SIMULATION OF CONTAMINANT TRANSPORT IN THE PRESENCE OF COLLOIDS AND BACTERIA USING PARTICLE TRACKING METHOD

By

Ahmed Mohamed Sayed Ibrahim Hedia

A Thesis Submitted to the
Faculty of Engineering at Cairo University
in Partial Fulfillment of the
Requirements for the Degree of
MASTER OF SCIENCE

In

IRRIGATION AND HYDRAULICS ENGINEERING

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Title of Thesis:

Simulation of Contaminant Transport in the Presence of Colloids and Bacteria Using Particle Tracking Method

Key Words:
Co-transport of Contaminant and Colloids; Bactria; Chemical Processes; Biological Processes; RWPT.

Summary:

In this study, an existing RWPT code has been adapted to simulate contaminant transport in the presence of colloids and bacteria. The existing RWPT simulate the contaminant migration in porous medium under assumption of conservative transport. Modifications are made to consider the chemical reactions between contaminant and surrounding solid mass. The modified RWPT code is verified with several available sources and shows well performance in simulation of contaminant transport in porous medium in the presence of colloids and bacteria. An investigation of impacts of various parameters has been performed to study the contaminant fate in the domain under influence of physical, chemical, and biological parameters.

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Nomenclature

α_l	longitudinal dispersivity [L]
α_t	transverse dispersivity[L]
β	conservation factor using in bacterial lysing
μ	specific growth rate of bacteria [T^{-1}]
μ_{max}	maximum specific growth rate of bacteria [T^{-1}]
μ_{ba}	specific growth rates of bacteria in aqueous phase [T^{-1}]
μ_{bs}	specific growth rates of bacteria attached on solid matrix phase [T^{-1}]
μ_{bDa}	specific growth rates of bacteria attached to mobile colloid [T^{-1}]
μ_{bDs}	specific growth rates of bacteria attached to immobile colloid [T^{-1}]
θ	porosity of porous medium [1]
Δt	time step interval [T]
C_{ca}	contaminant mass concentration for aqueous contaminant [ML^{-3}]
C_{cs}	mass concentration of contaminant which sorbed on the solid matrix [ML^{-3}]
C_{cDa}	mass concentration of contaminant which sorbed on mobile colloid [ML^{-3}]
C_{cDs}	mass concentration of contaminant which sorbed on immobile colloid [ML^{-3}]
C_{cba}	contaminant mass concentration for contaminant in phases cba [ML^{-3}]
C_{cbs}	contaminant mass concentration of contaminant in phases cbs [ML^{-3}]
C_{cbDa}	contaminant mass concentration for contaminant in phases cbDa [ML^{-3}]
C_{cbDs}	contaminant mass concentration of contaminant in phases cbDs [ML^{-3}]
C_{ba}	mass concentration of bacteria in phase ba [ML^{-3}]
C_{bs}	mass concentration of bacteria in phase bs [ML^{-3}]
C_{bDa}	mass concentration of bacterial cells which attached to mobile colloid [ML^{-3}]
C_{bDs}	mass concentration of bacterial cells which attached to immobile colloid [ML^{-3}]
C_{Da}	mobile mass concentration of colloids [ML^{-3}]
C_{Ds}	immobile mass concentration of colloids [ML^{-3}]
ca	contaminant in aqueous phase
cs	contaminant sorbed on solid matrix
cDs	contaminant sorbed to immobile colloid particle
cDa	contaminant sorbed to mobile colloid particle

cba	contaminant sorbed to bacteria particle in aqueous phase
cbs	contaminant sorbed to bacteria cell attached to solid matrix
cbDs	contaminant sorbed to bacteria stacked on immobile colloid
cbDa	contaminant sorbed to bacteria stacked on mobile colloid
C	the dissolved substance concentration $[ML^{-3}]$
C_b	concentration of bacteria in the domain $[ML^{-3}]$
ba	bacteria in aqueous phase
bs	bacteria sorbed on solid matrix
bDs	bacteria attached to immobile colloid particle
bDa	bacteria attached to mobile colloid particle
D^*	molecular diffusion coefficient of aqueous substance in porous media$[L^2T^{-1}]$
Da	colloid in aqueous phase – mobile phase
Ds	colloid Sorbed on solid matrix – immobile phase
D_{ca}	the dispersion tensor for contaminant
D_{ba}	the dispersion tensor for bacteria
D_{Da}	the dispersion tensor for colloids
FE	finite elements
FD	finite differences
K_a	ratio between forward reaction rates for aqueous contaminant to be sorbed on solid matrix and backward reaction rates for the reverse processes
K_d	specific decay rate $[T^{-1}]$
K_f	forward reaction rates $[T^{-1}]$
K_b	backward reaction rates $[T^{-1}]$
K_d^{ba}	specific decay rates of bacteria in aqueous phase $[T^{-1}]$
K_d^{bs}	specific decay rates of bacteria in bs phase $[T^{-1}]$
K_d^{bDa}	specific decay rates of bacteria in bDa phase $[T^{-1}]$
K_d^{bDs}	specific decay rates of bacteria in bDs phase$[T^{-1}]$
K_s	half saturation constant $[ML^{-3}]$
K_{Da}^{Ds}	coefficient of deposition rates for colloids $[T^{-1}]$
K_{Ds}^{Da}	coefficient of release rates for colloids $[T^{-1}]$
K_{ba}^{bs}	attachment reaction rate coefficients of bacteria, which is in aqueous phase, for attachment processes to solid matrix $[T^{-1}]$

