Modelling E. coli transport in soil columns: simulation of wastewater reuse in agriculture
Edward Smith and Aimen Badawy

ABSTRACT
Transport of E. coli bacteria was investigated in laboratory soil columns for three Egyptian agricultural soils, with aim toward determining a set of site specific criteria for safe and sustainable use of treated wastewater in irrigation in Egypt. In particular, the impacts of varying soil type and hydraulic loading rate (HLR) on E. coli effluent breakthrough curves were examined in the laboratory and simulated using the CXTFIT package to solve a one-dimensional mass transport equation that included advection, dispersion, adsorption, and straining/filtration. The attempt was made to measure the coefficients associated with each mass transfer process from independent experiments. The HLR used in irrigation was found to exert considerable influence on the impact of transport processes on E. coli breakthrough. At low HLRs, adsorption and straining/filtration are significant in addition to advection and dispersion. However, at high HLRs approaching flood irrigation, E. coli is essentially unaffected by reaction processes, with breakthrough a function of advection and dispersion only. Estimating $K_d$ via independent batch experiments did not provide a suitable description of adsorption of E. coli in soil columns. To ensure safe and sustainable reuse of reclaimed wastewater in irrigation, guidelines should account for physical and chemical properties of the soil and other local conditions that may impact residual contaminant transport.

Key words | adsorption, dispersion, E. coli, modelling, soil columns, wastewater reuse

INTRODUCTION
Reclaimed wastewater use in agriculture is an important component of sound water resource management policy as it promotes conservation of water resources. However, reclaimed wastewater may often contain constituents that pose a potential communal health risk either directly or indirectly through contamination of soil and groundwater resources. Assessing these risks together with the fate and transport of these constituents in typical agricultural soils under local conditions will lead to the safe and sustainable use of this resource. This is important in countries such as Egypt where the agricultural sector consumes 85% of the national water resources (UN-FAO 2005), but where currently less than 10% of wastewater is reused (UN-FAO 2000). This work investigated the fate and transport of one important wastewater constituent, E. coli bacteria, in three Egyptian agricultural soils, with aim toward a longer-range goal of determining a set of site specific criteria for safe and sustainable use of treated wastewater in irrigation in Egypt. A series of laboratory experiments and model simulations using a material balance equation were conducted to determine the impacts of varying soil type and hydraulic loading rate (HLR) on E. coli transport. The experiments included a set of laboratory soil columns, and the CXTFIT package (version 2.1) was used to solve a one-dimensional mass transport equation that included advection, dispersion, adsorption, and straining/filtration.

The CXTFIT code, developed at the U.S. Salinity Laboratory for the U.S. Department of Agriculture (Toride et al. 2000), was used to simulate the transport of E. coli in the laboratory soil columns. The model was calibrated using the CXTFIT software version 2.1, which is a widely used and validated tool for simulating mass transport in porous media. The model was run for different hydraulic loading rates (HLRs) and soil types to evaluate the impact on E. coli transport. The results showed that at low hydraulic loading rates, adsorption and straining/filtration are significant, in addition to advection and dispersion. However, at high hydraulic loading rates approaching flood irrigation, E. coli is essentially unaffected by reaction processes, with breakthrough a function of advection and dispersion only. Estimating $K_d$ via independent batch experiments did not provide a suitable description of adsorption of E. coli in soil columns. To ensure safe and sustainable reuse of reclaimed wastewater in irrigation, guidelines should account for physical and chemical properties of the soil and other local conditions that may impact residual contaminant transport.
et al. 1999), has been used by other investigators to simulate mass transport of bacteria in unsaturated soil (Powelson & Mills 2001; Dong et al. 2002; Andres et al. 2004). In addition to incorporating the known important transport processes for contaminant migration in soil, the model can be used to estimate transport parameters (e.g., dispersion coefficients) from independently obtained laboratory or field data. The form of the mass transport equation used in this work is:

\[
\frac{\partial C}{\partial t} = D \frac{\partial^2 C}{\partial z^2} - v_p \frac{\partial C}{\partial z} - \mu C
\]

