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Evidence of Low-dimensional Determinism in Short Time Series of Solute Transport

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Fall 2013

Evidence of Low-dimensional Determinism in Short Time Series of Solute Transport

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Fall 2013**

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Abstract

Investigating the vadose zone, the physics behind the temporal and spatial instabilities of flow (in unsaturated media) is still of question. Although chaotic approaches have been widely employed for identifying different surface hydrology processes, such as rainfall, runoff, lake volume, etc., they were not applied for subsurface systems as much. On this ground, the present study attempts to investigate nonlinear determinism in solute transport processes in vadose zone. Previously, a few studies have investigated/examined solute transport processes from the view point of nonlinear chaos. However, this is the first study that is directly analyzing solute transport time series from field experiments. Also, it is analyzing short time series (68 data points) from a soil profile (62 measurement probes). For this purpose, Correlation Dimension Method is used as the most celebrated nonlinear chaotic technique in the hydrological studies. In general, the results of correlation dimension analysis provide the minimum number of ordinary differential equations needed to map a given dynamics. This study placed its main focus on the evolution of Correlation Exponent (CE) vs. Embedding Dimension (EM). The oscillation of correlation exponents between different values (2-4) which is referred to as Instable Saturation (IS) has been observed. Plausible explanations for this instability is discussed. The values of correlation dimensions for stable saturation are 2 and 3 among which $CD=3$ is the most frequent CD for SS is 3; for the rest of SS, CD is 2. In case of instable saturation, however, CD values are varying between 2 and 4 where IS-2, 3 is the most frequent one. Although the results are not as 'accurate' as other hydro-chaotic studies which dealt with longer time series, the consistent pattern and the order of magnitude in the results are in good agreement with previous findings. On a large scheme, the results encouragingly indicate a promising avenue from the presuppositional perspective of stochasticism towards nonlinear determinism for hydrological studies especially subsurface processes.

Keywords: Nonlinear time series analysis, Chaos Theory, Correlation Dimension Method, Solute transport, short time series, unsaturated zone, vadose zone.

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Sina

30 October 2013, Lund

Acronyms and Abbreviations

CC	Correlation Coefficient
CE	Correlation Exponent
CDM	Correlation Dimension Method
DOF	Degree of Freedom
EM	Embedding Dimension
FNA	False Neighbors Algorithm
FNN	False Nearest Neighbors
GKA	Gaussian Kernel Algorithm
GPA	Grassberger-Procaccia Algorithm
KEM	Kolmogorov Entropy Method
LEM	Lyapunov Exponent Method
ODE	Ordinary Differential Equation
NPM	Nonlinear Prediction Method
RC	Relative Concentration
ST	Solute Transport

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1 INTRODUCTION

Investigating hydrologic processes from the view point of Chaos Theory has been of great interest during recent times. For one thing, possible presence of nonlinear determinism in such systems could be utilized to model and predict the dynamics of these hydrologic systems. The favorable outcomes of such studies together with the great performance and predictability of nonlinear techniques in comparison to other methods (Sivakumar, Persson, Berndtsson, & Uvo, 2002), such as stochastic, neural networks, indicate a promising avenue towards the extension of the applications of nonlinear deterministic approaches for solving hydrological problems.

So far, one of the main challenges of chaos application in hydrology has been its limited scope; it was mainly concentrated on surface hydrologic processes such as rainfall, rainfall-runoff, river flow, lake volume and sediment transport. Despite the fact that the results of these studies are promising, nonlinear determinism framework has not received much attention in order to be employed for subsurface problems (Sivakumar, Harter, & Zhang, 2005). This is due to the fact that it is generally presupposed that the heterogeneous – essentially nonuniform in composition/character – nature of soil and aquifers would result in random behavior (dynamics) of flow and transport. This presupposition has been justified by the temporal and spatial variability exhibited by these processes. Therefore, flow and transport models most commonly employ the concept of stochastic process. Especially the fact that these models fairly represent the basic statistical properties (e.g. mean, variance) of flow and transport processes may have further strengthened the view on the usefulness of stochastic field/process concept for subsurface problems (Sivakumar et al., 2005).

One of the most challenging problems in the modern subsurface hydrology/hydrogeology is the characterization of unstable flow and transport in unsaturated zones and rocks. The unsaturated zone, also known as vadose zone, is situated between the soil surface and the groundwater table (saturated zone). Based upon this layer the food chain is built; plants take up water and nutrient from this zone. Therefore, it plays an essential role in the ecosystem (Persson, 1999). Understanding the nature of unsaturated flow in fractures is imperative to incorporate a foundation for resolving practical problems related to hydrogeological systems including the vadose zone (Faybishenko, 2002). Unstable flow has various fundamental applications, both theoretically and practically:

- Theoretically speaking, wetting-front instability can invalidate our best-laid theories of vertical infiltration and groundwater recharge (Hillel, 1987).

- Moreover, it can have important practical consequences. For example, unstable flow can allow small ‘outlaw’ streams of water to flow directly, and carry raw pollutants, into the groundwater while avoiding the profile’s filtration and purification mechanisms (Hillel, 1987). It could also be utilized for developing technical and economic programs for environmental remediation; the exploitation of oil, gas, and geothermal reservoirs; and nuclear waste disposal in fractured rock (Faybishenko, 2002).

Transport and flow processes in fractured rocks occur, generally, in a “nonvolume-averaged” fashion; relatively slow flow through the rock matrices and fast flow in localized preferential pathways within fractures. Currently, nevertheless, modeling of these processes in unsaturated fractured rocks utilizes macro-scale continuum concepts based upon large-scale volume averaging. Such models would be well fitted to represent large-scale features of fractured-rock, yet would be insufficient for resolving time varying and spatially localized flow phenomena. This causes serious challenges for mathematical modeling and demands alternative methods of modeling for a given site. As it is explained earlier, the common approach has been based upon stochastic techniques in order to describe the seemingly random data sets, overlooking the fact that deterministic nonperiodic (chaotic) processes could yield ostensible randomness (Faybishenko, 2002). In light of the above, it is crucially important to identify chaotic processes in subsurface systems in order to develop appropriate models for short- and long-term predictions. The very first step in this direction would be to investigate the possible presence of low-dimensional determinism in the underlying dynamics of subsurface systems such as solute transport process(es).

1.1. Problem Definition

Within the field of hydrogeology and specifically investigating the vadose zone, the physics behind the temporal and spatial instabilities of flow (in unsaturated media) is still of question. In addition, it is yet unclear how laboratory and field experiments should be optimized and also how some paradoxes in unsaturated flow theory (Gray & Hassanizadeh, 1991) could be explained (Faybishenko, 2002). On this ground, the main objective of the present study is to investigate the potential utilization of a nonlinear deterministic framework for understanding the underlying dynamics of Solute Transport (ST) processes. In other words, this study attempts to explore the possible presence of low-dimensional determinism in short time series of solute transport. Pursuing this goal, Correlation Dimension Method (CDM) as a celebrated technique of nonlinear time series analysis is employed to distinguish determinism and stochasticity.

The possibility of the existence of chaotic behavior in transport processes in the soil stems from the fact that such transport processes and also most of the models used to exhibit them

are nonlinear (Addiscott & Mirza, 1998). Faybishenko (2002) and Sivakumar et al. (2005) have examined the possible existence of chaotic behavior in flow and transport processes using different data sets. Nonetheless, no study has so far placed its main focus on the evolution of Correlation Exponent (CE) vs. Embedding Dimension (EM). Almost all studies in this realm with the objective of ‘system identification’ have attempted to simply calculate the Correlation Dimension (CD) as the diagnostic parameter of deterministic chaos. However, it is very important to look at the unfolding behavior of CE vs. EM considering the time series length and also the nature of the studied system(s).

It is vitally crucial to keep this possibility open that there might be chaotic systems where the number of generating mechanisms – the number of governing autonomous Ordinary Differential Equations (ODE) – are not constant during the evolution of the system; that is, instability in the mechanisms generating the dynamic of the process. Not just the results of a few interacting mechanisms are hugely different based upon their initial conditions (the essence of Chaos Theory), but also as the system evolves its generating mechanisms/variables and their number could be highly dependent on the conditions of the process in which initial conditions could be one of them. Therefore, in light of the above, CDM analysis has been conducted on a data set of solute transport signals measured at different levels of a soil profile; that is, to see if any pattern could be discerned in the evolution of CE vs. EM, horizontally or vertically.

2 LITERATURE REVIEW

After presenting a brief history of Chaos Theory, Khatami (2013) has thoroughly explained its fundamental elements and concepts, namely, phase-space, trajectory and attractor. Further, he has discussed various aspects and criticisms on the application of Chaos Theory in hydrological studies. Therefore, this study would not explore the theory and its related issues but put its main focus on its application in solute transport process.

