2015), and storm water detention ponds (Khan et al., 2013). With the improvement in CFD and computing resources, increasingly complex models are becoming prevalent. It is therefore pertinent to discuss an important aspect of CFD modelling that has been overlooked by pervious researchers and is crucial to correctly account for the physics observed in maturation ponds and the coupled effects for the disinfection of pathogens. That is, the treatment of buoyancy in CFD models for maturation ponds.

Modelling the diurnal cycle of thermal stratification and natural convection is important for the prediction of pathogen disinfection. Consistent cycles of thermal stratification and night-time natural convection in maturation ponds have been reported (e.g. Gu and Stefan, 1995; Brissaud et al., 2003; Dahl et al., 2017a,b). Modelling and experimental evidence reported that the combination of thermal stratification and vertically attenuated sunlight in the water column is the cause for greater die-off in the near surface region of the water column during the day (Brissaud et al., 2003; Dahl et al., 2017a,b). This has also generated interest in developing sunlight disinfection models that resolve disinfection in a spatially dependent manner (e.g.

Maraccini et al., 2016) and take wavelength dependence into account (e.g. Fisher et al., 2011; Nguyen et al., 2014, 2015; Silverman and Nelson, 2016). Previous work by the authors (Dahl et al., 2017b) on modelling of *Escherichia coli* disinfection showed that surface die-off is significantly different to spatial-averaged results and to completely mixed models. The present study focuses on the treatment of buoyancy and the effects to the turbulence which was not fully expounded in our previous work.

The large physical size and mismatch between thermal mixing time-scales (seconds), diurnal time cycles (day) and pathogen-residence times (weeks) necessitates the use of turbulence models for CFD simulation of maturation ponds (Dahl et al., 2017b). Turbulent flow modelling of thermal energy was only undertaken by Dahl et al. (2017b) for maturation ponds and by Sah et al. (2011) for facultative ponds and possibly by Sweeney et al. (2005) and Badrot-Nico et al. (2009). Laminar flow models have been employed by Wood et al. (1995) and Olukanni and Ducoste (2011). The most widely used turbulence model is the $k-\varepsilon$ model and has been used by many researchers (e.g. Wood et al., 1998; Peterson et al., 2000; Sweeney et al., 2005; Shilton et al., 2008; Alvarado et al., 2012a,b). At this point, it is noted that the short-comings of unsteady Reynolds-averaged Navier-Stokes (URANS) turbulence models have been discussed in the context of chemical UV reactors (Wols et al., 2010). It was shown that more sophisticated means of resolving turbulent fluctuations can make a marked impact on disinfection distributions. However, practical modelling with such methods is restricted by insufficient computing resources except for short periods of time, rendering a full diurnal cycle unfeasible (or rather ambitious). Hence for URANS simulations, buoyancy effects are required to be added to the turbulence models, hence requiring thermal modelling, the exact equations of which were discussed early by Rodi (1984, 1987). Thus, the implementation of these aspects for modelling of pathogen die-off (or disinfection) by CFD methods has not been addressed adequately.

In terms of CFD modelling for pond disinfection, the cross-discipline knowledge (e.g. Rodi, 1984, 1987) of how thermal gradients affect the turbulent transport has not been transferred or sufficiently highlighted for pond modelling. Particularly relevant is the demonstration of its effect on sunlight disinfection throughout a typical day. We therefore fill a gap by experimentally and numerically evaluating the effect and importance of resolving buoyancy in a maturation pond and providing guidance on implementation of turbulence models with respect to ultraviolet driven disinfection.

Methods

Experimental data comprising of meteorological information, pond bathymetry, and vertical temperature distributions were taken in a maturation pond. CFD equations including turbulence model selection are described before detailed boundary conditions are given which applies the CFD model to the physical case. CFD numerical implementation is detailed.

Fieldwork

The maturation pond under investigation is located in South East Queensland and has been the subject of a number of studies (Sheludchenko et al. 2016; Dahl et al. 2017a,b). Fig. 1 shows the layout of the pond. The volume of water in the pond was 1380 m^3 and the average inflow rate was $\sim 10^{-3}$ m^3 s^{-1} at the time of investigation with an average horizontal velocity component of 0.36 m s^{-1} and a drop height of 0.05 m. The inflow rate was measured at various points throughout the day and found to be approximately steady with a variation of $\pm 15\%$. Inlet enumeration of *E. coli* was measured and found to vary in a diurnal pattern with minimum concentrations at 2pm ($4 \square 10^3$ CFU 100 mL^{-1}) and a maximum concentration in early morning

(6am $2\square10^{6}$ CFU 100 mL^{-1}). *E. coli* data for the study period has been reported for this pond in Dahl et al. (2017a).

