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Field Trials of Subsurface Chaotic Advection: Stirred Reactive Reservoirs

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Abstract

Chaotic advection refers to the mixing of fluid elements which arise from repeated stretching and folding of fluid parcels [7,8]. Chaotic advection can be generated by time-dependent Darcy flows and has the potential to enhance mixing under laminar conditions in subsurface reservoirs or other porous media [3,4,10]. Enhanced mixing has many possible applications in environmental science and engineering. Remediation of contaminated aquifers is particularly relevant where mixing between the injected reagent and contaminant is a critical step. To assess whether chaos can be invoked at scale in a natural porous medium, a field trial is being designed in the sandpit area at the University of Waterloo Groundwater Research Facility at CFB Borden located near Alliston, ON, Canada, where we propose to use a transient reoriented dipole flow for subsurface stirring. This paper describes the design criteria associated with this phase of the field trial and presents preliminary modelling results for the determination of key flow system parameters. The Borden aquifer was modelled using Visual MODFLOW® Flex, a 3-D software for groundwater flow and heat/contaminant transport. Assumptions included aquifer homogeneity and isotropic and confined flow. At this initial screening stage, focus was given to horizontal flow fields generated. Simulation results showed that after at least four periodic reorientations of dipoles spaced 1.50 m apart with a pumping rate and duration of 2.50 m^3/d and 3 hours, respectively, there is significant crossing of flow paths in the Borden aquifer that indicates high potential for rapid mixing.

Introduction

Effective delivery of reagents is a key factor for the successful implementation of *in situ* remediation methods where chemical/biological amendments are injected into the subsurface to promote contaminant degradation. For desired reactions to occur, the injected reagent and contaminant must come into contact in the porous medium where significant mixing is desired. As flow in groundwater systems falls typically in the low-Reynolds number domain and lacks turbulent dispersion, mixing is limited to rates which are orders of magnitude lower than those encountered in open channel flow [2]. As such, mixing at the pore-scale relies predominantly on molecular diffusion as the critical mass transfer mechanism, leading to the overlapping of dissolved compounds. Since effective aqueous molecular diffusion coefficients range from 10^{-11} to 10^{-9} m^2/s in porous media, mixing is often ineffective at the timescales associated with remediation efforts [1,2]. Thus, transport is the rate limiting step that governs the overall rate of contaminant degradation, rendering remediation activities both costly and unpredictable [2,10].

Conversely, repeated stretching and folding of material lines and surfaces brings about a well-mixed state. If laminar Darcy flows can be designed such that transient crossing of path lines results in the required repeated stretching and folding , then we may be able to achieve the desired remediation reactions in the contaminated aquifers. This type of mixing is known as chaotic advection; moreover, it has been demonstrated previously that chaotic advection can be generated in porous media by time-dependent Darcy flows [6,10]. One configuration used to achieve chaotic advection involves creating periodically reoriented dipole flow through the transient switching of pressures at a series of wells surrounding the treatment zone. This configuration has been termed the rotated potential mixing (“RPM”) flow, and can lead to enhanced mixing and confinement of injected reagents in a porous medium. In RPM flow, a dipole well pair undergoes pumping for a specified duration of time (τ) before being reoriented by angle, θ. This chaotic flow behaviour by RPM flow has been verified mathematically and experimentally in the laboratory under controlled conditions [3,4,6,10]. If chaotic advection can be created and controlled *in situ*, then effective reaction rates and therefore the rate of contaminant remediation can be significantly increased.

In this initial phase of investigation, we study the behaviour of a conservative tracer in a sandy aquifer under chaotic groundwater flow conditions. This paper describes the design criteria associated with this initial phase of the field trial and presents preliminary modelling results that we are using to determine the key RPM flow system parameters to implement a field RPM experiment at Borden.