Chaos Theory attempts to study dynamical systems and how they behave with their highly dependence on initial conditions – dynamical instability. A chaotic process or system evolves in a deterministic way that its current state depends unequivocally on its previous state (Addiscott & Mirza, 1998). Chaos theory could be seen and employed on a larger scheme as “complexity theory”, “complex systems theory,” “synergetics”, and “nonlinear dynamics”. Nevertheless, to the present time, application of chaos theory in practical problems remains as much an art as a science (Faybishenko, 2002). So far, different methods have been employed in order to investigate deterministic chaos in hydrological processes. The simplest tool is the phase diagram plot of a dynamical system which is in fact a visual evaluation of the process investigating preliminary evidence on deterministic chaotic behavior. Sophisticated diagnostic techniques, namely, Correlation Dimension Method (CDM), Lyapunov Exponent Method (LEM), Kolmogorov Entropy Method (KEM), Nonlinear Prediction Method (NPM), Gaussian Kernel Algorithm (GKA), and False Neighbors Algorithm (FNA) or False Nearest Neighbors (FNN), could also be employed for different purposes. In principle, these methods are tests examining whether a given system/process is deterministic chaotic or stochastic. Among which CDM is the fundamental approach and it has been widely used in hydrological studies.

2.1. Chaos Theory in Solute Transport

Addiscott and Mirza (1998) was the first study – to the knowledge of the author – that has proposed a paradigm shift from stochastic to deterministic chaos in order to investigate and/or model transport processes in soil. Their proposition was based upon studies by Flühler, Durner, and Flury (1996) and Steenhuis et al. (1998). Experimental observations by Flühler et al. (1996) has shown that the variable extent and rates of lateral mixing cause substantially different transport regimes which could neither be explained nor predicted mechanistically in terms of known state variables. They have speculated that solute flow may not only be chaotic but may also have further complication as the chaotic processes depend upon randomly distributed state variables. This might explain the transport regimes found by Flühler et al. (1996), i.e., “neither be predicted nor explained mechanistically in terms of

known state variables”. Therefore, they have proposed an even more complex approach of modeling in which deterministic chaos is interacting with stochastic distribution of state variables. To their opinion, suppose one can show chaotic behavior in a transport model, then two fundamental questions should be met; ‘So what?’ and ‘What then?’. The former, calls attention to careful and critical thinking about the way in which the models are used. The latter, nonetheless, could be answered in various ways. One possibility is to reformulate the theoretical approach to transport processes endorsing their chaotic natures. Study by Rodriguez-Iturbe, Entekhabi, Lee, and Bras (1991) could be an example for this case. Addiscott and Mirza (1998) have looked through this question and discussed several different options as well.

Faybishenko (2002) has compared the results of Persoff–Pruess experiments (Persoff & Pruess, 1995) with nonlinear chaotic analyses of both laboratory dripping-water experiments in fracture models and field-infiltration experiments in fractured basalt. Based upon this comparison he has hypothesized that processes of intrinsic fracture flow and dripping as well as extrinsic water dripping from a fracture subjected to a capillary-barrier effect are deterministic chaotic systems with a certain random component. In brief, it has been concluded that the unsaturated fractured rock is a chaotic dynamic system as the flow processes are dissipative, nonlinear, and sensitive to initial conditions. These flow processes are exhibiting chaotic oscillations generated by intrinsic properties of the system, not external random factors. Identifying such systems as deterministic is a crucial turning point in terms of developing well-defined models for short- and long-term predictions of these dynamic systems, evaluating the uncertainty inherent to the system and its predictions, assessing the spatial distribution of flow characteristics from solute transport time series, and ultimately improving chemical-transport simulations.

Sivakumar et al. (2005) have employed CDM in order to investigate deterministic behavior in solute particle transport time series in a heterogeneous aquifer medium. They have studied simulated time series for different scenarios using an integrated probability/Markov chain (IP/MC) model. The phase-space is reconstructed in two dimensions (i.e. $m=2$), with 1 year delay time which is a typical sampling interval for groundwater monitoring. CDM nonlinear analyses of solute transport processes have interestingly yielded correlation dimension of 2 for a two facies medium (sand 20%, clay 80%), and correlation dimension of 3 for a three facies medium (sand 21.26%, clay 53.28%, loam 25.46%). It should be noted that anisotropy conditions have been considered for different simulation scenarios and different number of facies.

As Khatami (2013) has summarized major studies of Chaos Theory in hydrology, summary of its main applications in ST processes are presented in **TABLE 1**.

Table 1. *Classified summary of nonlinear chaotic analyses of solute transport processes*

Study	Results	Summary
Addiscott and Mirza (1998)	-	Proposes a paradigm shift from stochastic to deterministic chaos for investigating transport processes in soil
Faybishenko (2002)	CD=2-4	“The unsaturated fractured-rock system is chaotic as the flow processes are sensitive to initial conditions, nonlinear and dissipative. The presence of chaotic behavior is confirmed by calculating diagnostic chaotic parameters for gas, liquid, and capillary pressures, measured during the water–gas injection in fractures, as well as laboratory and field dripping-water experiments.”
Sivakumar et al. (2005)	CE=1.33 & 2.12, CD=2-3	Simulated solute transport through the two and three facies media in a heterogeneous aquifer medium

3 MATERIAL & METHODS

3.1. Data Sets & Study Area

Solute transport time series are collected from the field experiments that has been carried out in a site situated in Löddeköpinge in southern Sweden by Persson (1999). The soil in this field consists of 4 horizons, namely, Ap (topsoil or surface mineral horizons with anthropogenic disturbances e.g. ploughing, deep ripping), E (eluviated), B (subsoil), and C (parent material). Details of each horizon are presented in table below.

Table 2. *Soil properties (Persson & Berndtsson, 2002)*

Horizon	Depth (cm)	Sand (%)	Silt (%)	Clay (%)	Organic C (%)	Bulk Density (g/cm ³)	Porosity (m ³ /m ³)
Ap	0-20	80	16.5	3.5	4.3	1.53	0.40
E	20-45	78.8	18.3	2.9	3.4	1.55	0.39
B	45-70	84.3	11.8	3.9	2.6	1.55	0.39
C	>70	93.4	4.8	1.8	0.5	1.56	0.39

Measurement probes are planted in the soil profile as it is schematically portrayed in **FIGURE 1**. Data derive from this probes are not point measurements. Each probe measures an average Relative Concentration (RC) over an approximate cylindrical volume with a diameter of about 5 cm around a 30-cm probe.

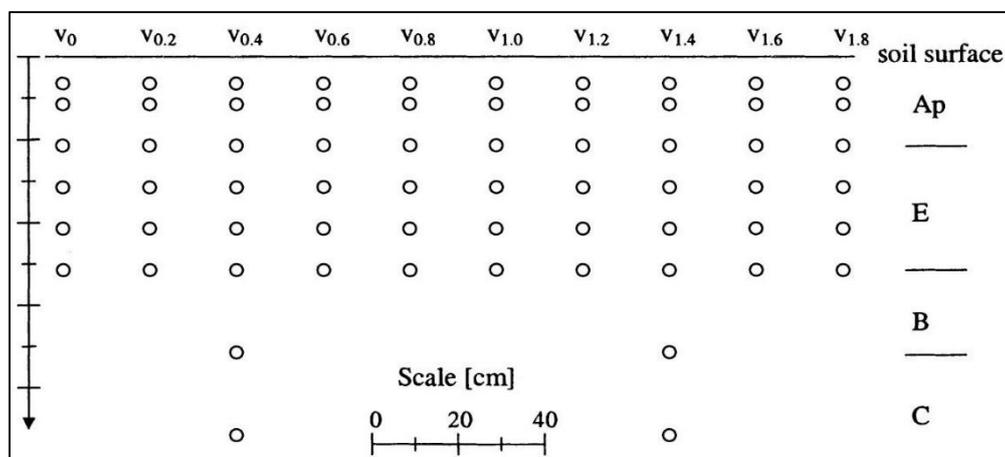


Figure 1. *Schematic location of TDR probes on the soil profile (Persson & Berndtsson, 2002)*

The temporal resolution of time series is 12 h and the measurement is began 132 h (i.e. 11 time steps) prior to applying the tracer into the soil. Each time series contains 68 data points from which 57 values are after the tracer is applied. Overall, 64 probes are placed at 8 different depths of 5, 10, 20, 30, 40, 50, 70, and 90 cm. The first 6 depths contain 10 probes each, and the two deepest ones include 2 each. It should be noted that two sensors were broken and so only 62 signals are at hand. These two sensors are number 48 at depth 40 cm and number 59 at depth 50 cm. Further information about the field experiments and data collection are explained by Persson (1999) and Persson and Berndtsson (2002).