(1)

where, \( C \) is the contaminant concentration in the liquid phase (number/L\(^2\)); \( t \) is time; \( z \) is the vertical dimension of flow (L); \( v_p \) is the pore velocity; \( D \) is the longitudinal dispersion coefficient (L\(^2\)/t); and \( \mu \) is an overall first-order decay coefficient that includes straining/filtration (1/t). In addition,

\[ R = \left[ 1 + \left( \frac{\rho_b K_d}{\theta} \right) \right], \]

the retardation factor due to adsorption (dimensionless);

where \( \rho_b \) is the soil bulk density (M/L\(^3\)); \( \theta \) is the volumetric water content; and \( K_d \) is the partitioning coefficient (L\(^3\)/M) describing the adsorption equilibrium relationship between \( C \) and \( S \), the contaminant concentration in the solid phase (number/M\(_{soil}\)).

**MATERIALS AND METHODS**

An American Type Culture *Escherichia coli* Strain (ATCC 25922 - from the Naval American Marine Research Unit in Cairo) was obtained on a MacConkey culture plate. Buffer solutions were prepared to achieve aqueous phase concentrations in the range \( 10^3 \) to \( 10^4 \) CFU/100 mL. A new buffer solution was prepared prior to each experiment in distilled, de-ionized water. All bacterial enumeration was performed using the standard membrane filter technique for fecal coliforms, Method 9222 D from *Standard Methods* (1998).

The only deviation was the incubation of bacteria in a thermostatically and humidity controlled air incubator rather than a water bath. In a comparative experiment with a water bath, statistical analysis using the f-test demonstrated that the data belonged to the same population with 95% confidence.

Soil 1 is a slightly clayey, slightly loamy sandy soil from an irrigated field at the Red Sea coast 350 km southeast of Cairo. Soil 2 is a sandy desert soil from South Tahrir City reclaimed for agricultural use using disinfected manure. Soil 3 is also from a land reclamation project in Sadat City, but is a more clayey, fine-textured soil. Prior to experimental investigations, the soil was sieved through a U.S. Standard No. 10 sieve to remove stones, sterilized, cooled, and placed in sterilized polyurethane containers until use. Some relevant soil properties are listed later in Table 1 together with corresponding mass transport parameters for the various test cases.

For each of the three test soils, column experiments were conducted for three different hydraulic loading rates (HLR) used in Egyptian agricultural practice: (1) 5 cm/h (3 mL/min) simulating unsaturated flow at a relatively low HLR; (2) 13 cm/h (8 mL/min) corresponding to unsaturated flow at a higher delivery rate; and, (3) 66 cm/h (40 mL/min) simulating ponded flow or “flood” irrigation. Flood irrigation is still the most common used in Egypt. Schemes such as subsurface trickle irrigation are practised to a limited degree, but were not addressed in this work. Buffer feed solution containing *E. coli* at a concentration averaging approximately 8,000 CFU/100 mL was delivered to the columns in downflow mode using a peristaltic pump. The column design and setup, rigorous soil packing procedures to attain consistency (Powelson et al. 1991; Abu-Ashour et al. 1994), and effluent sampling are detailed in a previous paper (Smith & Hegazy 2006). The soil

<table>
<thead>
<tr>
<th>HLR (cm/hr)</th>
<th>( \Phi ) (%)</th>
<th>( f_{oc} ) (batch)</th>
<th>( D ) (cm(^2)/hr)</th>
<th>( K_d ) (batch)</th>
<th>( \mu ) (1/hr)</th>
</tr>
</thead>
<tbody>
<tr>
<td>5</td>
<td>27.0</td>
<td>24.3</td>
<td>23.2</td>
<td>0.382</td>
<td>0.0274</td>
</tr>
<tr>
<td>13</td>
<td>33.1</td>
<td>49.0</td>
<td>17.9</td>
<td>0.318</td>
<td>–</td>
</tr>
<tr>
<td>66</td>
<td>39.3</td>
<td>192.4</td>
<td>29.1</td>
<td>0.026</td>
<td>–</td>
</tr>
<tr>
<td>5</td>
<td>23.7</td>
<td>22.2</td>
<td>12.0</td>
<td>0.0139</td>
<td>0.0065</td>
</tr>
<tr>
<td>13</td>
<td>28.3</td>
<td>52.1</td>
<td>7.8</td>
<td>0.100</td>
<td>–</td>
</tr>
<tr>
<td>66</td>
<td>33.4</td>
<td>213.4</td>
<td>26.3</td>
<td>0.018</td>
<td>–</td>
</tr>
<tr>
<td>5</td>
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<td>18.3</td>
<td>11.9</td>
<td>1.125</td>
<td>0.0348</td>
</tr>
<tr>
<td>13</td>
<td>40.0</td>
<td>28.5</td>
<td>22.0</td>
<td>0.895</td>
<td>–</td>
</tr>
</tbody>
</table>

