Budget Analysis of *Escherichia coli* at a Southern Lake Michigan Beach

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Nearshore Processes

Nearshore processes influencing *E. coli* (EC) concentrations are complex and often interrelated. An assessment of the importance of these processes (including buoyancy, waves and major annually-occurring sediment resuspension events) is available in Liu et al. [1] (Supplementary Information).

Governing Equations

The governing equations for momentum (1-3), temperature (4) and EC (5) appear as shown below.

\[
\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} + v \frac{\partial u}{\partial y} + w \frac{\partial u}{\partial z} - f v = - \frac{1}{\rho_0} \frac{\partial P}{\partial x} + \frac{\partial}{\partial x} \left( 2 A_M \frac{\partial u}{\partial x} \right) + \frac{\partial}{\partial y} \left( A_M \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial z} \left( K_{VM} \frac{\partial u}{\partial z} \right)
\]

\[
\frac{\partial v}{\partial t} + u \frac{\partial v}{\partial x} + v \frac{\partial v}{\partial y} + w \frac{\partial v}{\partial z} + f u = - \frac{1}{\rho_0} \frac{\partial P}{\partial y} + \frac{\partial}{\partial x} \left( 2 A_M \frac{\partial v}{\partial y} \right) + \frac{\partial}{\partial y} \left( A_M \frac{\partial v}{\partial y} + \frac{\partial v}{\partial x} \right) + \frac{\partial}{\partial z} \left( K_{VM} \frac{\partial v}{\partial z} \right)
\]

\[
\frac{\partial P}{\partial z} = -\rho g
\]

\[
\frac{\partial T}{\partial t} + \frac{\partial (uT)}{\partial x} + \frac{\partial (vT)}{\partial y} + \frac{\partial (wT)}{\partial z} = \frac{\partial}{\partial x} \left( A_H \frac{\partial T}{\partial x} \right) + \frac{\partial}{\partial y} \left( A_H \frac{\partial T}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_V \frac{\partial T}{\partial z} \right) + S_T
\]

\[
\frac{\partial c}{\partial t} + \frac{\partial (uc)}{\partial x} + \frac{\partial (vc)}{\partial y} + \frac{\partial (wc)}{\partial z} = \frac{\partial}{\partial x} \left( A_H \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y} \left( A_H \frac{\partial c}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_V \frac{\partial c}{\partial z} \right) + k_c
\]

\[
k = -\left( \frac{f_P v_S}{\Delta z_i} - \frac{f_P v_S}{\Delta z_{i-1}} + k_I \theta \right)
\]

where \( P \) and \( \rho_0 \) denote the pressure and reference density, \( T \) and \( c \) denote the water temperature and EC concentration, \( (u, v, w) \) are the components of the velocity vector in the three coordinate directions \( (x, y, z) \) respectively, \( f \) is the latitudinal variation of the Coriolis parameter and \( K_{VM} \), \( K_V \) denote the vertical eddy diffusivity of turbulent momentum mixing and mixing for temperature or EC respectively. \( S_T \) is a general term that denotes sources and sinks in the temperature equation. In the equation for EC loss rate \( k \), \( f_P \) denotes the fraction of EC attached to particles, \( v_S \) is the settling velocity, \( \Delta z_i \) and \( \Delta z_{i-1} \) are the thicknesses of the vertical layers, \( k_I \) is the sun light-dependent inactivation rate, \( I_0(t) \) is the sun light at the surface, \( k_c \) denotes the extinction coefficient for light and \( k_d \) is the base mortality rate (also called the dark death rate). The first two terms in equation (6) denote the settling terms (loss to the layer below and gain from the layer above). The attenuation of sunlight within the water column is modeled using the Beer-Lamberts relation. Dependence of the loss rate \( k \) on temperature is modeled using the Arrhenius relation as shown in equation (6). Horizontal mixing was described using the Smagorinsky formulation and vertical mixing was described using the Mellor-Yamada turbulence model. Horizontal eddy viscosity in the momentum equations \( A_M \) was calculated using the Smagorinsky model:

\[
A_M = C \Delta x \Delta y \frac{1}{2} \left[ \left( \frac{\partial u}{\partial x} \right)^2 + \frac{1}{2} \left( \frac{\partial u}{\partial y} + \frac{\partial v}{\partial x} \right)^2 + \left( \frac{\partial v}{\partial y} \right)^2 \right]
\]

\[
Pr_t = \frac{A_M}{A_H}
\]