Site Description

A field trial is being designed in the sandpit area at the University of Waterloo Groundwater Research Facility at CFB Borden located near Alliston, ON, Canada. The sandpit area has been described in broad terms as an unconfined aquifer of thickness ranging from 9 to 11 m underlain by an aquitard ~8 m thick. The aquifer consists of fine to medium-grained well sorted sand of glaciofluvial origin (porosity of 0.33, specific storage of $1\text{x}10^{-3}$/m, and hydraulic conductivity of 6.0×10^{-6} to 2.0×10^{-4} m/s) with some microscale heterogeneity in the form of silty sand and coarse sand lenses [5]. The water table is ~0.5 m below ground surface (“m bgs”) and varies seasonally. Groundwater flows in the north and northeast direction with a hydraulic gradient of 0.0039 and an average linear groundwater velocity of 0.091 m/d.

This field trial will take place in a 3 m x 10 m experimental cell which has been hydraulically isolated from the aquifer on three sides by sheet pilings driven down to ~2 m bgs. The fourth side of the cell is open. This cell has been designed to retain aqueous phase constituents and assess remedial technologies.

Design Considerations & Criteria

To support the experimental design, numerical simulations were performed to determine key RPM flow system parameters, including: base pumping rate (*Q*), pumping duration prior to switching (τ), re-orientation angle (θ), number of iterations of the RPM flow (*n*), and the distance between the dipole pairs (*d*).

Simulations represent a scenario in which a reagent solution previously injected at the centre of the domain was mixed by RPM flows. Ultimately, we were interested in the set of system parameters that would result in enhanced mixing of the injected reagent in the domain while minimizing the reagent mass leaving the system. Particle trajectories (i.e., streaklines) were used as indicators of mixing. At this initial screening stage, simulation results were visually compared using the spatial distribution of particle trajectories as a criterion for selecting the optimal set of parameters. More specifically, optimal RPM flow parameters were considered to be those that produced the greatest lateral spreading of the reagent relative to its initial position and the spatial dimensions of the RPM domain with minimal reagent mass exiting the system. This visually corresponds to streakline distributions that provide the greatest spatial coverage throughout the RPM domain relative to the initial area occupied by the particles representing reagent mass. The optimal set of RPM flow parameters should also produce densely distributed streaklines with visible points of intersection along these trajectories corresponding to the crossing of fluid path lines characteristic of chaotic advection mixing.

Total duration of the proposed test was also was an important design criterion. Due to practical considerations and costs associated with implementation, a shorter test was desirable. The maximum duration of the field trial was not to exceed 14 days.

Methodology

All simulations were executed using the MODFLOW and MODPATH engines in Visual MODFLOW® Flex, a 3-D software for groundwater flow and heat/contaminant transport. MODFLOW is a finite difference groundwater flow model. MODPATH uses velocity field outputs from MODFLOW to track particle locations in space and time. At this initial screening stage, our focus is on the horizontal flow fields generated.

The experimental cell was discretised into a finite difference grid comprised of 30 rows, 100 columns and 1 layer ($\Delta x = 0.1$ m, $\Delta y = 0.1$ m and $\Delta z = 2$ m, respectively). Since solute transport was not a focus at this stage, this coarse discretisation was considered to be sufficient for this effort. The aquifer material was assumed to be isotropic and assigned a specific storage, porosity and hydraulic conductivity of 0.001 m^{-1}, 0.33, and $8.0 x 10^{-5}$ m/s respectively. A constant hydraulic head boundary condition of 8.5 m was applied at the open (left) face of the cell to indicate the average depth to the water table. No-flow boundary conditions were assumed at all other faces of the grid to represent the hydraulically isolated conditions of the cell. Confined flow was assumed for simplicity.

All wells were assigned as a pumping well boundary condition with a time-dependent pumping schedule. The wells were assigned an internal diameter of 5 cm (~ 2 inches) and a screen length of 1.5 metres. Each well was screened from 0.5 to 2 m bgs, corresponding to the depth to water table and the sheet pilings, respectively.

The MODFLOW engine was run using transient flow settings to capture the time-dependent pumping schedule. Under transient flow conditions, MODPATH generates streaklines which represent particle trajectories. Thirty five (35) massless particles were released from a circular area in the centre of the RPM flow domain with a diameter that is 3/5 of the distance between the dipole pairs (i.e, 0.6*d*). These particles represent the approximate initial location of a reagent solution previously injected at the centre of the RPM domain within a non-mobile contaminant treatment zone.