K_{ba}^{bDa} attachment reaction rate coefficients of bacteria, which is in aqueous phase, for attachment processes to mobile colloid [T^{-1}]

K_{ba}^{bDs} attachment reaction rate coefficients of bacteria, which is in aqueous phase, for attachment processes to immobile colloid [T^{-1}]

K_{bs}^{ba} detachment reaction rate coefficients of bacteria for detachment processes from solid matrix [T^{-1}]

K_{bDa}^{ba} detachment reaction rate coefficients of bacteria for detachment processes from mobile colloid [T^{-1}]

K_{bDs}^{ba} detachment reaction rate coefficients of bacteria for detachment processes from immobile colloid [T^{-1}]

K_{ca}^{cs} sorption reaction rate coefficients of contaminant, which is in aqueous phase, for sorption processes to solid matrix [T^{-1}]

K_{ca}^{cDa} sorption reaction rate coefficients of contaminant, which is in aqueous phase, for sorption processes to mobile colloid [T^{-1}]

K_{ca}^{cDs} sorption reaction rate coefficients of contaminant, which is in aqueous phase, for sorption processes to immobile colloid [T^{-1}]

K_{ca}^{cba} sorption reaction rate coefficients of contaminant, which is in aqueous phase, for sorption processes to bacteria in aqueous phase [T^{-1}]

K_{ca}^{cbs} sorption reaction rate coefficients of contaminant, which is in aqueous phase, for sorption actions to bacteria in phase bs [T^{-1}]

K_{ca}^{cbDa} sorption reaction rate coefficients of contaminant, which is in aqueous phase, for sorption actions to bacteria in phase bDa [T^{-1}]

K_{ca}^{cbDs} sorption reaction rate coefficients of contaminant, which is in aqueous phase, for sorption actions to bacteria in phase bDs [T^{-1}]

K_{cs}^{ca} desorption reaction rate coefficients of contaminant for desorption processes from solid matrix[T^{-1}]

K_{cDa}^{ca} desorption reaction rate coefficients of contaminant for desorption processes from mobile colloid[T^{-1}]

K_{cDs}^{ca} desorption reaction rate coefficients of contaminant for desorption processes from immobile colloid[T^{-1}]

K_{cba}^{ca} desorption reaction rate coefficients of contaminant for desorption processes from aqueous bacterial cell surfaces [T^{-1}]

K_{cbs}^{ca} desorption reaction rate coefficients of contaminant for desorption processes from bacterial cells in phase bs $[T^{-1}]$

K_{cbDa}^{ca} desorption reaction rate coefficients of contaminant for desorption processes from bacterial cells in phase bDa $[T^{-1}]$

K_{cbDs}^{ca} desorption reaction rate coefficients of contaminant for desorption processes from bacterial cells in phase bDs $[T^{-1}]$

n_p number of assigned particles in RWPT model [1]

PDEs partial differential equations

PT Partial tracking technique

Q_g mass growth rate of bacteria $[ML^{-3}T^{-1}]$

Q_d mass decay rate of bacteria $[ML^{-3}T^{-1}]$

Q_g^{ba} mass growth rates of bacteria in aqueous phase $[ML^{-3}T^{-1}]$

Q_g^{bs} mass growth rates of bacteria attached on solid matrix phase $[ML^{-3}T^{-1}]$

Q_g^{bDa} mass growth rates bacteria attached to mobile colloid $[ML^{-3}T^{-1}]$

Q_g^{bDs} mass growth rates of bacteria attached to immobile colloid $[ML^{-3}T^{-1}]$

R contaminant utilization rate $[ML^{-3}T^{-1}]$

R_{ca} contaminant utilization rate for aqueous contaminant by bacterial cells $[ML^{-3}T^{-1}]$

R_{cba} contaminant utilization rate, for contaminant in phase cba, by the carrier bacterial cells $[ML^{-3}T^{-1}]$

R_{cbs} contaminant utilization rate, for contaminant in phase cbs, by the carrier bacterial cells $[ML^{-3}T^{-1}]$

R_{cbDa} contaminant utilization rate, for contaminant in phase cba, by the carrier bacterial cells $[ML^{-3}T^{-1}]$

R_{cbDs} contaminant utilization rate, for contaminant in phase cbDs, by the carrier bacterial cells $[ML^{-3}T^{-1}]$

RWPT Random walk particles tracking techniques

TCM Total remaining contaminant mass in the domain

TVD third-order, total variance-diminishing scheme

V_p pore water velocity $[LT^{-1}]$

X random number normally distributed with unit variance

X_1 contaminant mass in aqueous phase [M], used in mass balance equations