3.2. Correlation Dimension Method

Due to the fact that sophisticated mathematics behind Chaos Theory has been explained thoroughly in several authentic sources (e.g.(Broer & Takens, 2011; Gidea & Niculescu, 2002; Ivancevic & Ivancevic, 2008), the present study only focuses on the application aspect of the theory and CDM technique in particular.

There are different methods discerning low-order deterministic chaotic processes from stochastic ones. Among those, CDM is almost certainly the most fundamental one that has been used in a wide range of subjects. In simple words, CDM attempts to estimate the dimension of a dynamic system's attractor. CDM is established upon the concept of the *correlation integral* (or *correlation function*). The concept is that an ostensibly irregular phenomenon could arise from deterministic dynamic. Therefore, such systems will have a limited number of DOF equal to the smallest number of first order differential equations that capture the most important features of their dynamic. From different approaches in estimating the correlation dimension, the present study utilizes the Grassberger-Procaccia Algorithm (GPA)(Grassberger & Procaccia, 1983).

The reconstruction of the phase-space of a scalar time series and, hence, its attractor is the first important step in any chaos identification approach. Such a reconstruction method uses the concept of embedding a single-variable series in a multi-dimensional phase-space to represent its underlying dynamic (Sivakumar & Jayawardena, 2002). As the present study aims to analyze discrete time series of ST observations, hence, the phase-space reconstruction method is explained for discrete scalar time series.

For an autonomous system characterized by d interacting state variables (a d -dimensional state space \mathbf{z}) the associated dynamics could be represented as:

$$\frac{d\mathbf{z}(t)}{dt} = F(\mathbf{z}(t)) \quad (\text{Equation 1})$$

Assume a scalar univariate time series $x(t)$, $t=1, 2, \dots, N$ for one of the d state variables (i.e. RC in this study), generated by this system. This system can be rewritten as a high-ordered differential equation in terms of the single state variable x as follow:

$$x^{(d)} = f(x, x', \dots, x^{(d-1)}) \quad (\text{Equation 2})$$

Based upon the notion of phase-space reconstruction (Packard, Crutchfield, Farmer, & Shaw, 1980; Takens, 1981) a pseudophase-space could be defined using delay coordinates by defining a delay vector \mathbf{Y}_t :

$$\mathbf{Y}_t = \{x(t), x(t - \tau), \dots, x(t - (m - 1)\tau)\} \quad (\text{Equation 3})$$

where τ is delay time, appropriately chosen as an integer multiple of sampling time Δt , and m is an integer embedding dimension. If the solution of the equations lies on an attractor of dimension d_A ($d_A < d$), choosing the integer m ($m > 2d_A$) is a sufficient condition for unfolding the attractor from time series $x(t)$. Subjecting to generic assumptions on F and Δt , for any delay time τ and forecast period T , the underlying dynamics could be represented by a smooth (i.e. differentiable) map:

$$\begin{aligned} \mathbf{Y}_{t+T} &= f^T(x(t), x(t - \tau), x(t - 2\tau), \dots, x(t - (m - 1)\tau)) = f^T(\mathbf{Y}_t) \\ f^T: \mathbb{R}^m &\rightarrow \mathbb{R} \end{aligned} \quad (\text{Equation 4})$$

Where \mathbf{Y}_t and \mathbf{Y}_{t+T} are vectors of dimension m , describing the system state at current state t and future state $t+T$, respectively. Equation 4 is a basis for reconstructing the phase-space of the underlying dynamic of a given scalar time series by providing the map f^T if appropriate values of τ and m are chosen.

Simply put, the reconstruction of the phase-space from a discrete time series (pseudophase-space) can be achieved with the help of an m -dimensional ‘‘embedding space’’, EM, which is spanned by delay vectors for any given (integer) time delay τ . For a scalar univariate time series X_i , where $i=1, 2, \dots, N$ the phase-space could be reconstructed as (Sivakumar, Berndtsson, Olsson, & Jinno, 2001):

$$\mathbf{Y}_j = (X_j, X_{j+\tau}, X_{j+2\tau}, \dots, X_{j+(m-1)\tau}) \quad (\text{Equation 5})$$

where $j=1, 2, \dots, N-(m-1)\tau/\Delta t$, m is the embedding dimension (dimension of vector \mathbf{Y}_i) and τ is delay time. τ is almost an ‘arbitrary’, but fixed time delay for an infinite amount of noise-free data (Takens, 1981). τ should be a suitable integer multiple of the sampling time Δt (Packard et al., 1980; Takens, 1981). m is the number of coordinate of the embedding space.

Despite the basic assumption of phase-space reconstruction method that for an infinite noise-free time series, τ is an almost ‘arbitrary’, there is no such time series in real life problems and hydrological time series are no exceptions to this. Therefore, there has been a quest finding the optimal delay time for practical problems. In practical problems and in particular hydrological studies investigating the existence of chaos in hydrological time series (e.g. Jayawardena & Lai, 1994; Khatami, 2013; Puente & Obregón, 1996; Rodriguez-Iturbe, Febres De Power, Sharifi, & Georgakakos, 1989; Sharifi, Georgakakos, & Rodriguez-Iturbe, 1990; Sivakumar et al., 2001; Sivakumar et al., 2005; Sivakumar, Liang, Liaw, & Phoon, 1999; Sivakumar, Woldemeskel, & Puente, 2013), the first zero-crossing of the autocorrelation function has been commonly used as the proper delay time.

Based upon **EQUATION 5**, a trajectory in an m -dimensional space can be constructed. Therefore, moving along with time t , a series of m -dimensional vectors will be obtained which represent the m -dimensional phase-space of the system. Suppose a circle (a sphere for $m=3$ or a hypersphere for $m \geq 4$) of radius r centered about an arbitrary point of the m -dimensional set of vectors (see Figure 2) and count the number of points $N(r)$ located inside the circle. Normalizing such a count, the so called *correlation integral* $C(r)$ of the process will be obtained (Rodriguez-Iturbe et al., 1989).

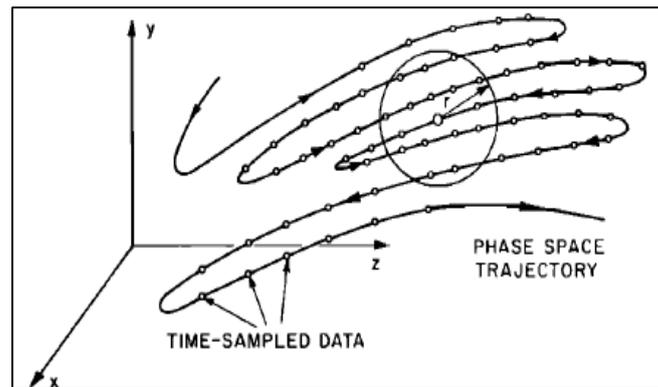


Figure 2. The counting sphere in a longtime trajectory in phase-space (Rodriguez-Iturbe et al., 1989)

The GPA uses the described concept of phase-space reconstruction to represent the system’s dynamic. According to GPA, for an m -dimensional phase-space (m is an integer), the correlation function $C(r)$ of an infinite time series is (Grassberger & Procaccia, 1983):

$$C(r) = \lim_{N \rightarrow \infty} \frac{2}{N(N-1)} \sum_{\substack{i,j \\ 1 \leq i < j \leq N}} H(r - \|Y_i - Y_j\|) \quad i \neq j \quad (\text{Equation 6})$$

where N is the number of data point, r is the vector norm (radius of a sphere) centered on \mathbf{Y}_i or \mathbf{Y}_j and H is the Heaviside step function or the unit step function defined as below:

$$H(u) = \begin{cases} 0, & u < 0 \\ 1, & u \geq 0 \end{cases} \quad (\text{Equation 7})$$

$C(r)$ is also called the correlation function or correlation integral. The correlation integral $C(r)$ is used to describe the dimension of the attractor (Berndtsson et al., 2001). It defines the density of points around a specific coordinate x_i . In other words, it measures how densely the trajectories populate phase-space. If the time series is characterized by an attractor, according to **EQUATION 8**, the correlation function $C(r)$ and radius r for positive values, are related:

$$C(r) \underset{\substack{r \rightarrow \infty \\ N \rightarrow \infty}}{\approx} \alpha r^v \quad (\text{Equation 8})$$

where α is constant and v is the *correlation exponent*. In case the values of v are not integers, it is implied that the attractor is fractal and thus chaotic (Berndtsson et al., 2001). Correlation exponent v , as the slope of $\log C(r)$ vs. $\log r$, could be simply obtained as follow:

$$v = \lim_{\substack{r \rightarrow \infty \\ N \rightarrow \infty}} \frac{\log C(r)}{\log r} \quad (\text{Equation 9})$$

Generally, the slope is estimated by a least-squares fit of a straight line over a certain range of r known as the *scaling region* or *scaling regime* (Rodriguez-Iturbe et al., 1989; Sangoyomi et al., 1996; Sivakumar et al., 2001). The scaling region is not visually obvious, thus to make it easier, the local slope of the curve $\log C(r)$ vs. $\log r$ should be calculated:

$$\Delta_t = \frac{\log[C(r)]_{t+1} - \log[C(r)]_{t-1}}{\log(r)_{t+1} - \log(r)_{t-1}} \quad (\text{Equation 10})$$

The local slopes, then, should be plotted versus $\log r$ so that scaling region could be seen (see Figure 3).