Air temperature, solar radiation, relative humidity, absolute pressure, wind speed and wind direction were recorded on site at 15 minute intervals. Wind speed was corrected to a height of 10 m (Dahl et al., 2017a). The atmospheric data recorded is presented in Fig. 2 and is used for boundary conditions of the CFD simulations. Water temperatures were recorded at five different depths (0, 0.1, 0.3, 0.5 and 0.9 m from the water surface down) as shown in Fig. 1b. The Beer-Lambert law was used to regress attenuation coefficients from vertical sunlight profiles of UVB 39.2 m^{-1} UVA 44.5 m^{-1}, and photosynthetically active radiation (PAR) 18.5 m^{-1} (see Dahl et al. (2017a) for further details).

Modelling via Computational Fluid Dynamics

The CFD model is built on governing equations for fluid flow, energy and scalar transport (*E. coli*) which are listed. Closure of the momentum equations is via the Boussinesq approach and by directly modelling the Reynolds Stresses. Boundary conditions and sources are detailed. Information about the level of grid independence is given. The CFD simulations are two dimensional, vertical-horizontal in orientation and align with the cross sectional location noted on Fig. 1.

Governing Equations

Conservation of mass is given by Eq. (1), conservation of momentum by Eq. (2) and conservation of energy by Eq. (3). They are solved for incompressible flow.

$$\frac{\partial \rho}{\partial t}+\frac{\partial}{\partial x_i}(\rho u_i)=0 \tag{1}$$

$$\frac{\partial}{\partial t}(\rho u_i)+\frac{\partial}{\partial x_j}(\rho u_i u_j)=-\frac{\partial p}{\partial x_i}+\rho g_i+\frac{\partial}{\partial x_j}\left[\mu\left(\frac{\partial u_i}{\partial x_j}+\frac{\partial u_j}{\partial x_i}-\frac{2}{3}\delta_{ij}\frac{\partial u_l}{\partial x_l}\right)\right]+\frac{\partial}{\partial x_j}\left(-\rho\overline{u_i' u_j'}\right) \tag{2}$$

$$\frac{\partial}{\partial t}(\rho U)+\frac{\partial}{\partial x_i}(u_i(\rho U+p))=\frac{\partial}{\partial x_j}\left[\left(k_l+\frac{c_p\mu_t}{Pr_t}\right)\frac{\partial T}{\partial x_j}+u_i(\tau_{ij})_{eff}\right]+S_U \tag{3}$$

where ρ, t, u and p are the density, time, Reynolds-averaged velocity and pressure respectively, g_i is the gravitational vector and $\rho\overline{u_i' u_j'}$ are the Reynolds stresses. U is the specific internal energy, T is the temperature, k_l is molecular thermal conductivity, c_p is the specific heat, μ_t is the turbulent viscosity, Pr_t is the turbulent energy Prandtl number (assumed to be 0.7), and $u_i(\tau_{ij})_{eff}$ involves viscous dissipation. This study assumes a Lewis number of unity and given the Schmidt number below, the Prandtl number is assumed to be the same.

Scalar transport, representing the transport of *E. coli*, is modelled by the convective-diffusion equation (Eq. (4)). ϕ represents the dimensionless *E. coli* concentration (normalised to the inlet concentration).

$$\frac{\partial \rho\phi}{\partial t}+\frac{\partial}{\partial x_i}(\rho u_i\phi)=\frac{\partial}{\partial x_j}\left[\left(\frac{k_l}{c_p Le_l}+\frac{\mu_t}{Sc_t}\right)\frac{\partial \phi}{\partial x_j}\right]+S_\phi \tag{4}$$

The turbulent Schmidt number and Lewis number for molecular diffusion Le_l are assumed to be 0.7 and 1, respectively. The assumption of the turbulent Schmidt number is follows Elyasi and Taghipour (2006).

Closure of Turbulence via Boussinesq Approach

A turbulence closure model is needed to close Eq. (2) and thus account for the turbulence introduced by wind shear, velocity gradients and inform stratification and natural convection arising from buoyancy forces. For this study, multiple turbulence closure models were investigated for their effect on thermal profiles and velocity field predictions. Closure of the Reynolds stresses $\left(-\rho\overline{u_i'u_j'}\right)$ in Eq. (2) via the Boussinesq approximation relates the Reynolds stresses to the mean velocity gradients and is modelled by Eq. (5).

$$-\rho\overline{u_i'u_j'} = \mu_t\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial u_i}\right) - \frac{2}{3}\rho k\delta_{ij} \tag{5}$$

Within Eq. (5), μ_t and k (turbulent kinetic energy) are modelled by different closure models ($k-\varepsilon$ (Launder and Spalding, 1972), $k-\omega$ (Wilcox, 1998), the shear-stress transport model (SST) (Menter, 1994) and a scale adaptive simulation (SAS) (Menter and Egorov, 2010)). Turbulent kinetic energy in the turbulence models is according to:

$$\frac{\partial \rho k}{\partial t} + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{Pr_k}\right)\frac{\partial k}{\partial x_j}\right] + G_k + G_b - Y_k + S_k \tag{6}$$