Here \( C \) is a non-dimensional constant dependant on grid resolution. A constant value of \( C = 0.15 \) was used in the present work after carefully studying the effect of this parameter on model results. The horizontal eddy diffusivity in the equation for EC (\( A_H \)) is related to the eddy viscosity (\( A_M \)) in the momentum equations through the turbulent Prandtl number, Eq. 8. In addition to the above equations, the model uses the Mellor-Yamada 2.5 level turbulence parameterization and solves two prognostic equations for turbulent kinetic energy and turbulence length scale. Details of these equations, the boundary conditions for the momentum and scalar transport equations as well as the transformed equations (in the \( \sigma \)-coordinate or terrain-following system) are available in the POM manual [2].

Details of loading from the two creeks based on observations for summer 2004 are published in Liu et al. [1] and the information is included here for the sake of completeness (Figure S1). Finite-difference grids used
in the computation of lake-wide as well as nearshore circulations are shown in Figure S2. Initial conditions for EC used a zero concentration value throughout the study area. The model comparisons for EC presented in the paper used a mean eddy diffusivity of 5.4 m$^2$/s in the nearshore region. This value is consistent with our observations and dye studies conducted at the site as well as with earlier dye release studies at beaches and shallow lakes with shear-augmented diffusion [3,4,5,6,7]. Comparisons between observed and simulated water surface elevations, temperature and solar radiation are summarized in Figures S3, S4 and S5. The radiation algorithm (also used for simulating temperature in the POM model) is based on the EPA algorithm described in [8]. The model did a reasonable job of describing the observed radiation although the EPA algorithm was originally developed to make predictions at sea level and is known to underpredict radiation at higher latitudes [9]. Probability plots based on the observed and simulated EC concentrations are summarized in Figure S6. The comparisons indicate that the model was able to describe both lower and higher values of EC concentration.

**Budget Analysis**

To examine fluxes in different coordinate directions and to understand the importance of processes in the nearshore region, we focus attention on a control volume near the Central Avenue beach that is 100 m long in the along-shore direction and 100 m wide in the cross-shore direction. The mean depth at the center of the cell is 4.5 m. POM uses a staggered grid in the horizontal (referred to as the Arakawa-C grid) in which variables such as EC concentration and temperature are defined at the cell centers and velocities are defined at cell faces (Figure S7). To calculate the fluxes at the cell faces, concentrations at the cell faces are needed. These were calculated as the arithmetic averages of the concentrations at the neighboring cell centers since uniform grid spacing was used in our computations. The fluxes (units: $ML^{-2}T^{-1}$) are defined and computed as shown below. Advective Fluxes in the $x$ and $y$ directions:

\[
J_{adv,x} = uc, \quad J_{adv,y} = vc
\]

Diffusive Fluxes in the $x$ and $y$ directions:

\[
J_{diff,x} = -AH \frac{\partial c}{\partial x} \\
J_{diff,y} = -AH \frac{\partial c}{\partial y}
\]

Net Fluxes in the $x$ and $y$ directions:

\[
J_{net,x} = uc - AH \frac{\partial c}{\partial x} = J_{net,adv,x} + J_{net,dif,x} \\
J_{net,y} = vc - AH \frac{\partial c}{\partial y} = J_{net,adv,y} + J_{net,dif,y}
\]

Using the staggered grid shown in Figure S7, these fluxes are approximated as shown below. Net advective flux in the $x$ and $y$ directions:

\[
J_{adv,x,in} = u_{i,j} \left( \frac{c_{i-1,j} + c_{i,j}}{2} \right); \quad J_{adv,y,in} = v_{i,j} \left( \frac{c_{i,j-1} + c_{i,j}}{2} \right) \\
J_{adv,x,out} = u_{i+1,j} \left( \frac{c_{i,j} + c_{i+1,j}}{2} \right); \quad J_{adv,y,out} = v_{i,j+1} \left( \frac{c_{i,j} + c_{i,j+1}}{2} \right) \\
\therefore J_{net,adv,x} = u_{i,j} \left( \frac{c_{i-1,j} + c_{i,j}}{2} \right) - u_{i+1,j} \left( \frac{c_{i,j} + c_{i+1,j}}{2} \right) \\
J_{net,adv,y} = v_{i,j} \left( \frac{c_{i,j-1} + c_{i,j}}{2} \right)
\]
- \nu_{i,j+1} \left( \frac{c_{i,j} + c_{i,j+1}}{2} \right) \tag{16}