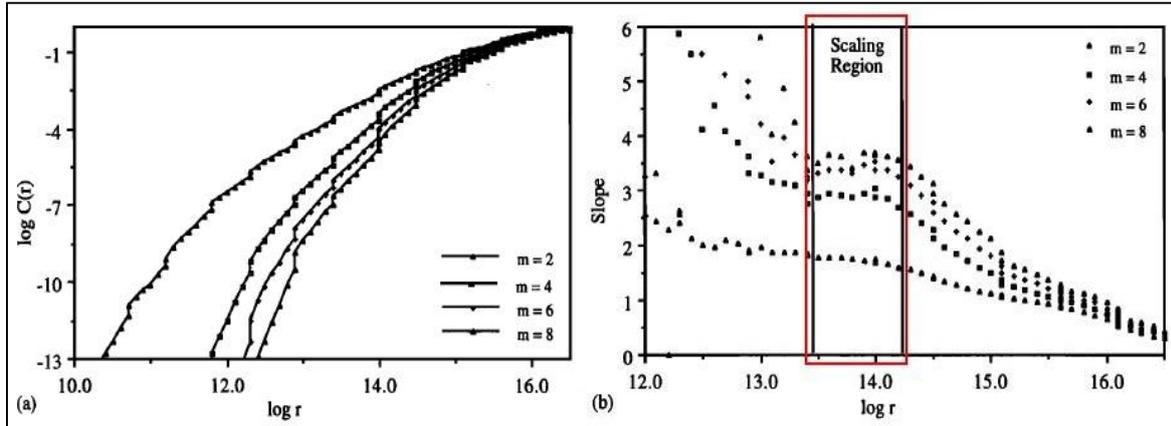


Figure 3. (a) $\log C(r)$ vs. $\log r$ for the time series of Great Salt Lake volume and (b) Local slope of the curve (a) vs. $\log r$ (Sangoyomi, Lall, & Abarbanel, 1996)

It has to be noted that Lai and Lerner (1998) have probed the dependency of the scaling region on fundamental parameters τ , m , and $m\tau$. The results suggested that the effective linear scaling region used for reliably estimating correlation dimension, is highly sensitive to the choice of delay time employed in the phase-space reconstruction. It is always desirable to have a larger scaling region to determine the slope, since the determination of the slope for a smaller scaling region may be difficult and could possibly give rise to errors.

For a random process, correlation exponent ν varies linearly as m increases without reaching a saturation value; on the contrary, in case of a deterministic processes the estimated correlation intergral of the reconstructed attractor (i.e. correlation exponent ν) reaches a plateau from which the dimension estimate ν is relatively constant for a large range of embedding dimensions m (see **FIGURE 4-G** & **FIGURE 4-H**). It is assumed that the plateau dimension ν is an estimate of the attractor dimension d_A in the original full phase-space (Ding, Grebogi, Ott, Sauer, & Yorke, 1993). It is due to fact that a widely fluctuating and seemingly irregular process stems from a deterministic dynamic which has a limited number of DOF. Hence, in constructing the phase-space of higher dimensions, a point will be reached at which the dimension equals the DOF and increasing the dimension will not affect the relation $N(r) \sim r^\nu$ for an infinite time series. In other words, the saturation value d_A (attractor dimension) is defined as the correlation dimension of the attractor (or the time series) (Rodriguez-Iturbe et al., 1989). Therefore, d – the nearest integer above d_A – suggests the the minimum number of variables essential to understand/capture the dynamic of the system i.e. minimum number of embedding dimensions required to unfold the attractor and subsequently, the dynamic of the system (Jayawardena & Lai, 1994). In other words, the smallest number of first-order differential equations that capture the main feature of the process dynamics may be determined.

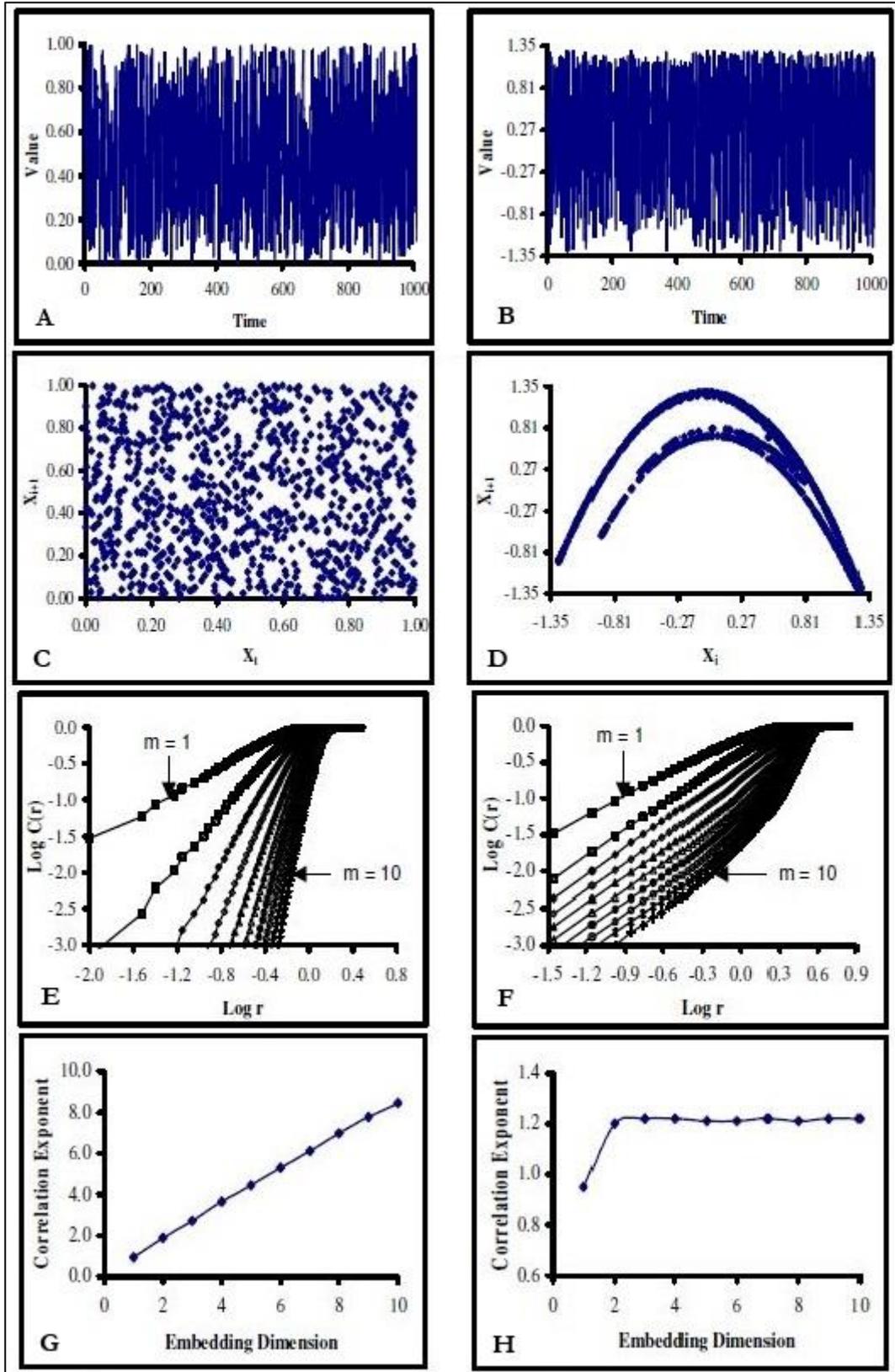


Figure 4. Signal (A, B), phase-space attractors (C, D), correlation integral (E, F), and correlation exponent (CE vs. EM) of random vs. chaotic time series, respectively (Sivakumar & Berndtsson, 2010).

