

## COMPARISON OF CHAOTIC FLOWS FOR PLUME SPREADING IN AQUIFERS

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### 1 INTRODUCTION

Groundwater is a crucial resource, containing 99% of the world's fresh water.<sup>1</sup> Accordingly, remediation of groundwater contamination resulting from historical waste disposal or accidental spills is a multi-billion dollar industry and a major focus in hydrology.<sup>2</sup> Because of the well-known limitations of pump-and-treat remediation, in which contaminated groundwater is extracted for treatment by an engineered system, the last few decades have seen widespread acceptance of the alternative approach of in situ remediation, in which treatment takes place within the aquifer. In situ remediation promotes degradation reactions that generally take place at the *fluid interface* between the contaminated groundwater and a plume of injected treatment solution containing chemical or biological amendments. Although major advances have been made with regard to chemical and biological aspects of in situ remediation, and numerous studies have investigated the effect of non-uniform velocity fields resulting from aquifer heterogeneity, the prospect of improving remediation by imposing engineered velocity fields has received less attention. Therefore, the general approach of the present research is to improve in situ remediation by hydraulic means.

Why engineer velocity fields by injection and extraction? Because doing so provides a mechanism to overcome a fundamental limitation of groundwater remediation, or any application where reactions take place against the background of laminar flow imposed by porous media. The fundamental limitation is that laminar flows lack the turbulent velocity structure that provides efficient mixing in streams and engineered reactors. Fortunately, the fluid mechanics literature indicates that mixing under laminar conditions can be optimized by using a chaotic flow, that is, a deterministic flow with sensitive dependence on initial conditions.<sup>3</sup> To create such a chaotic flow, a periodic velocity field can be engineered to create stretching and folding of

fluid interfaces. Indeed, stretching and folding has been called the essence of mixing.<sup>4</sup> Therefore a promising approach to improve in situ remediation by hydraulic means is to design a chaotic flow that will stretch and fold the fluid interface between the contaminated groundwater and the treatment solution, which will elongate the fluid interface, leading to enhanced reaction and accelerated remediation.

## 2 BACKGROUND

Previous studies have considered a model system whose initial condition is a cylindrical plume of treatment solution surrounded by four injection-extraction wells, located at a unit distance in each of the cardinal directions, in a confined, homogeneous, isotropic aquifer of infinite extent with contamination in the region between the wells (Figure 1). Stretching and folding is imposed by a series of injections and extractions at the four wells, shown conceptually as the first cycle in Table 1, and with details provided elsewhere.<sup>5</sup> In order to avoid clogging at wells, the fluid interface (*i.e.*, the reactive surface) cannot be extracted. Neglecting diffusion, dispersion, sorption, and transient effects following changes in the injection-extraction scheme, the first cycle in Table 1 turns the initially circular fluid interface into contorted geometry shown in Figure 2a. Later studies have generalized this injection-extraction scheme to include diffusion and dispersion,<sup>6</sup> and have analyzed this injection-extraction scheme using analysis tools from the field of dynamical systems.<sup>7</sup> Specifically, the analysis tools from dynamical systems are (1) to identify periodic points, which are points to which fluid particles return in later cycles; (2) to categorize these periodic points as elliptic points or hyperbolic points; (3) to plot the stable and unstable manifolds associated with the hyperbolic periodic points; and (4) to identify heteroclinic points, located at the intersection of stable and unstable manifolds, which confirm the presence of deterministic chaos.

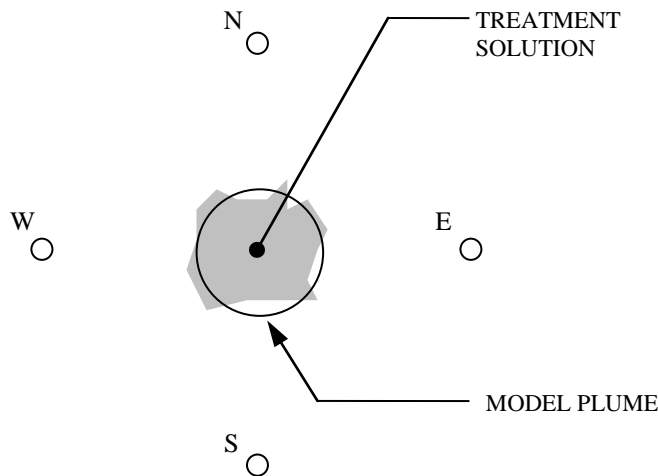


Figure 1: Aquifer schematic, with treatment solution injected at center, and surrounding wells N-W-S-E.

cycle	+	+	-	-	-	-	+	+	-	-	-	-
1	W	E	W	E	W	E	S	N	S	N	S	N
2	E	W	E	W	E	W	N	S	N	S	N	S
3	W	E	W	E	W	E	S	N	S	N	S	N
4	E	W	E	W	E	W	N	S	N	S	N	S

Table 1: New injection and extraction scheme, where (+) indicates injection and (-) indicates extraction.