The diffusive fluxes can be computed in a similar way:

\[ J_{\text{net}, \text{diff}, x} = \left( - \frac{(A_{H_{i,j}} c_{i,j} - A_{H_{i-1,j}} c_{i-1,j})}{\Delta x} \right) - \]

\[ - \frac{(A_{H_{i,j+1}} c_{i,j+1} - A_{H_{i,j}} c_{i,j})}{\Delta x} \] \tag{17}

\[ J_{\text{net}, \text{diff}, y} = \left( - \frac{(A_{H_{i,j}} c_{i,j} - A_{H_{i,j-1}} c_{i,j-1})}{\Delta y} \right) - \]

\[ - \frac{(A_{H_{i,j+1}} c_{i,j+1} - A_{H_{i,j}} c_{i,j})}{\Delta y} \] \tag{18}

Similar expressions were used to compute the vertical fluxes in the z-direction. For the budget analysis, the 3D transport equation is used to understand the relative importance of different processes. The transport equation for EC (equation 5) can be written in terms of the above fluxes as shown below:

\[ \frac{\partial c}{\partial t} + \frac{\partial (uc)}{\partial x} + \frac{\partial (vc)}{\partial y} + \frac{\partial (wc)}{\partial z} = \frac{\partial}{\partial x} \left( A_H \frac{\partial c}{\partial x} \right) + \frac{\partial}{\partial y} \left( A_H \frac{\partial c}{\partial y} \right) + \frac{\partial}{\partial z} \left( K_v \frac{\partial c}{\partial z} \right) + kc \] \tag{19}

\[ \frac{\partial c}{\partial t} + \frac{\partial (J_{\text{adv}, x})}{\partial x} + \frac{\partial (J_{\text{adv}, y})}{\partial y} + \frac{\partial (J_{\text{adv}, z})}{\partial z} + \frac{\partial (J_{\text{diff}, x})}{\partial x} + \frac{\partial (J_{\text{diff}, y})}{\partial y} + \frac{\partial (J_{\text{diff}, z})}{\partial z} = kc \] \tag{20}

Once the fluxes in equations (9) - (12) are computed, they can be used to evaluate the different terms in equation (20) by evaluating each term as the difference between the fluxes entering and leaving a control volume divided by the step size in the appropriate direction. For example, the advective flux in the along-shore direction can be approximated as:

\[ \frac{\partial (J_{\text{adv}, x})}{\partial x} = \frac{J_{\text{adv}, x, \text{in}} - J_{\text{adv}, x, \text{out}}}{\Delta x} \] \tag{21}

To understand the relative magnitude of the advective and diffusive fluxes of EC at a point in the nearshore region, we plotted the fluxes \( J_{\text{adv}, x}, J_{\text{adv}, y}, J_{\text{adv}, z}, J_{\text{diff}, x}, J_{\text{diff}, y}, J_{\text{diff}, z} \) as defined in equations (9) - (12) (similar equations were used for the vertical) in Figure S10. Since \( u \) is positive in the position x-direction (to the right), the along-shore advective velocity \( u \) is negative going towards the cell near Central Avenue and positive away from it. Similarly positive \( v \) is in the positive y-direction (from the shoreline towards the lake) in Figure S10. Horizontal fluxes are the fluxes in the x and y directions and vertical fluxes are in the z direction. Each term in the transport equation (20) represents a mass flow rate for EC with units \( ML^{-3}T^{-1} \). Mass flow rate results are presented in Figures 5 and 6 in the paper. Each term in (20) is evaluated as the difference of the flux entering the cell (treated as being positive) and the flux leaving the cell (negative) as shown in equation (21). The fluxes presented in Figure S10 indicate that the horizontal fluxes are an order of magnitude higher compared to the vertical fluxes, however, the relative importance of a process is controlled by the gradients and the length scales involved, therefore the mass flow rate results (Figures 5 and 6 in the paper) should be used to understand the importance of various processes.

**Flow Reversals**

Flow reversals are an important aspect of the transport in the present study. More details of flow reversals and their impact on beach water quality are described in Nevers et al. [10]. Simulated EC concentrations on Julian day 217 showed flow reversals as shown in Figure S8. Red patches indicate areas of the plume in which the concentrations were either equal to or exceeded the Indiana standard of 235 CFU/100 mL.
Figure S1: Loading from Trail Creek and Kintzele Ditch during summer 2004 used as model inputs for the simulation period [1].