In Eq. (6), G_k is the turbulent generation of kinetic energy due to velocity gradients, G_b is the generation/suppression of TKE due to buoyancy (the focus of this study) and Y_k is the dissipation of TKE. ε and ω are modelled by Eq. (7) and (8) respectively.

$$\frac{\partial \rho \varepsilon}{\partial t} + \frac{\partial}{\partial x_i}(\rho \varepsilon u_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{Pr_\varepsilon}\right)\frac{\partial \varepsilon}{\partial x_j}\right] + G_\varepsilon + G_{b\varepsilon} - Y_\varepsilon + S_\varepsilon \tag{7}$$

$$\frac{\partial \rho \omega}{\partial t} + \frac{\partial}{\partial x_i}(\rho \omega u_i) = \frac{\partial}{\partial x_j}\left[\left(\mu + \frac{\mu_t}{Pr_\omega}\right)\frac{\partial \omega}{\partial x_j}\right] + G_\omega + G_{b\omega} - Y_\omega + S_\omega \tag{8}$$

where Pr_ε and Pr_ω are the turbulent Prandtl numbers, G_ε and G_ω are the production terms, $G_{b\varepsilon}$ and $G_{b\omega}$ involve the effect of buoyancy production on ε and ω, and Y_ε and Y_ω represent the dissipation terms. Generation of TKE follows the Boussinesq hypothesis and is proportional to the modulus of the mean rate-of-strain tensor $\left(S = \sqrt{2S_{ij}S_{ij}}\right)$.

$$G_k = \mu_t S^2 \tag{9}$$

Generation/suppression of turbulence due to buoyancy is necessary to account for stratification and natural convection which occurs frequently within waste stabilisation pond (see Dahl et al., 2017a,b). Rodi (1987) provides an excellent discussion on the inclusion of buoyancy production terms in the TKE and dissipative equations. It is made clear that stable buoyancy augments mixing, supressing turbulence $(G_b < 0)$, while unstable buoyancy enhances turbulent mixing $(G_b > 0)$. Numerically this is introduced within the coefficient of $C_{3\varepsilon}$ (noted in Rodi, 1984) and is evaluated as $C_{3\varepsilon} = \tanh\left|v/u\right|$. Eq. (10) gives the form of G_b used in the turbulence closure model equations. Note the dependence on the thermal gradient which acts to supress turbulence in stable stratification and enhance turbulence in unstable stratification.

$$G_b = \alpha_v g_i \frac{\mu_t}{Pr_t} \frac{\partial T}{\partial x_i} \tag{10}$$

where α_v is the coefficient of volumetric expansion (K^{-1}). The individual terms within Eqs. (7)–(9) are provided in more detail in Table 1 which also includes the calculation of turbulent viscosity (μ_t).

A limitation of the SST model is the tendency to over-predict turbulent length scales and turbulent viscosity. Menter and Egorov (2010) proposed the addition of a source term to the SST model that allows the turbulent length scales to be resolved in a dynamic nature, thus resolving the unsteady flow when mesh density and time step resolution are fine enough and reverting to unsteady Reynolds-averaged velocity simulations otherwise. The term responsible for this dynamic scaling is added as an additional source term to the ω equation (Eq. (8)) and is given as

$$S_{\omega} = \rho \max\left[\zeta_2 \kappa S^2 \left(\frac{L}{L_{v\kappa}} \right)^2 - 6k \max\left(\frac{1}{\omega^2} \frac{\partial \omega}{\partial x_j} \frac{\partial \omega}{\partial x_j}, \frac{1}{k^2} \frac{\partial k}{\partial x_j} \frac{\partial k}{\partial x_j} \right), 0 \right] \tag{11}$$

where $\zeta_2 = 3.51$, the von Karman constant is $\kappa = 0.41$, S is the magnitude of the shear strain rate, L and $L_{v\kappa}$ are the length scales (m) of the modelled turbulence and von Karman scales, respectively. The turbulent length scale given by the SAS model is

$$L = \frac{\sqrt{k}}{C_{\mu}^{0.25} \omega} \tag{12}$$

Closure of Turbulence via a Complete Reynolds Stress Model

Closure of the Reynolds Stresses are additionally modelled by the Reynolds Stress Model (RSM). As opposed to Boussinesq closure models, the RSM computes the Reynolds Stresses (Eq. (13)) directly and calculates TKE from these stresses as $k = 1/2\left(\overline{u_i u_i}\right)$ and includes the transport of ε which is modelled in the same manner as the $k-\varepsilon$ model. The stress equations are complex and we refer the reader to the literature for further explanation (e.g. Rodi, 1984).