Table 1 | Transport parameters for test soils
column depth was 5 cm in every case, and the packing executed to achieve the same bulk density as measured for field soil for column experiments of a respective soil type. An independent tracer column experiment (without bacteria in the feed solution) was performed for each soil-HLR case using bromophenol blue as tracer in order to characterize dispersive transport. Bromophenol blue concentrations in effluent samples were measured by visible light spectroscopy using a DR 2000 spectrophotometer (HACH) and employing a four-point calibration curve. Batch adsorption experiments were used to independently determine the soil-water partitioning of bacteria given by the parameter, $K_d$. The methodology is described in a companion paper (Smith & Badawy 2007).

RESULTS AND DISCUSSION

Previous research indicated that careful packing of laboratory columns could not only reproduce field soil bulk density values, but also consistent volumetric water content, $\theta$, for a given HLR (Smith & Hegazy 2006). This enables the conducting of independent tracer studies to characterize flow and dispersion in laboratory columns for a given soil. Figure 1 includes the tracer breakthrough curve for Soil 1 for the mid-range HLR, namely 13 cm/h. This data was used together with CXTFIT simulations (setting $R = 1$ and $\mu = 0$) to estimate $v_p$ and $D$ by an optimization routine that minimizes the error between model and experimental values. The adsorption partitioning coefficient ($K_d$) was determined from batch equilibrium experiments. CXTFIT was then applied to predict the $E. coli$ breakthrough curves for the various cases using mass transport parameters determined from independent experiments (i.e., $v_p$, $D$, $K_d$). If substantial discrepancies between model simulations and breakthrough data were observed, $K_d$ and/or $\mu$ were adjusted to obtain a good fit of the data. The objective was to determine a consistent set of transport coefficients that aid in identifying the relationships between the important transport processes and the key variables of the
system. This is illustrated in Figure 1. Curve 1 is the CXTFIT calibration of tracer data to obtain $v$ and $D$. Using these values, Curve 2 is the model simulation using the experimentally determined value of $K_d$. It is obvious that *E. coli* retardation is greatly overestimated when using $K_d$ values from independent batch isotherm experiments. Changing $K_d$ shifts the breakthrough curve horizontally; Curve 3 is the fitted curve and corresponds to a $K_d$ value (0.32 mL/g) that is more than an order of magnitude less than that estimated from the batch isotherm (6.4 mL/g).

The fitted $K_d$ value for this case (0.32 mL/g) was found to adequately simulate the timing of *E. coli* breakthrough for Soil 1 at a low HLR (5 cm/hr) as depicted by Curve 3 in Figure 2. However, Figure 2 also indicates that at this HLR the bacterial breakthrough levels off at about 70 percent of the influent value. This suggests that bacterial transport is also affected by soil-flow relations whereby bacterial cells are retained by a mechanism in addition to adsorption such as straining or filtration. A model search for the overall decay parameter $\mu$ (the last term in Equation 1) results in Curve 4 of Figure 2. At high HLR simulating flood irrigation, a common scenario in Egypt, very little adsorption was observed; thus the retardation of bacteria was overpredicted when using a $K_d$ value of 0.32 mL/g. This is depicted in Figure 3. It is worthy to note from Figures 1–3 that the tracer and bacteria breakthrough curves for respective HLRs are essentially displaced images of one another, indicating the consistency of packing and flow pattern through the columns. Moreover, $v_p$ values from model calibration of tracer data match quite closely with theoretical values calculated from consideration of the HLR, the column cross-sectional area, the void ratio, and $\theta$.