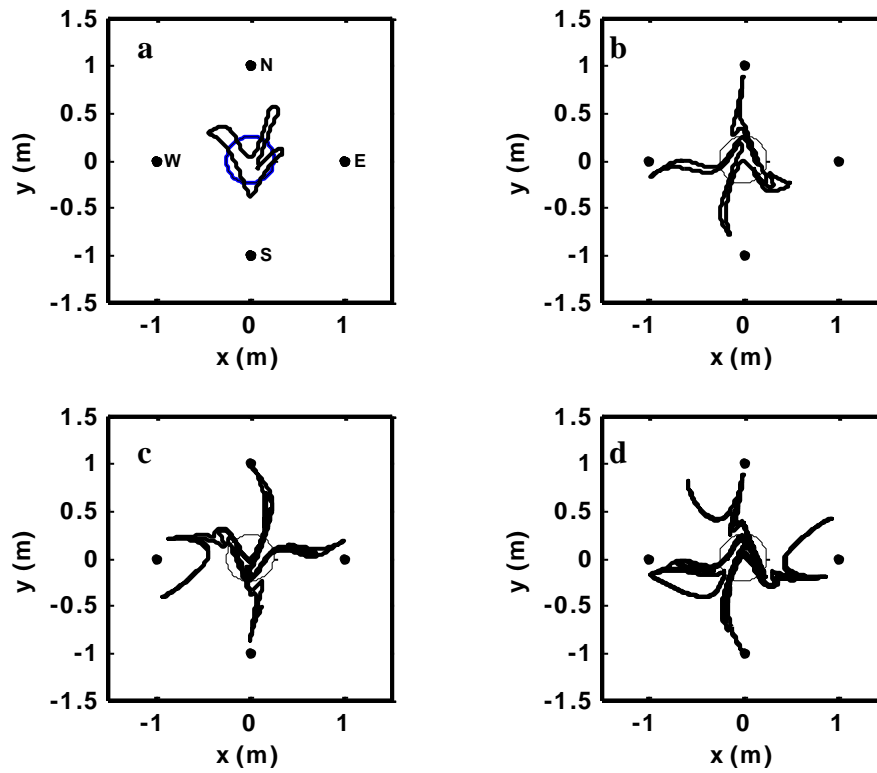


Figure 2: Fluid interface after cycle 1 (a), cycle 2 (b), cycle 3 (c), and cycle 4 (d) shown in Table 1.

Although the first cycle on Table 1 achieved plume spreading by stretching and folding, it has not been optimized, and should therefore be viewed as a proof-of-principle design. The analysis described above has identified a number of limitations in this specific injection-extraction scheme. Therefore the goal of the present study is to investigate plume stretching and folding by an alternative injection-extraction scheme.

### 3 ANALYSIS

The first cycle on Table 1 comprises two 6-step building blocks. The first 6-step building block starts with well W, then uses wells W and E to stretch and fold the initially circular fluid interface into a geometry resembling a flattened crescent. The second 6-step building block is identical to the first, except that it begins with well S, and uses wells S and N. Given the initial condition resembling a flattened crescent, the second 6-step building block generates the interface is shown in Figure 2a. Previous studies have treated these two 6-step building blocks as a single 12-step cycle, which was then repeated.

In the present study, the 6-step building block is the same, but instead of alternating the initial well between W and S, the initial well rotates in the order  $W \rightarrow S \rightarrow E \rightarrow N$ . The two 6-step building blocks starting with  $W \rightarrow S$  form the first and third 12-step cycles on Table 1, and the two 6-step building blocks starting with  $E \rightarrow N$  form the second and fourth cycles on Table 1.