$$\frac{\partial}{\partial t}\left(\rho \overline{u_i' u_j'}\right) + \frac{\partial}{\partial x_k}\left(\rho u_k \overline{u_i' u_j'}\right) = \frac{\partial}{\partial x_k}\left(\left(\mu + \frac{\mu_t}{Pr_k} \right) \frac{\partial \overline{u_i' u_j'}}{\partial x_k} \right) - \rho \left(\overline{u_i' u_k'} \frac{\partial u_j}{\partial x_k} + \overline{u_j' u_k'} \frac{\partial u_i}{\partial x_k} \right)$$

$$- \rho a_v \left(g_i \frac{\mu_t}{Pr_t} \frac{\partial T}{\partial x_j} + g_j \frac{\mu_t}{Pr_t} \frac{\partial T}{\partial x_i} \right) + p' \left(\frac{\partial u_i'}{\partial x_j} + \frac{\partial u_j'}{\partial x_i} \right) - 2\mu \overline{\frac{\partial u_i'}{\partial x_k} \frac{\partial u_j'}{\partial x_k}} \tag{13}$$

where the final two terms on the right hand side are required to be modelled by approximations. It can be seen that the buoyancy effects (third term on right hand side) are reproduced directly without requiring explicit inclusion. Turbulent viscosity is calculated in the same way as the $k-\varepsilon$ model (Table 1).

Boundary Conditions

At the water-atmosphere boundary, heat fluxes and shear stresses are applied to account for the environmental conditions. The momentum boundary condition in the x direction is modelled entirely by the wind shear given by Eq. (14).

$$\tau_i = \rho_a C_d \left|u_{10i} - u_i\right|\left(u_{10_i} - u_i\right) \tag{14}$$

where τ, ρ_a and C_d are the shear stress ambient air density and the coefficient of aerodynamic resistance respectively (taken as 10^{-3}). u_{10} is the wind speed 10 m above the water surface.

To account for the inflow of water from the inlet pipe, a point source is added to the horizontal and vertical momentum equations and is calculated to be proportional to the product of mass rate inflow and velocity difference between the inlet water and simulated surface velocity. As the inlet pipe of the pond is 5 cm above the pond surface, the inlet velocity in the vertical component is assumed to obey projectile motion. Water properties at the inlet are assumed to be the same as the computational cell that the momentum is applied to. Hence it was assumed that no heat transfer occurred with the inlet water. A 'plug-flow' background velocity occurs in the pond due to a net flow of mass entering via the inlet pipe and exiting at the exit region. This velocity effect is accounted for by the addition and subtraction of mass, proportional to the inflow rate, at the inlet (the same location as the momentum addition) and exit regions, respectively.

Shortwave and longwave radiation and sensible and evaporative heat fluxes model the energy boundary condition at the water-atmospheric boundary (Eq. (15)).

$$-k_{eff}\frac{\partial T}{\partial y}=(1-r_{albedo})r_{sa}q_{sw}+q_{lw}+q_{conv}+q_{evap} \tag{15}$$

where k_{eff}, r_{albedo} and r_{sa} are the effective thermal conductivity, the albedo of sunlight and the fraction of irradiance absorbed at the water-atmospheric interface. q_{sw} is the experimentally-measured irradiance in the UV and PAR radiation bands. q_{lw}, q_{conv}, q_{evap} are the longwave radiation, sensible heat and evaporative heat fluxes.

Longwave radiation is modelled using Eq. (16).

$$q_{lw}=\varepsilon_w\sigma A\left(T_{sky}^4-T_s^4\right) \tag{16}$$

where T_{sky} is the effective sky temperature and is estimated to be a constant 273.15 K, T_s is the simulated surface temperature (K) (Dahl et al., 2017a).

Sensible heat and evaporation are modelled using the Chilton-Colburn analogy:

$$q_{conv}=h_{conv}\left(T_\infty-T_s\right) \tag{17}$$

$$q_{evap}=h_{fg}h_{evap}\left(\rho_{v,\infty}-\rho_{v,sat}\right) \tag{18}$$

where h_{conv} is the local heat transfer coefficient, T_∞ is the ambient air temperature, h_{fg} is the latent heat of vapourisation at the water surface, h_{evap} is the local mass transfer coefficient,

$\rho_{v,\infty}$ is the water vapour density recorded on site and $\rho_{v,sat}$ is the saturated vapour density at the water surface. h_{evap} is evaluated by $\left(Sh_x \cdot D_{AB} \cdot x^{-1}\right)$ where Sh_x is the local Sherwood number (Eq. (19)) and D_{AB} is the binary diffusion coefficient. Similarly, h_{conv} is evaluated as $\left(Nu_x \cdot k_l \cdot x^{-1}\right)$ where Nu_x is the local Nusselt number determined in the same manner as Sh_x, except replacing the Schmidt number with the Prandtl number.

$$\begin{cases} Sh_x \\ Nu_x \end{cases} = 0.0296 Re_x^{4/5} \cdot \begin{cases} Sc^{1/3} \\ Pr^{1/3} \end{cases} \tag{19}$$

where Sc and Pr are the Schmidt and Prandtl numbers for air and Re_x is the length scale Reynolds number. Convective heat transfer and momentum from wind stress are included to the full extent of the boundary.