There could be a suspicion of stochastic chaos when one deals with a low-length finite data (Schertzer et al., 2002). Phase-space – or better say pseudophase-space – could be a helpful tool for providing reliable evidence that the system is not stochastic indeed. In case of a stochastic time series, one would expect a space-filling phase-space diagram in all embedding dimensions m . (see **FIGURE 4-C**) Nonetheless, Figure 4 vividly represents that despite the phase-space of a purely stochastic time series (**FIGURE 4-C**), when phase-space of a chaotic time series is embedded in a 2-dimensional space (**FIGURE 4-D**), it fills up the space only partially. As it was mentioned earlier, for measuring the dimension of the strange attractor i.e. correlation exponent, $\log C(r)$ vs. $\log r$ plot should be plotted. As it could be seen from **FIGURE 4**, in case of a stochastic process (**FIGURE 4-G**), the correlation exponent is increasing as the embedding dimension increases. However, for a chaotic process (**FIGURE 4-H**), correlation exponent saturates beyond a certain embedding dimension.

4 RESULTS & DISCUSSIONS

A series of 62 solute transport signals are examined using the nonlinear analysis of Correlation Dimension Method. The results of CE vs. EM for all signals have been analyzed both individually and comparatively; measurements are assessed horizontally and vertically in order to obtain a larger scheme of the ST dynamics considering the variation of depth and soil horizon. The results generally imply the nonlinear low-dimensional nature of solute transport process. That is, the dynamics are dominantly governed by a few variables, majorly on the order of 2-4 – with a few exceptions. Although the nature of the studied time series in this project are different from previous ones, the results are in a good agreement with the correlation dimensions that have been reported by previous studies on subsurface hydrology. Faybishenko (2002) has reported CD of 2-4 for the flow processes in the unsaturated fractured-rock system for both laboratory and field dripping-water experiments. Sivakumar et al. (2005) have also computed correlation dimensions of 2-3 for simulated solute transport through the two and three facies media in a heterogeneous aquifer medium. Even so, there is still an essential difference between the results and implications of this study and prior ones – chaotic analysis of hydrologic time series using CDM. This difference together with its probable causes are discussed.

4.1. Analysis

Firstly, each signal is plotted on a schematic map of its location on the soil profile (see **FIGURE 5**). Secondly, for each signal the 2D pseudophase-space attractor is plotted (see **FIGURE 6**). Then, the first zero-crossing of the autocorrelation function is computed as the proper delay time for phase-space reconstruction (see **FIGURE 7**); corresponding delay time for each signal is presented in **TABLE 3**. Afterwards, correlation integral is calculated and from which CE is derived (see **FIGURE 8 & FIGURE 9**). Further details about each signal are presented in the **APPENDIX**.

4.1.1. Solute Transport Signals

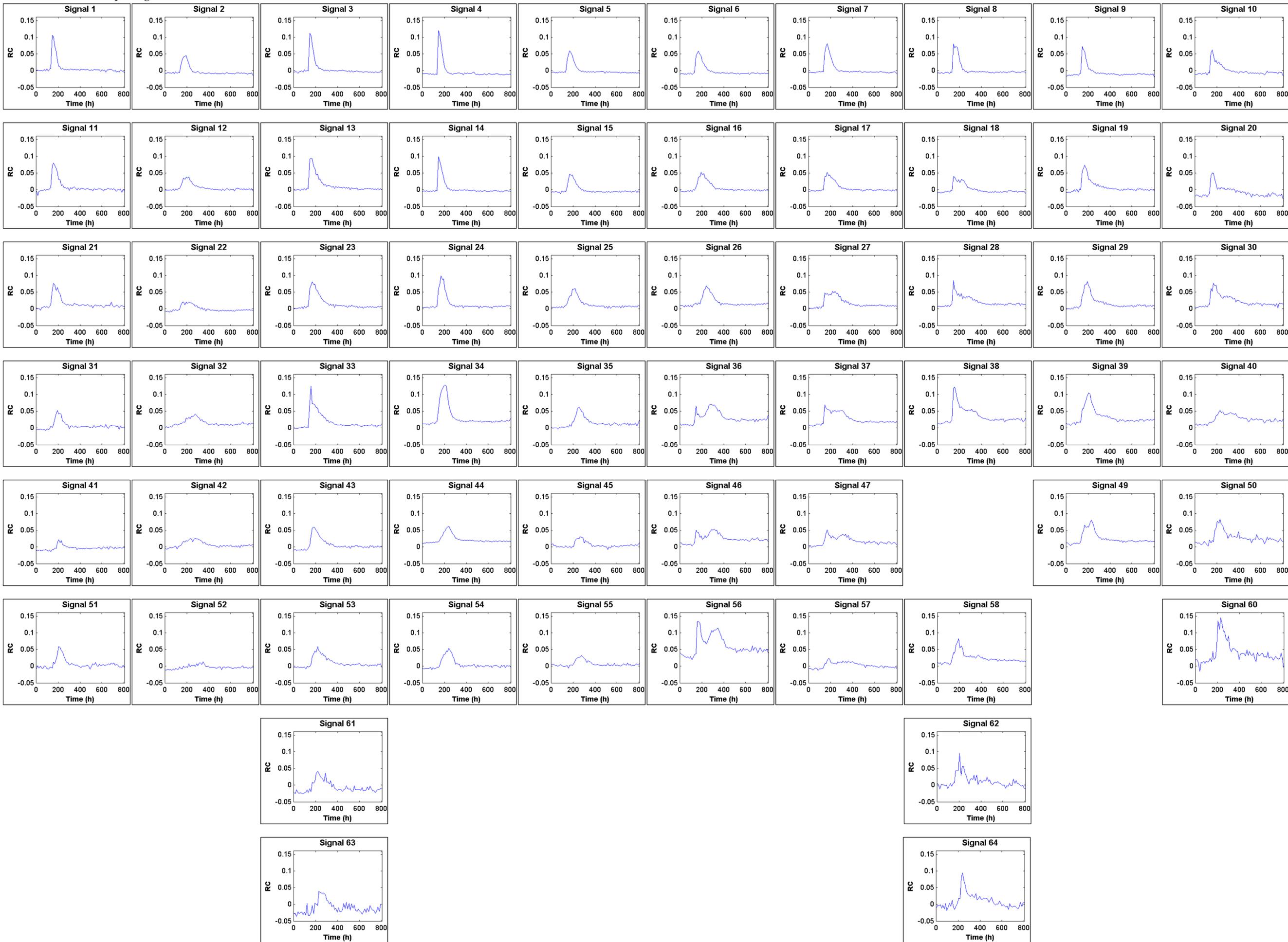


Figure 5. Schematic presentation of solute transport signals placed at the location of their corresponding measurement probes.