### 4 RESULTS

The fluid interface after each of the four cycles on Table 1 is shown in Figure 2. Visual inspection reveals that stretching and folding in each of the cardinal directions generates additional elongation of the fluid interface compared to previous studies.<sup>5-7</sup>

Preliminary results have identified periodic points, which are the basis for more advanced dynamical systems analysis. To identify the location of periodic points, an initial matrix of particle positions was defined, then tracked through each of the four cycles on Table 1, from which the magnitude of the particle displacement  $|\vec{x} - \vec{x}_o|$  was calculated and plotted as a contour map at the initial position. Results for the first cycle on Table 1 are shown in Figure 3. In this

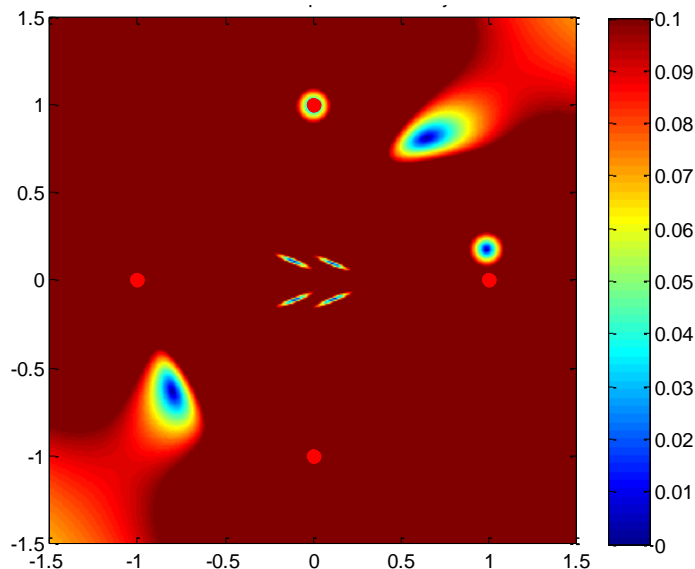


Figure 3: Particle separation distance from initial position after cycle 1 in Table 1.

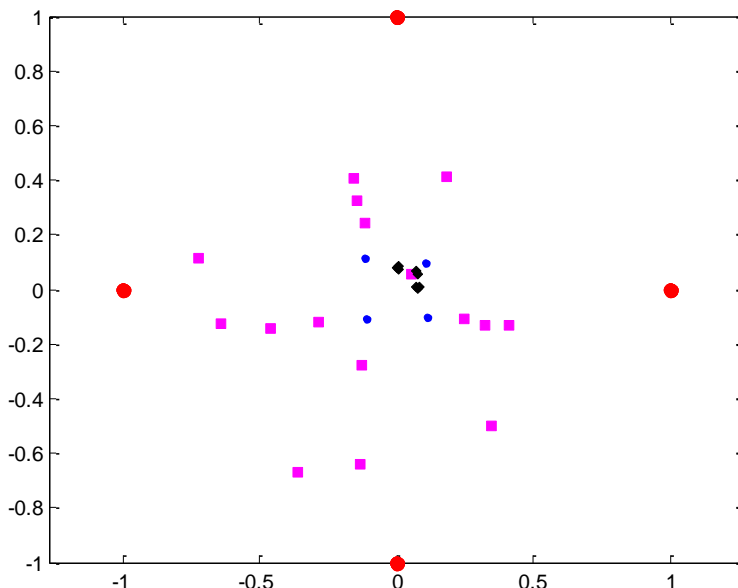


Figure 4: Periodic points for periods 1, 2, and 4. Large red circles are wells; small purple circles are period 1 periodic points; blue squares are period 2 periodic points; black diamonds are period 4 periodic points.

plot, the four disk-shaped minima near the origin are of primary importance because of their proximity to the initial position of the fluid interface.

The minima (*i.e.*, zeros) on Figure 3 indicate the locations of period 1 periodic points. Equivalent plots after the second, third, and fourth cycles of Table 1 identify the location of period 2, 3, and 4 periodic points. No period 3 periodic points were identified, but period 1, 2, and 4 periodic points are shown on Figure 4. Compared to the equivalent plot in previous work,<sup>7</sup> the periodic points fill a larger proportion of the area between the four wells. Because chaotic mixing is associated with periodic points, the more extensive spatial distribution of periodic points in the present study suggests that simply changing the starting wells from  $W \rightarrow S$  to  $W \rightarrow S \rightarrow E \rightarrow N$  will result in improved spreading. Testing this hypothesis is the subject of ongoing research.

## 5 CONCLUSIONS

The work reported here suggests that a diversity of injection-extraction schemes can achieve improved plume spreading by stretching and folding. In other words, the particular injection-extraction scheme analyzed in previous studies<sup>5-7</sup> is not unique. Both it and the modification presented here show that the basic idea of improved spreading in laminar chaotic flows is sound. Ongoing research will relax the assumptions used here, particularly with regard to aquifer heterogeneity and contaminant (or treatment solution) sorption, and will employ optimization tools to further improve the injection-extraction scheme. More generally, these results are encouraging from the perspective of using well hydraulics to complement other advances in chemical and biological aspects of in situ groundwater remediation.

## 6 ACKNOWLEDGMENTS

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