Attenuation of shortwave radiation in the water column creates thermal energy generation which is accounted for by the source term in Eq. (3) and calculated by Eq. (20) (W m^{-3}). Irradiance reaching the boundary of the soli-water interface is distributed to the soil and water at an 80 to 20 ratio.

$$S_U = \left(1 - r_{albedo}\right)\left(1 - r_{sa}\right) q_{sw} \eta \psi e^{\eta \psi y} \tag{20}$$

The disinfection of *E. coli* is modelled via the source term in Eq. (4) using Nguyen's die-off term (Nguyen et al., 2015; Dahl et al., 2017a,b).

$$S_\phi = \rho \phi \left(-3.8 \times 0.836 \cdot 10^{-8} \int_{\lambda=280}^{\lambda=400} I(\lambda, z) \lambda \, \partial \lambda \right) \tag{21}$$

Water Properties

Within the simulation domain, fluid properties are calculated by linear interpolation according to standard water properties. Water properties were defined at 5 K increments. Such properties included density, viscosity, thermal conductivity, specific heat and the thermal expansion coefficient.

Numerical Implementation

Temporal discretisation was done using a bounded seconded order scheme and pressure-velocity coupling using the Pressure Implicit with Splitting of Operators (PISO) scheme (Issa, 1986). All other scalar quantities were discretised as second order with Gauss node based gradient scheme, except for the momentum equation in the SAS turbulence model simulations which was discretised as bounded central differencing with least squares spatial gradient scheme. The model was implemented through extensive use of user-defined functions in the CFD fluids package ANSYS FLUENT 16.0.

The convergence criteria for all CFD simulations was 10^{-4} for the continuity equation and 10^{-6} for all other quantities. It should be noted that one of the Reynolds Stress components in the RSM had difficulty in consistently achieving convergence to a level of 10^{-6} and instead only achieved a value of 10^{-5}. Further iterations to reduce this Reynolds Stress component residual proved ineffective. Given the results are extremely similar to all other turbulence models it was deemed not to be critical.

Grid Independence

To test grid independence, simulations were run with three meshes (14 400, 77 000 and 315 000 mesh elements) and a time-step of 0:25 s. Due to the long runtime of the grids, results are reported for two times of the day, 10 am and 2pm. Results are reported for the average surface temperature $\left(\overline{T}_s\right)$, average surface velocity $\left(\overline{u}_s\right)$, average surface *E. coli* concentration $\left(\overline{\phi}_s\right)$

and the volume averaged *E. coli* concentrations at the exit region (see Fig. 3). The results of the three meshes are shown in Table 2. Model results presented in this study are all run with a timestep of 0.25 s. Testing with larger timesteps showed little change in the results, highlighting that for timesteps less than 1 second the grid convergence was more critical than timestep size.

Results demonstrate that grid independence is confirmed at 10 AM of the simulation (4 hours into a simulation), however there is still a level of dependence for the results at 2 PM. It therefore appears as though an even finer grid is required to capture surface effects, however this was considered unfeasible.

The chosen two-dimensional grid for all simulations is that with 14400 grid elements and is shown in Fig. 3. Considering the lengthy runtime, a finer grid resolution was not feasible. The corners are truncated to avoid singularity (Lei and Patterson, 2002) and the exit region where the baffle ceases is shown. Note that the coordinate axis of the simulation represents x to be aligned with the *width* of the pond (in line with the cross sectional location shown in Fig. 1) and y is the vertical depth along this cross sectional location.

Results and Discussion

Thermal profiles of the experiment and simulations are compared. Results of the vertical velocity distributions predicted by the turbulence model simulations are shown to highlight the effect of buoyancy production. Distributions of velocity within the entire domain demonstrate the importance of buoyancy production to initiate natural convection. Finally, the application of *E. coli* die-off is shown and the significance of the turbulence model and terms within are concluded.

Thermal distributions and stratification

The effect that G_b in the turbulence closure models has to vertical temperature distributions and reproducing stratification is presented in Fig. 4. In comparing the results of turbulence models including G_b (Fig. 4b,d) to the experiment (Fig. 4a), it can be seen that the simulations reproduce stratification during the midday and exhibit similar night-time surface cooling with the maximum temperatures being close to that of the experiment. The effect of excluding G_b can be seen by comparing Figs. 4b and 4c (or 4d and 4e). In Figs 4c and 4e, the water column is well mixed with only a very weak vertical thermal distribution observed. When compared to the experimental data (Fig. 4a) it is clear that neglecting the buoyancy production term over estimates mixing to an unacceptable level. Here, temperature profiles S_1 to S_5 in Fig. 4a are related to Fig. 1b.

Thermal comparisons between models indicate that treatment of buoyancy production in the turbulence closure models is more significant to thermal stratification than the choice of turbulence model itself. This is evident in Fig. 4 by noting that 4b and 4d are very similar. In fact, all of the turbulent models show a similar pattern (as previously noted by Dahl et al. (2017b)). Neglecting G_b over predicts mixing to an unacceptable level, while the inclusion has more sensible surface temperatures and stratification present but under predicts mixing in the lower half of the water column.