4.1.2. Pseudo-Phase Space Attractors of Solute Transport Signals

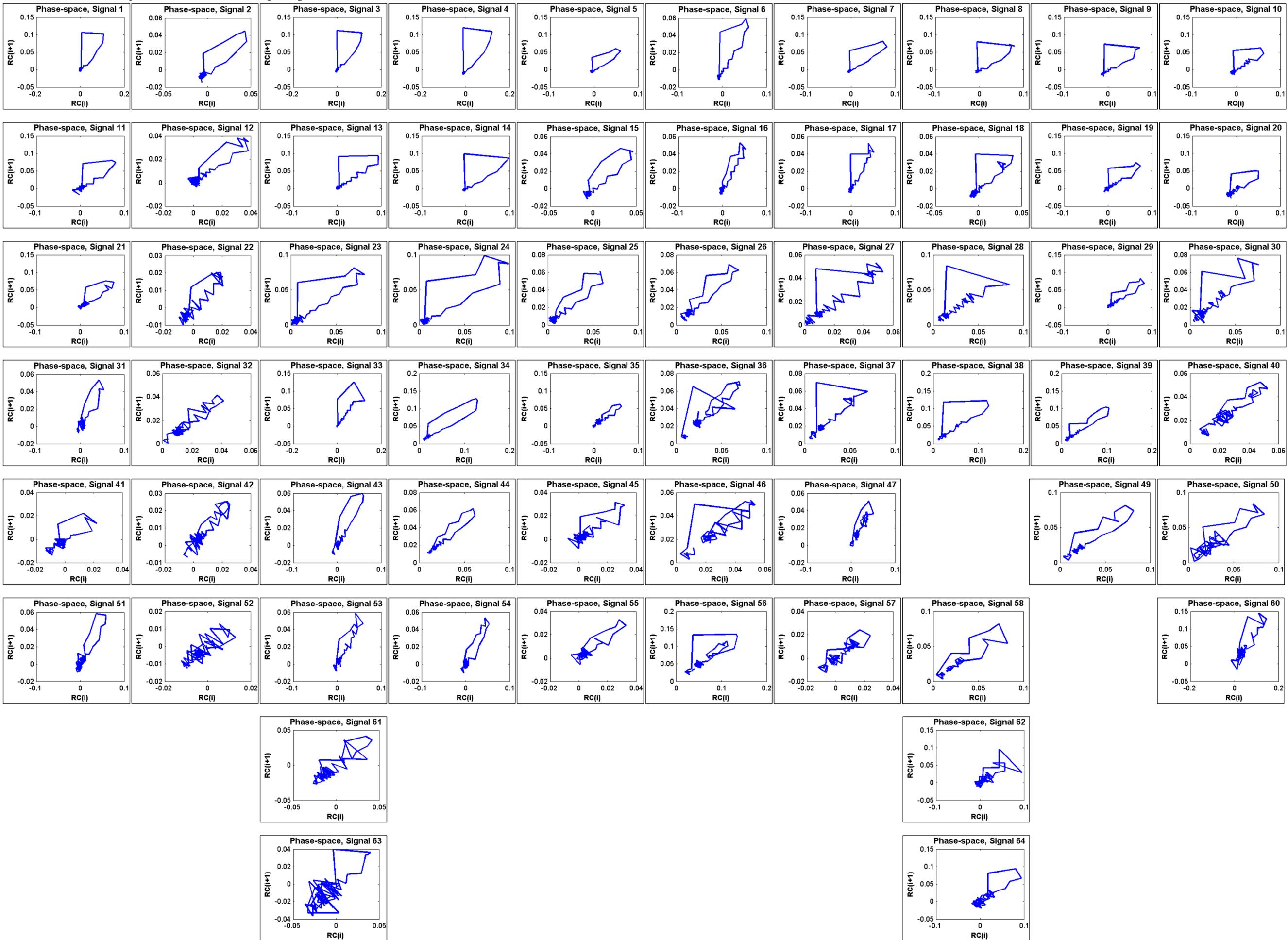


Figure 6. Schematic presentation of 2D projections of pseudo-phase space attractors (lag 1) of solute transport signals placed at the location of their corresponding measurement probes.

4.1.3. Autocorrelation

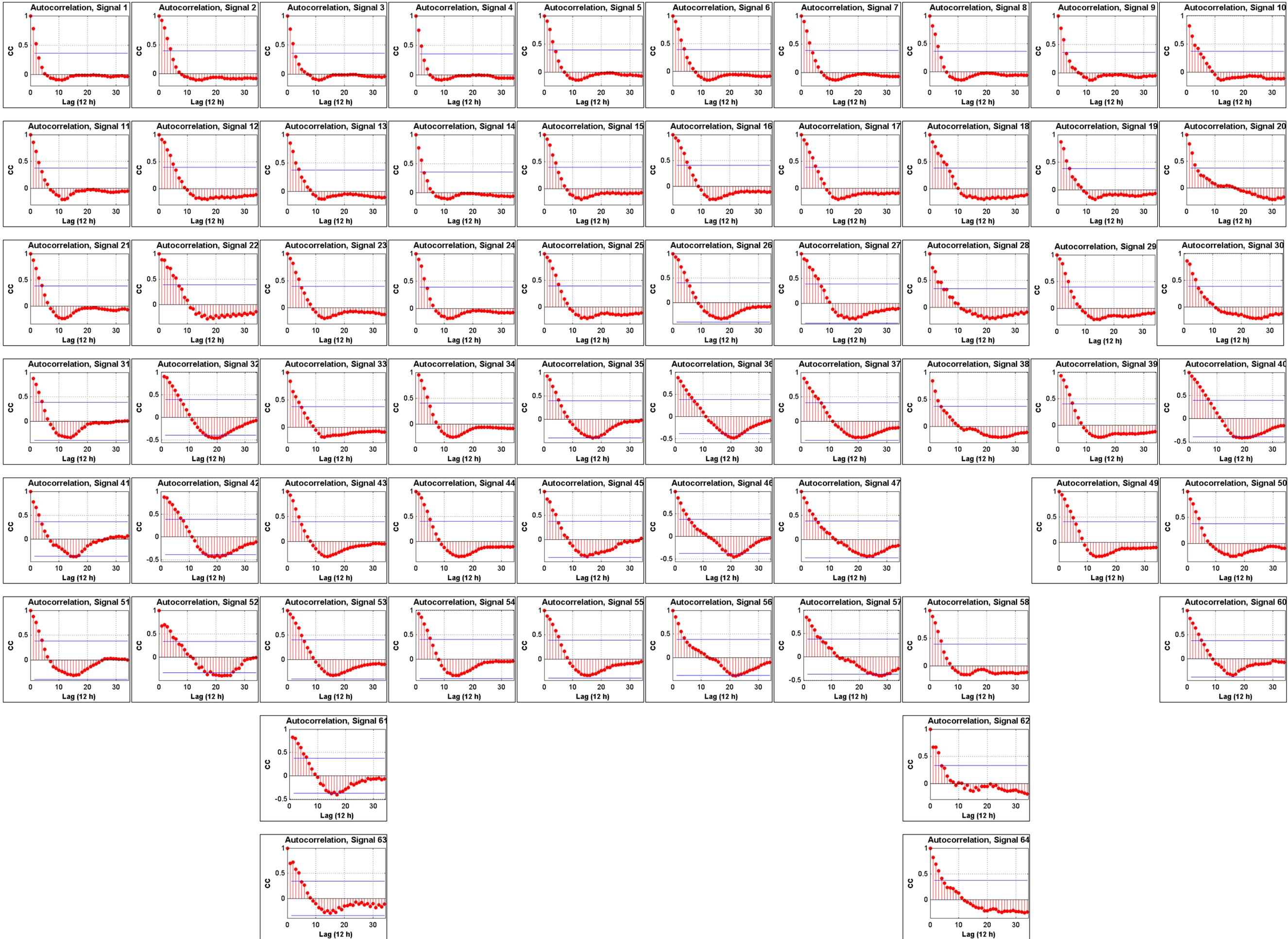


Figure 7. Schematic presentation of autocorrelation diagrams of solute transport signals placed at the location of their corresponding measurement probes.

4.1.4. Correlation Dimension: $\log C(r)$ vs. $\log r$



Figure 8. Schematic presentation of the plot of $\log C(r)$ vs. $\log r$ for solute transport signals placed at the location of their corresponding measurement probes.