In total, the RPM flow system was designed to include eight (8) wells in a circular array with $\theta = \pi/4$ being the angular offset between neighbouring dipoles. The number of wells was based on practical considerations and previous experience, and was deemed to be sufficient to induce RPM flow. Figure 1 shows a plan view of the finite difference grid with the proposed well locations and initial particle locations.

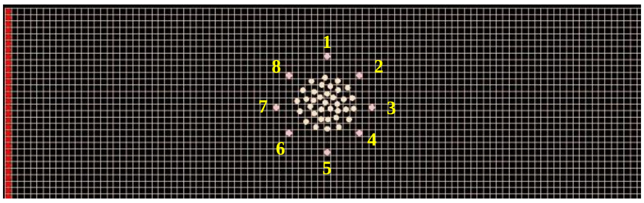


Figure 1. Finite difference grid in Visual MODFLOW® Flex. Red symbols along the left-hand side indicate the constant hydraulic head boundary and the pink symbols indicate the location of the 8 pumping wells. Initial particle locations are shown by white symbols.

The range of pumping rates used in these simulations was determined based on previous experience at the site and capacity of available equipment. For a given time interval τ, a single dipole well pair was set to operate, consisting of one injection and one extraction well. All other wells were turned off at this time. For example, at a given time, only Well 1 (injection) and Well 5 (extraction) would operate as a dipole for τ with equal pumping rates, *Q*. After τ, Wells 1 and 5 would be switched off, and Well 2 would commence operation as the injection well with extraction simultaneously occurring in Well 6. This sequence was repeated around the circular network of wells for a period of 2π.

Parameters and the respective values used in the simulations are summarized in table 1.

Parameter	**Values**
Distance between well pairs, *d* (m)	1.25, 1.5
Pumping duration, τ (hrs)	2, 3, 4
Base pumping rate, *Q* (m^3/d)	1 to 10
Number of iterations, *n*	1 to 8

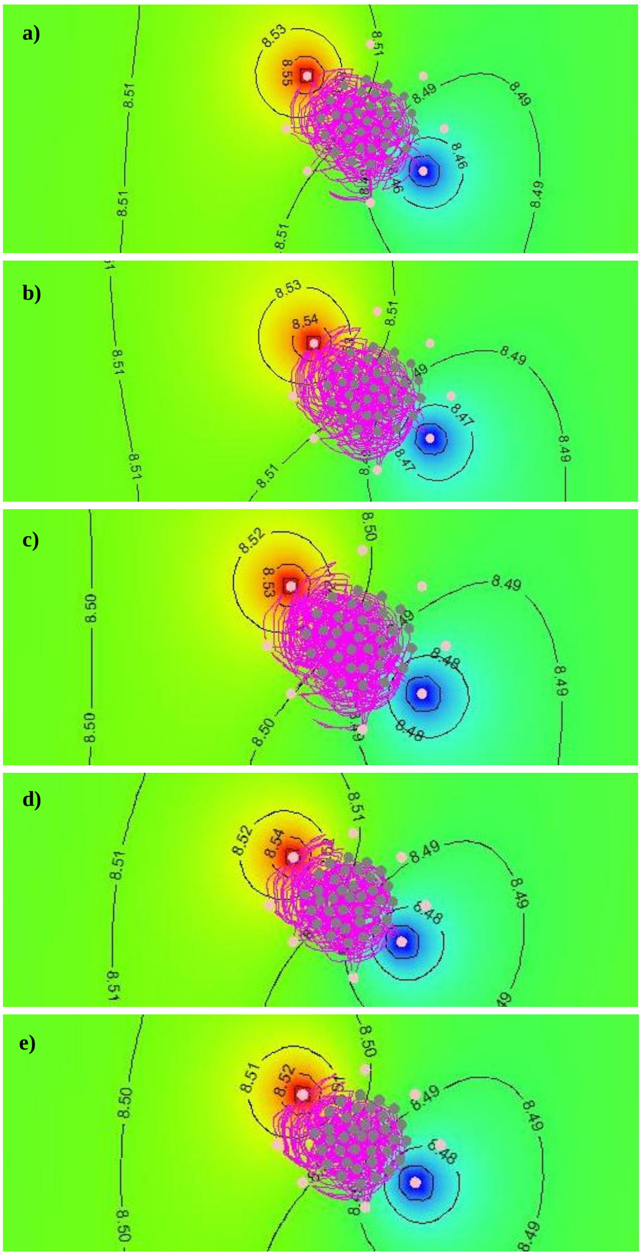
Table 1. RPM flow system parameters used in the simulations.