Flow patterns

During the diurnal cycle, different flow regimes occur corresponding to the thermal regime occurring. The primary regimes are those of complete stratification that occur during peak daytime stratification (e.g. 2 pm; c.f. Fig. 4a) and that of complete natural convection during night time. Intermediate flow regimes between the two exist, but here we choose to demonstrate the effect of G_b on velocity flow patterns at two representative times during the day. These are presented in Fig. 5. The two selected times correspond to strong stratification at 2 pm and to the occurrence of natural convection at midnight. The simulation results shown were computed by the SST model, with and without G_b present in the turbulence model.

In Fig. 4a and 4b, it can be seen that with G_b included (Fig. 5a), there are multiple vertically layered current structures that are complex. Conversely, a simple velocity distribution is predicted for the simulation where G_b is neglected (Fig. 5b). Similar trends were seen for all other turbulence models comparing with and without G_b. Moreover, similar dramatic differences can be observed in different thermal regimes. This is evident in Figs. 4c and 4d for the natural convection dominated flow fields that occur during the night.

The physics of natural convection consists of random plumes, penetrating downward into the water column (c.f. Bednarz et al. 2009a,b) causing chaotic turbulent structures that eventually form more structured convective cells. Because we are relying on a turbulence model to account for the fine structures of natural convection, results of the SST model with G_b show structured convective cells but do not resolve the random plumes (Fig. 5c). Thus the effect of the plumes is accounted for by turbulent thermal diffusivity. In contrast, without G_b in the turbulence model, convective cells did not occur at all. This is shown in Fig. 5d at midnight, where numerous convective cells should be present and when the surface temperature continues to cool. This clearly demonstrates that to resolve natural convection, even coarsely, G_b is an important and significant part of the turbulence model.

Similar flow patterns to those shown in Fig. 5a,c were observed for all simulations that contained the term G_b and significantly less complex for $G_b = 0$. To illustrate the effect of buoyancy production terms in the turbulence model, the vertical profile of horizontal velocity at the midpoint of the domain is shown in Fig. 6. The times of these results are at 2 pm and 6 pm on the 6th March. It can been seen that the results of the $k - \omega$ and SST models without G_b is less complex with a single forward and reverse circulation current beneath the surface driven shear stress. Simply by including G_b, the thermal profiles (see Fig. 4b,d) and the velocity structure is altered (c.f. Fig. 5). Fig. 6 shows that the other turbulence closure models $(G_b \neq 0)$ behave similarly with multiple current directions down the depth of the water column. It should be noted that field measurements to verify the presence of multiple current directions was not undertaken and further validation work is still required.

Significance of G_b on E. coli die-off

The significance of G_b is shown to have major implications to *E. coli* die-off, primarily arising from how G_b influences the reproduction and approximation of the underlying physics. Numerically, *E. coli* is modelled via the scalar transport equation (Eq. (4)) with the source term accounting for die-off (Eq. (21)). The source term is calculated by integrating over each computation cell using Gauss's theorem. UV intensities (280 to 400 nm) in the pond are distributed in a log-linear form with an order of magnitude drop every 5 cm of depth. For an indication of the magnitude of UV irradiance in the pond, at a depth of 2.5cm there is in excess of 10 W m^{-2} of UV irradiance for the duration of 10AM to 3 PM. Take-off points from maturation ponds for discharge are most typically at the surface via gravity feed. Therefore, we show the results of *E. coli* die-off over a diurnal cycle at the surface of the pond in the exit region for simulations with and without G_b in Fig. 7.

In Fig. 7 the die-off can be seen to increase in late morning and peak near mid-afternoon before increasing in concentration during the night-time. The differences between simulations with and without G_b are most prominent during sunlight hours and into the early evening. Both groups of simulations decrease in concentration as the morning proceeds, however the inclusion of G_b causes the concentration to decrease more greatly than without G_b. Considering the physics occurring in the water column, this phenomenon occurs due to stratification which restricts and allows the near-surface concentrations to be affected by UV sunlight to a greater extent. However, when G_b is absent from the turbulence model, only weak stratification is created (c.f. Fig. 4c,e) and this causes mixing over the whole water column to occur which continues to transport *E. coli* cells into the near-surface region to be affected by UV sunlight. Thus, during the flow regime of stratification, the inclusion of G_b is important in recreating the stratification effect that holds significant influence over the connected transport and sunlight die-off. This effect is also in agreement with the experimental data shown as average points and limits for the time of day. Experimental data is from Dahl et al. (2017a) and has been altered to represent the range of values at three points in the day.