4.1.5. Correlation Dimension vs. Embedding Dimension

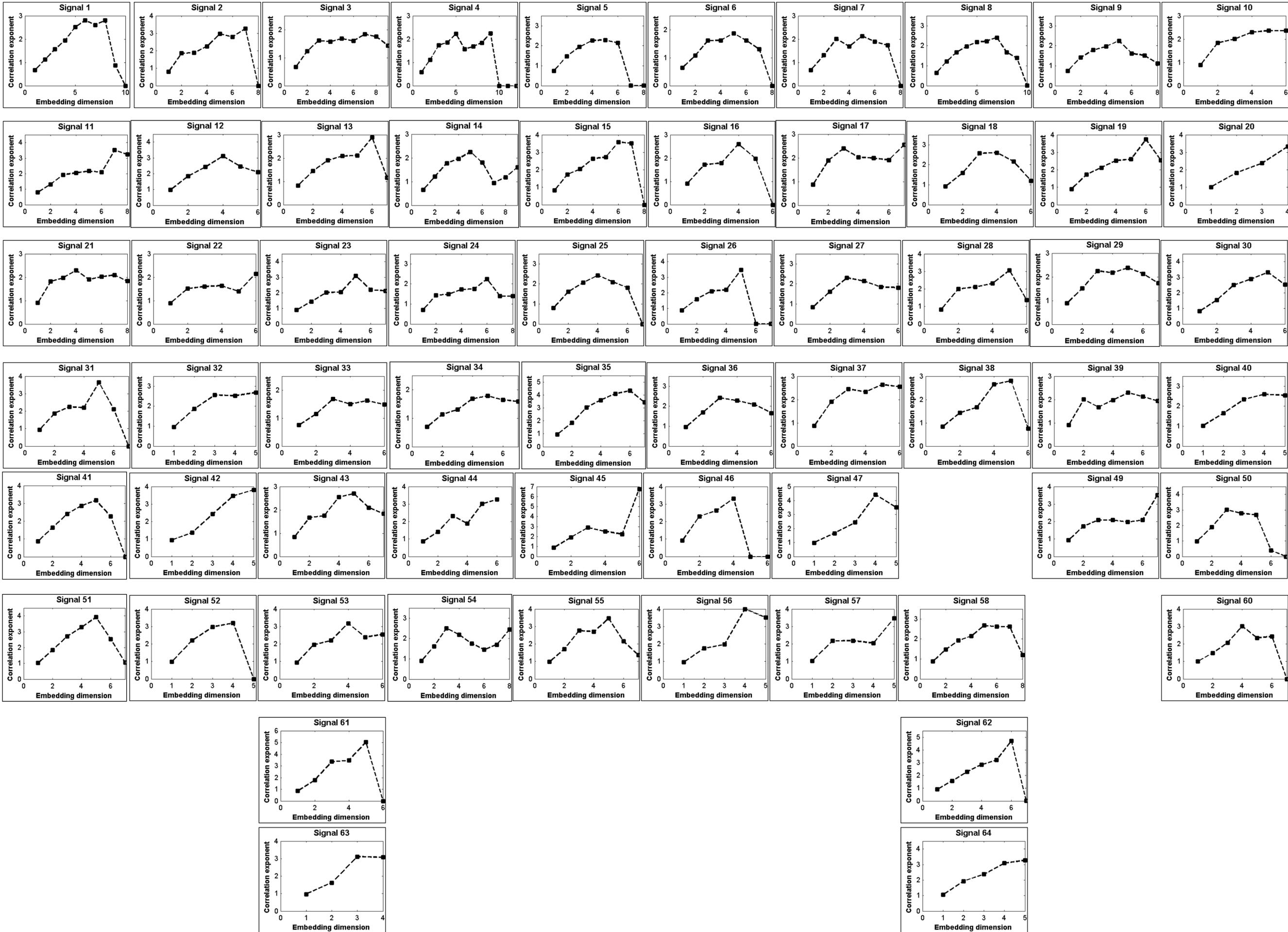


Figure 9. Schematic presentation of CE vs. EM plots placed at the location of their corresponding measurement probes.

4.2. Discussion of the Results

4.2.1. Time Series Length

No study has so far investigated such short time series (68 data points) using nonlinear chaotic techniques. For one reason, it is normally presumed that short time series do not contain enough information about the evolution of the given dynamic system to be captured, therefore, time series length is a limiting factor for CDM analysis. As it is discussed by Khatami (2013), due to inherent qualitative characteristics that would be different in dynamical systems, it is not practically nor theoretically possible to formulate a criterion of minimum data length. So far, the shortest time series – to the knowledge of author – analyzed by CDM are (Sivakumar, 2005):

- 100-point time series for an artificially generated chaotic time series (using the Henon map equation)
- and 360-point time series for a hydrological data set (real monthly flow series from Göta River basin, Sweden (Sivakumar et al., 2001) where generating mechanisms are not known *a priori*).

Nonetheless, the results of the present study suggest that short time series might contain essential information about the characteristics of their generating dynamics as it is well reflected in CE vs. EM dimensions. This is implying that no time series should be ruled out of chaotic investigation solely due to its size; even short hydrologic time series are potential to reveal fundamental information about the underlying dynamics of their processes.

4.2.2. Classification of the Dynamics

As it is thoroughly explained by Khatami (2013) the diagram of CE vs. EM could be used in order to differentiate stochastic and chaotic systems considering that their characteristics are known *a priori*. In case of a stochastic process, there is a linear relationship of $\nu = m$ for any m (see **FIGURE 4-G**). On the other hand, for a chaotic time series the ν is increasing as m increases on the basis of $\nu = m$ (in practice it is $\nu \approx m$) until a certain m at which ν saturates (see **FIGURE 4-H**). Be that as it may, for hydrologic time series, which their characteristics are not known *a priori*, it would not always be a clear steady saturation. Therefore, the nature of hydrological processes is an ongoing question, deterministic chaotic versus stochastic.

Due to possible causes, which will be discussed in **SECTION 4.2.2.1**, in some cases there are instable or fluctuating saturations that in this study are called Instable Saturation (IS) as opposed to Stable Saturation (SS) where a clear steady saturation is evident. Therefore, the re-

sults of this investigation are classified into two groups of SS and IS. In each case, the value(s) of the (potential) correlation dimension(s), i.e. number of autonomous ODE needed to determine the dynamic of the system, is (are) presented in **TABLE 3**. For instance, in case of **SIGNAL 3** there is a steady saturation of CE with CD=2 (coded as SS-2); while for **SIGNAL 4** the saturation is instable and CE values are fluctuating between 2 and 3 (coded as IS-2, 3). In some cases such as **SIGNAL 49** correlation exponents are varying between more than two values. Nonetheless, in cases like **SIGNAL 18**, **SIGNAL 47**, **SIGNAL 51** and etc. it is difficult to easily classify the signals as either SS or IS. Such signals are coded as N/A.

In order to clearly demonstrate the saturation of CE values after a certain m , generally in chaos studies, CEs are computed and presented for embedding dimensions up to 10 or 20. However, in this study as time series are very short for CDM analysis, CEs could not usually be calculated for embedding dimensions greater than 7 (see **FIGURE 9**). In many cases, regardless of stable or instable saturation, there is a breakdown in CE values after a certain m . For example, in case of **SIGNAL 1** and after EM=8, CE values start breaking down to zero. Therefore, in **TABLE 3** the maximum number of EMs until which the computed CEs are considered to be valid are presented. It should be noted that one should make a distinction between a breakdown, which is due to data size, and fluctuations of correlation exponents (SS vs. IS) which is not necessarily due to data length (see **SECTION 4.2.2.1**).

The values of correlation dimensions for signals with stable saturation are either 2 or 3, among which CD=3 is the most frequent. In the study by Sivakumar et al. (2005) the CD values for simulated solute transport were also 2 and 3. In case of instable saturation, however, CD values are varying between 2 and 4 from which IS-2, 3 is the most frequent one.

4.2.2.1. Stability vs. Instability

Instability in the CE saturation of solute transport signals could be explained from three standpoints: (1) the data properties, (2) numerical computation, and (3) the physical process of solute transport – and certainly a combination of the above.

(1) Using a short time series of a given dynamic for the CDM could result in a significant underestimation of the CD value. Further, the presence of noise in the observed data may lead to an overestimation of the CD (Ma, 2013). However, in this study the CD values are in good agreement with previous studies by (Faybishenko, 2002; Sivakumar et al., 2005); in both cases of SS and SI signals, the CD values are in the range of 2-4. Therefore, it could be argued that the data properties (size and noise) may not significantly influence the CD values (at least its order of magnitude), but the instability in the CE values in SI cases could be due to the noise and the limited length of the signals.

(2) In addition to the data properties, numerical computation could be a source for the instabilities. In essence, correlation integral is the normalized count of the points inside a circle/sphere/hyper-sphere centered about an arbitrary point of the m -dimensional set of vectors (see **FIGURE 2, SECTION 3.2**). Further, determining the scaling region is the main problem with many of the earlier methods to estimate correlation dimension (Judd, 1992). Therefore, it is difficult to solely rely on CDM results in order to obtain intrinsic information about the underlying mechanism of solute transport process.

(3) Another explanation for the fluctuation of CE values is from a different perspective than the previous two. The previous two explanations are discussing the SI from a mathematical/numerical view point. Nonetheless, it is worthwhile to bring a physical interpretation into the discussion. On a more sophisticated level, the CE variations could be due to instability on a far more complex level; a highly complex nonlinear system of preferential flows formation and solute transport. Although there is a link between preferential flows and solute transport to some extent (e.g. solutes can travel from macropores out to the soil matrix during low flow periods), they are two isolated processes. Strictly speaking, formation of preferential flows is a 4D system. It is a spatially dependent time variant process. In other words, it is dependent on specifics such as soil properties, texture, structure, seasonal variabilities, etc. It is also a delicate function of time. Assuming the preferential flows to be constant – the path is not changing throughout time and space – the solute transport process itself could be chaotic, i.e., deterministic but highly instable due to crucial dependence on initial conditions. ST process, however, is interconnected to the process of preferential flow formation. In fact, they are highly interactive. In fact, preferential flows could be chaotic as well. Consequently, the combination of these two supposedly chaotic systems could lead to a highly instable nonlinear dynamical system where the generating mechanisms, both the mechanisms and their numbers, could vary throughout time and space. As much tentative is this speculation, studies on solute transport process using large data matrices (long solute transport signals on a soil profile) could test this hypothesis.

4.2.3. Consistent Pattern of Correlation Dimensions

The results of CDM analysis are presented as a schematic map in **FIGURE 10**. As it could be seen, adjacent probes are closely revealing the same results. Horizontal and vertical patterns (similar results) of CD values are signified by green rectangles. In general, the results are alluding to a consistent meaningful pattern of solute transport dynamics on a larger scheme of a soil profile. Further, all stable saturations (SS) are observed at the soil horizons. So it is plausible that the soil texture has an influence on CE saturation instability.