The optimal set of RPM flow parameters were determined by a sequential process of trial and error. For every combination of *d* and τ, simulations were performed for pumping rates (*Q*) varying at increments of 1 m^3/d for the entire range of values listed in table 1. The goal here was to narrow down the lower and upper bounds of *Q* to a feasible range to observe indicators of mixing. For example, if the pumping rate is too high for a given *d* and τ, all particles would exit the system. Conversely, if a pumping rate is too low, there would be minimal spreading of particles. Once this new range was obtained, the values of *Q* were then refined using smaller increments (≤ 0.5 m^3/d) to determine an optimal pumping rate at which the spatial spread of streaklines and the particles remaining in the system were both maximized. Finally, at the determined optimal value of *Q*, simulations were repeated for $n = 1$ to 8 iterations around the RPM well network to find a value of *n* that minimizes the total test duration without compromising the distribution of streaklines and particles remaining in the system. This iterative process was repeated for every combination of d and τ.

Visual MODFLOW® Flex produced hydraulic head contour maps with particle trajectories at every hour of pumping. Simulation results were captured at the last hour of pumping. Streaklines produced by MODPATH were visually compared for the presence of enhanced mixing within the RPM domain. Mixing by chaotic advection was interpreted to be occurring if densely distributed streaklines were observed throughout the RPM domain in lateral directions relative to their initial position. The areas covered by streakline distributions were estimated relative to the initial area occupied by the particles. Visual estimations were performed by examining the area of streakline distributions as slices of the total RPM domain (expressed as a fraction of the total circular area) and dividing this area by the initial area of the treatment zone to determine spreading as a relative measure.

Results and Discussion

Figure 1 shows the hydraulic head contour maps with streaklines for the simulations that generate maximum spatial spreading and number of remaining particles with minimum duration at every combination of d and τ.



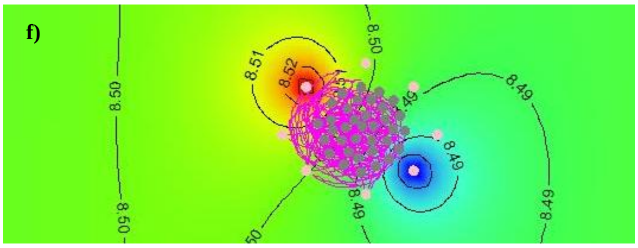


Figure 1. Hydraulic head contour map showing streaklines for: a) d = 1.5 m, τ = 2 hours, Q = 3 m^3/d, n = 4 at 2.67 days, b) d = 1.5 m, τ = 3 hours, Q = 2.50 m^3/d, n = 4 at 4 days, c) d = 1.5 m, τ = 4 hours, Q = 1.75 m^3/d, n = 5 at 6.67 days, d) d = 1.25 m, τ = 2 hours, Q = 2.25 m^3/d, n = 4 at 2.67 days, e) d = 1.25 m, τ = 3 hours, Q = 1.50 m^3/d, n = 4 at 4 days, and f) d = 1.25 m, τ = 4 hours, Q = 1.25 m^3/d, n = 3 at 4 days. Pink symbols indicate the location of the wells and the grey symbols indicates initial position of particles. Black contour lines represent hydraulic head and pink lines indicate streaklines.