As the flow regime moves from stratification and initiates natural convection, there is a sudden change in *E. coli* concentration. This change occurs around 6 pm in Fig. 7 (where G_b is included) and coincides with UV disinfection ceasing due to the sun setting. This sudden change is due to mixing of the surface and lower water column regions which contain low and high concentrations, respectively (when G_b is included). The mixing of these two regions is due to the combined effect of free convection and the increasing magnitude of mass diffusivity. Mass diffusivity is directly related to the turbulence models and for an unstable temperature gradient, G_b enhances mixing, while for a stable temperature gradient, G_b suppresses mixing. Therefore, the effects of including G_b are far more pronounced than simulations without G_b. *E. coli* concentrations with and without G_b are shown to increase throughout the remainder of the night (after 8 pm in Fig. 7). This is attributed to new cells entering at the inlet and UV disinfection having ceased at sunset. A similar trend is also observed for the experimental data showing an increase from peak daytime die-off to early night-time and continuing into early morning.

Significance of buoyancy production term in the turbulence model

The simulation results have demonstrated that G_b can create substantial differences in predictions. Of particular interest is the vertical turbulent transport of *E. coli* into the near surface region for UV disinfection. The primary mechanism for turbulent transport when relying on turbulence models is by turbulent diffusion. To understand the significance of G_b and the underlying turbulent transport mechanisms in different thermal regimes, the turbulent diffusivities predicted by the models are further investigated.

Fig. 8 shows how vertical profiles of effective (laminar + turbulent contributions) thermal diffusivity vary for the $k-\omega$ and SST models, with and without buoyancy production inclusion. To remove any short-term transient effects, time averaging has been performed on a two hour period in the middle of the day during peak stratification which shows the lower and upper bounds during this time.

Fig. 8a includes buoyancy production in the turbulence closure models, and demonstrates the change in diffusivity over the depth. It is immediately clear that the lower half of the water column experiences close-to-laminar diffusivities which explains why the thermal predictions in Fig. 4 $(\text{for } G_b \neq 0)$ show little change in temperature. The predicted diffusivities in the upper half of the water column however, reveal a surface mixed layer, being an order of magnitude greater than laminar conditions 50 % of the time. This turbulent diffusivity profile is also the reason for the large daytime surface die-off of *E. coli* predicted in Fig. 7; thermal and mass diffusivities being analogous due to the turbulent Lewis number assumed to be unity.

The effect of neglecting buoyancy production is shown in Fig. 8b for the same turbulence closure models. In contrast to buoyancy production inclusion, the diffusivity is consistent in time over the depth. In the middle of the water column, the diffusivities are an order of magnitude greater than the greatest diffusivities in the simulations with buoyancy production inclusion. With this in mind, it is not surprising that complete mixing was observed in the thermal stratification results in Fig. 4 with $G_b = 0$. This turbulent diffusivity profile (analogous to mass diffusivity) is why the die-off of *E. coli* at the surface in Fig. 7 is significantly less than that where G_b is included in the turbulence model. While daytime diffusivities, seen in Fig. 8a, suppress vertical mixing due to stratification, night-time thermal diffusivities are enhanced due to the occurrence of natural convection. This is shown in Fig. 9a for a two-hour period after midnight. The large diffusivity magnitudes close to the surface have now extended further towards the base as natural convection progressively mixes down the water column which is noted on the figure. Therefore, in addition to the natural convection cells seen in Fig. 5, G_b

also influences the vertical mixing. However, without G_b production in the turbulence closure model, the same magnitudes of diffusivities as during the day are seen (Fig. 9b).

From this discussion (Figs. 7 and 8) we can conclude that if the buoyancy production term is absent from the turbulence model equations, then natural convection is not resolved (see Fig. 5), even at the coarsest level, nor is the turbulent thermal diffusion (and by extension mass diffusion) reflected to be physically reasonable (Fig. 8 and 9). While simulations with buoyancy production may have over and under estimated turbulent thermal diffusivity in the diurnal cycle (evidenced by Fig. 4), the temperatures are in approximate agreement with experimental data and reproduce the experimentally observed physics. The effect of G_b has a marked impact on predictions to maturation pond *E. coli* performance, and by extension, similar pathogenic organisms. This information can also be useful for CFD modelling of other types of systems where thermal gradients are present.

Conclusion

A systematic evaluation of the effects of turbulence closure model choice to thermal distributions and velocity-field predictions has been performed. It has been shown that the choice of turbulence closure model is less significant than the inclusion of a buoyancy production term in the turbulence closure models. Vertical diffusivity profiles were shown to be significantly affected by the buoyancy production term which resulted in stratification occurring during daytime. Night-time destratification was characterised by greater turbulent diffusivities near the surface which increased as the unstable temperature gradient progressively mixed down the water column.

Without the buoyancy production term, greater overall die-off is predicted as turbulent diffusivity dominates the vertical transport of *E. coli* concentrations into the near surface region for sunlight disinfection. However, with the term, surface die-off dominates the *E. coli* reduction which represents observed trends. We therefore recommend the implementation of thermal energy and turbulence modelling for maturation ponds, incorporating the buoyancy production term.

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Figure Captions:

Fig. 1. (a) Pond layout (top view) showing locations of baffles, vertical temperature chain location and cross section location for CFD bathymetry generation. Inlet and outlet locations are given with pond dimensions and north direction. (b) Vertical thermistor chain schematic.