Table 1. List of Input Parameters
[RMSE = 0.41 (Mt. Baldy Beach)]

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
<th>Value</th>
</tr>
</thead>
<tbody>
<tr>
<td>$k_I$</td>
<td>Light-dependent inactivation rate</td>
<td>0.0026 W$^{-1}$m$^2$d$^{-1}$</td>
</tr>
<tr>
<td>$k_d$</td>
<td>Base mortality</td>
<td>$8.6 \times 10^{-5}$d$^{-1}$</td>
</tr>
<tr>
<td>$v_S$</td>
<td>Settling velocity</td>
<td>1 m d$^{-1}$</td>
</tr>
<tr>
<td>$f_P$</td>
<td>Fraction of EC attached</td>
<td>0.1</td>
</tr>
<tr>
<td>$k_e$</td>
<td>Light extinction coefficient</td>
<td>0.55 m$^{-1}$</td>
</tr>
<tr>
<td>$\theta$</td>
<td>Temperature correction factor</td>
<td>1.07</td>
</tr>
</tbody>
</table>
Figure S2: (a) Finite-difference mesh of Lake Michigan used to compute the lake-wide circulation (b) Part of the mesh used to compute nearshore circulation and *E. coli* transport showing the bathymetry.

**Bottom Shear Stress and *E. coli***

Although a comprehensive assessment of the role of sediment in contributing EC to the water column is beyond the scope of the present work, we computed the bottom shear stress to understand the relation between high shear-stress events and EC peaks. In the nearshore region, the shear stress exerted by currents is generally small compared to the contribution from waves and the total shear stress can be approximated as the sum of current and wave shear stresses [11]. Bottom shear stress due to currents was calculated using equation (22) neglecting wave-current interactions [11].

\[
\tau_C = C_D \rho V_B |V_B| 
\]  

(22)

where \(\tau_C\) is the bottom shear stress due to currents, \(V_B\) is the velocity at the bottom layer, \(\rho\) is the density of water and \(C_D\) is the drag coefficient calculated using the log law. In shallow waters near beaches bottom shear stress due to wind generated waves can be significant [11]. This was calculated using equation (23):

\[
\tau_W = H \left[ \rho \left( \frac{u}{\pi} \right)^3 \right]^{0.5} 
\]  

\[
\left( \frac{2 \pi d}{L} \right) 
\]  

(23)
Figure S3: Comparison of observed and simulated water surface elevations for summer 2006

Figure S4: Observed and simulated temperatures in the nearshore region
Figure S5: Comparison of observed and simulated shortwave radiation at Trail Creek

Figure S6: Probability plots of EC (observed versus simulated) for the two beaches
The wave height $H$, period $T$ and wave length $L$ are estimated for shallow waters using the relations (24-26):

$$\frac{g H}{U_W^2} = 0.283 \tanh \left[ 0.53 \left( \frac{g d}{U_W^2} \right)^{3/4} \right]$$
where $\tau_W$ is the bottom shear stress due to waves and $F$ is the fetch. A bottom roughness height $z_0$ of 1 cm has been used [12]. $U_W$ is the wind speed at 10 m above the water surface and $d$ is the water depth at the location. The net bottom shear stress can be expressed as:

$$\tau_{net} = \tau_C + \tau_W$$

To facilitate comparison between EC peaks and the bottom shear stress, the net bottom shear stress was normalized using the relation:

$$\tau' = \frac{\tau_{net} - \tau_{net,\text{min}}}{\tau_{net,\text{max}} - \tau_{net,\text{min}}}$$

where $\tau_{net,\text{max}}$ and $\tau_{net,\text{min}}$ are the maximum and minimum values of the bottom shear stress. The normalized shear stress and EC (also normalized in a similar way) are shown in Figure S9. The comparison shows that a majority of the peaks in EC are associated with high shear stress events. It is interesting to note that immediately after the high shear stress event around Julian day 218, no EC peaks were observed although there were multiple high shear stress events. The result points to the finite nature of the sediment as a source of EC.

![Figure S9: Normalized shear stress and EC for summer 2004](image-url)
**Figure S10:** Vertical (top panel) and horizontal (x and y) fluxes of EC plotted for all layers. The peaks are generally associated with the top layers.
References