Simulations results were assessed using the following criteria: spatial dispersion of particles relative to the initial area occupied by the particles, number of particles remaining in the system, and the total duration of the test. First, it is noted that the particle trajectories produced by MODPATH show a slight skew towards the left half of the RPM domain. This is likely a result of the constant hydraulic head boundary assigned to the open left face of the experimental cell. However, most of the reagent mass appears to remain inside the RPM domain for the duration of pumping despite this skew.

Visual screening and estimation of areas covered by the streaklines in figure 1 indicates that the particles trajectories in figures 1b), 1e) and 1f) provide the greatest spatial coverage of the RPM domain. The dense streakline distributions also indicate potential for occurrences of many intersection points (figure 2). The total duration of the test was the same for all three scenarios at four days. The number of particles remaining in the RPM domain after pumping was also similar in all three scenarios, with ~60% of particles retained.

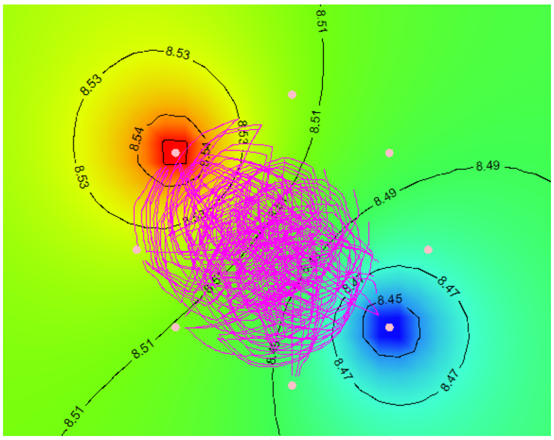


Figure 2. Close-up view of streaklines of scenario 1b).

As such, the set of RPM parameters used in figure 1b) was identified to be optimal to invoke mixing by chaotic advection. These results showed that after at least four periodic reorientations of dipoles spaced 1.50 m apart with a pumping rate and duration of 2.50 m^3/d and 3 hours, respectively, there is significant crossing of flow paths in the Borden aquifer that indicates high potential for rapid mixing.

Conclusions

Chaotic advection refers to mixing caused by the crossing of streamlines resulting in repeated stretching and folding of fluid parcels. One configuration used to achieve chaotic advection involves creating periodically reoriented dipole flow through the transient switching of pressures at a series of radial wells around the treatment zone (termed RPM flow). Key RPM flow parameters include base pumping rate (*Q*), pumping duration (τ), re-orientation angle (θ), number of periodic iterations (*n*), and the diameter between the dipole pairs (*d*).

A field trial is being designed in the sandpit area at the University of Waterloo Groundwater Research Facility at CFB Borden located near Alliston, ON, Canada. To determine the RPM flow parameters required to invoke chaos in the Borden aquifer, simulations were performed using the MODFLOW and MODPATH engines in Visual MODFLOW® Flex, a 3-D software for groundwater flow and heat/contaminant transport. The primary objective of numerical modelling was to determine the set of RPM parameters that would result in enhanced mixing of the injected reagent in the RPM domain while minimizing the reagent mass leaving the system. Particle trajectories generated by MODPATH were visually compared for indications of mixing. Optimal values of RPM flow parameters were determined to be those that produced the greatest lateral spreading of the reagent relative to its initial position in the RPM domain in all directions of horizontal flow while minimizing the reagent mass exiting the system. The total duration of the test was also considered in selection of the optimal RPM parameters. Simulation results confirmed the published theoretical and laboratory findings on chaotic advection. Furthermore, simulation results showed that after at least four periodic reorientations of dipoles spaced 1.50 m apart with a pumping rate and duration of 2.50 m^3/d and 3 hours, respectively, there is significant crossing of flow paths in the Borden aquifer that indicates high potential for rapid mixing.

The results presented in this paper represent initial modelling efforts to show the potential of using RPM flows to invoke chaotic advection in an aquifer. The next stage will focus on the development of a three-dimensional model that includes vertical flow fields.

Acknowledgements

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