Fig. 2. Experimental atmospheric conditions recorded over the experiment and used for CFD simulations.

Fig. 3. CFD geometry and mesh of the first baffled area shown in Fig. 1. Note that the depth and curvature are exaggerated.

Fig 4. Vertical temperatures profiles of (a) experimental data and (b-e) simulation data of various turbulence closure models.

Fig. 5. Velocity patterns computed by the SST model with (a,c) and without (b,d) the buoyancy production term at two representative times in the simulation period. The inlet is located at width = 0.

Fig. 6. Vertical profile of horizontal velocity for each turbulence model at the horizontal midsection at (a) 2 pm and (b) 6 pm of the 6th March 2015.

Fig. 7. Effect of turbulence closure model to simulated concentration at the surface of the exit region over the course of one day (6th – 7th March 2015). Simulation data has been raised to the power of 6 to show the complete pond die-off assuming consistent log removal in each baffled area.

Fig. 8. Time-averaged vertical profiles of thermal diffusivity $(Pr_t = 0.7)$ in the period of peak stratification (12pm – 2pm, 6th March 2015) for the three turbulence closure models $(k-\omega, \mathrm{SST}, \mathrm{SAS})$ with (a) inclusion and (b) exclusion of the buoyancy production term. The shaded area is limited by the 10th and 90th percentiles encountered during time averaging, while the thick centre line is the 50th percentile of the transient data for each height. Shown by blue lines for comparison are the molecular diffusivities assuming Prandtl numbers of 7 and 0.7.

Fig. 9. Time averaged vertical profiles of thermal diffusivity $(Pr_t = 0.7)$ in the period of night-time natural convection (12 am – 2 am, 7th March 2015) for the three turbulence closure models $(k-\omega, \mathrm{SST}, \mathrm{SAS})$ with (a) inclusion and (b) exclusion of the buoyancy production term. The shaded area is limited by the 10th and 90th percentiles, while the thick centre line is the 50th percentile of the transient data.

Table 1 and Caption:

Table 1. Generation rates and parameters used in the closure of turbulence.

Closure	Eqs.	Y_k	Y_ε / Y_ω	G_ε / G_ω	$G_{b\varepsilon} / G_{b\omega}$	$S_k / S_\varepsilon / S_\omega$	μ_t
$k-\varepsilon$	(6), (7)	$\rho\varepsilon$	$C_{2\varepsilon}\rho\frac{\varepsilon^2}{k}$	$C_{1\varepsilon}\frac{\varepsilon}{k}G_k$	$C_{1\varepsilon}C_{3\varepsilon}\frac{\varepsilon}{k}G_b$	-	$\rho C_\mu \frac{k^2}{\varepsilon}$
$k-\omega$	(6), (8)	$\rho\beta^* f_{\beta^*} k\omega$	$\rho\beta f_\beta \omega^2$	$\alpha\frac{\omega}{k}G_k$	$\frac{\omega}{k}G_b\left(C_{1\varepsilon}C_{3\varepsilon}-1\right)$	-	$\rho\frac{k}{\omega}$
SST	(6), (8)	$\rho\beta^* k\omega$	$\rho\beta\omega^2$	$\frac{\alpha}{\nu_t}G_k$	$\frac{\omega}{k}G_b\left(\left(1-\alpha\right)C_{3\varepsilon}-1\right)$	$S_\omega = 2\left(1-F_1\right)\rho\frac{1}{\omega Pr_{\omega 2}}\frac{\partial k}{\partial x_j}\frac{\partial \omega}{\partial x_j}$	$\rho\frac{k}{\omega}\frac{1}{\max\left[\frac{1}{\alpha^*}, \frac{SF_2}{a_1\omega}\right]}$

Note: The blending function of the SST model is shown here as a source term purely due to convenience and to avoid confusion with other closure models which do not have this term.

Table 2 and Caption:

Table 2. Grid independence results of three mesh sizes for time-averaged results of simulated quantities.

Elements	dt / s	$\overline{T}_s$ / °C		$\bar{u}_s$ / 10^{-3} m s^{-1}		$\overline{\phi}_s$		ϕ_{exit}	
		10 AM	2 PM	10 AM	2 PM	10 AM	2 PM	10 AM	2 PM
14400	0.25	27.45	32.54	41.95	20.31	0.6456	0.3775	0.6633	0.5879
		(0.18%)	(0.98%)	(-1.19%)	(14.28%)	(-1.07%)	(-9.03%)	(-0.14%)	(-0.83%)
77000	0.25	27.50	32.86	41.45	23.21	0.6387	0.3434	0.6624	0.5830
		(0.07%)		(-0.72%)		(0.11%)		(0.17%)	
315000	0.25	27.52		41.15		0.6394		0.6635	

For T_s, u_s and ϕ_s, spatial averaging has been performed representing an area-weighted average at the pond surface.
ϕ_{exit} is the volume averaged *E. coli* concentration in the exit region of the domain.
The percentage difference between successive grids is shown in parenthesis for each quantity.