The same trends were observed in Soils 2 and 3; however, the nature of the trends and parameter values varied considerably depending on the characteristics of the respective soils. Figures 4 and 5 illustrate the tracer and bacteria breakthrough curves together with model simulations for HLR = 5 cm/h and 13 cm/h, respectively. As in
the case of Soil 1, straining/filtration is observed in addition to adsorption at the lowest HLR examined, but this is eliminated for HLR = 13 cm/h and higher. There is apparently a threshold loading rate above which local retention forces associated with straining/filtration are exceeded by hydrodynamic turbulence, facilitating the breakthrough of bacteria through the column. Although the 66 cm/h HLR case is not shown, the result followed that of Soil 1, namely the bacteria breakthrough data was almost identical to the tracer data. Also evident is the over-prediction of E. coli retention when using $K_d$ from batch isotherm experiments. Moreover, comparing Figures 4 and 2 (5 cm/h) and Figures 5 and 1 (13 cm/h) indicates that E. coli adsorption capacity of Soil 1 is greater than Soil 2 as given by the timing of breakthrough. The extent of straining/filtration is also greater in Soil 1. These trends are quantified in the values of the the process coefficients presented in Table 1. For instance, $K_d$ estimated from column breakthrough data decreases for increasing HLR, but is close for the 5 and 13 cm/h cases as noted previously. Even in these two cases, however, $K_d$ is more than an order of magnitude less than that from batch isotherms. $K_d$ values for Soil 2 are less than for Soil 1 as indicated in the breakthrough curves. The magnitude of the decay coefficient, $\mu$, reflects the variable extent of straining/filtration for the different soils. Table 1 also includes the $\theta$ achieved for a given HLR together with comparative soil properties such as porosity ($\phi$) and soil organic fraction ($f_{oc}$).

Figures 6 and 7 depict tracer and bacteria breakthrough curves together with model simulations for Soil 3 at HLR = 5 cm/h and 13 cm/h, respectively. Because it is a more clayey and fine-textured soil, a HLR of 66 cm/h was not achievable. Once again, adsorption was overestimated by more than an order of magnitude by batch equilibria, straining/filtration is observed at 5 cm/h but not at 13 cm/h, and adsorption capacity is reduced for increasing HLR.
However, adsorption capacity as a whole and the extent of filtration is decidedly greater for Soil 3 than the other two soils. The increase in adsorption capacity is likely related to the considerably higher organic fraction, \( f_{oc} \), a phenomenon observed in other soil-bacteria studies (Johnson & Logan 1996; Pieper et al. 1997; Rogers & Logan 2000; Smith & Hegazy 2006). In fact, \( K_d \) values from both column and batch studies, while different in magnitude, follow the same trend of proportionality relative to \( f_{oc} \). The increase in straining/filtration of Soil 3 followed by Soil 1 and then Soil 2 may be associated with \( f_{oc} \) to some extent along with other properties of the soil; for instance the finer texture of Soil 3 or variable surface charge characteristics for the more clayey soil. Further investigations are required at additional HLRs, especially for lower values, and for other background solution- and soil-phase conditions to better understand these relationships and assess risks associated with residual contaminant transport resulting from reuse of treated wastewater in agriculture.

CONCLUSIONS

1. The HLR used in irrigation exerts considerable influence on the impact of transport processes on \( E. coli \) breakthrough. At low HLRs, adsorption and straining/filtration are significant transport processes in addition to advection and dispersion. However, at high HLRs approaching flood irrigation, \( E. coli \) is essentially unaffected by reaction processes, with breakthrough a function of advection and dispersion only.

2. Estimating \( K_d \) via batch experiments did not provide a suitable description of adsorption of \( E. coli \) in soil columns.

3. Wastewater reuse guidelines have normally been based on the type of crop and intended irrigation method and do not incorporate the significant impact of soil properties on fate and transport of the contaminant (UN-WHO 2000). To ensure sustainable development when reusing reclaimed wastewater for irrigation, a re-evaluation of guidelines taking into account physical and chemical properties of the soil in addition to other local/site-specific conditions is required.

REFERENCES