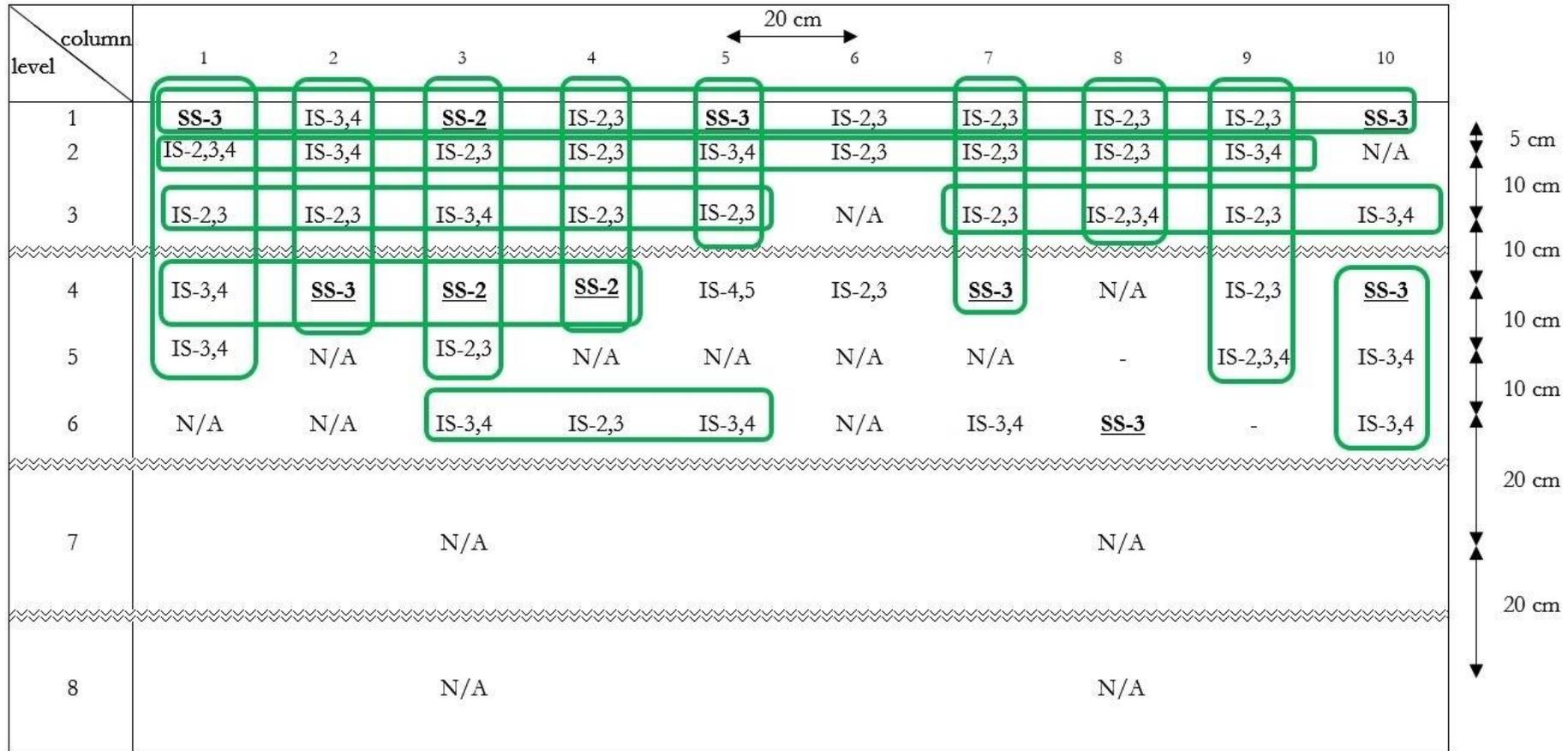


Figure 10. Scaled schematic map of CDM results. The results are presented at the locations of solute transport measurement probes; similar patterns of CD are discerned by colored rectangles, and soil horizons by double wavy lines.

It is important to note that the results of CDM analysis, i.e. CD values, and pseudo-phase space attractors are complementary. Although at lower levels it is not possible to get meaningful results from the CDM analysis (it is shown as N/A), the solute transport attractors are becoming more evident (see **FIGURE 9**). Therefore, in case CDM do not yield a meaningful CD values one cannot reject the possibility of low-dimensional chaos in the given system. It simply means that CDM cannot be applied for that specific data set and resolution. . In some cases, CDM could be applied to the time series by changing the temporal resolution of data.

Application of chaos, in general, and CDM, in particular, for hydrological studies has been criticized previously (Koutsoyiannis, 2006; Schertzer et al., 2002). Although the criticisms have been answered widely (Khatami, 2013; Ma, 2013; Sivakumar, 2000; Sivakumar, 2005; Sivakumar, Berndtsson, Olsson, & Jinno, 2002; Sivakumar, Persson, et al., 2002), it is vitally important to employ other chaotic methods such as Gaussian Kernel Algorithm (GKA) as well (Yu, Small, Harrison, & Diks, 2000). Scaling regions are problematic in chaos studies and GKA avoids some of these problems. Nonetheless, one is still fitting a function to a distribution and some problems remain. Further, other phase-space constructions should be engaged in ‘hydro-chaotic’¹ analyses. Revisiting previous studies with other chaotic methodologies would strengthen the argument for chaos determinism in hydrology and could promote breakthroughs in the field.

It is crucially important to note that the discussion on the present results could not be too detailed. First, although the observations are comprehensive in terms of collection from soil profile, there are limited to the soil type, data size, and existence of noise. Therefore, observation in other soil types are needed to confirm the results. As huge observed data sets could not be prepared easily, lab experiments are inevitable. Therefore, the next phase of this research will engage experimental data to see to what extent their outcome could be related to the field studies results.

¹ Hydrological studies that are using chaotic approaches for system identification, prediction, noise reduction or other purposes.

5 CONCLUSION

The physics behind the temporal and spatial instabilities of flow (in unsaturated media) is still of question. Therefore, the main objective of the present study was to investigate the potential utilization of a nonlinear deterministic framework for understanding the underlying dynamics of solute transport processes. Pursuing this objective, the nonlinear chaotic technique of correlation dimension method is employed to study short signals of solute transport (68 data points). Correlation dimension method can provide an assessment of the minimum number of processes that are governing a given dynamical system. Several issues have been raised against the application of chaos, in general, and CDM, in particular, for hydrological studies. Almost all these issues have been addressed by previous studies. Further, the consistent results of 'hydro-chaotic' are strengthening the interest in using CDM and other chaotic approaches in this area.

What make the present hydro-chaotic study special are:

- (1) the field of interest is subsurface process of solute transport than surface hydrology,
- (2) extremely short time series (68 points) are used,
- (3) and the spatial distribution of data set is taken into account, i.e., solute transport on a soil profile.

The results of CE vs. EM for all signals have been analyzed both individually and comparatively; measurement are assessed horizontally and vertically in order to obtain a larger scheme of the ST dynamics considering the variation of depth and soil horizon. Despite previous studies, the CE vs. EM is not always a stable saturated figure; therefore, there are two types of stable and instable saturations. The instability in the saturation of CE values could be explained by (1) data properties (data size and noise), (2) numerical computation (scaling region and phase-space reconstruction), and (3) physical interpretation.

The main results of this study could be summarized as follow:

- a) The outcome of CDM analyses suggest that the number of governing equations for solute transport are as low as 2-4 – i.e. low dimensional determinism. A consistent pattern has been observed in CD on the soil profile.
- b) Despite the claim of previous studies, time series length is not a limiting factor for hydro-chaos studies. Even short hydrologic time series are potential to reveal fundamental information about the underlying dynamics of a given process. The results of a short time series of only 68 data points, are in fairly good agreement with previous studies.

- c) Instability in the CE saturation of IS signals could be interpreted – only a speculation – as instability in the underlying dynamics of this process. Number of variables generating the mechanism are transitionally changing as the system evolves. In other words, depending on the status of the system throughout its evolution, number of determining variables – and most probably variables themselves – are changing; therefore, the dimension of the attractor is varying between different values. Consequently, no stable saturation could be observed.

The concluding remark from this study is therefore formed as a hypothesis. The implication of this hypothesis would be that although it is presumed that there are universal equations governing the solute transport process, the local conditions (soil texture and structure, soil horizon, elevation, preferential flows and macro pores, soil moisture distribution, time of day, evaporation, temperature and etc.) could intrinsically influence/change the dynamic of the process. In other words, the governing equations could change both spatially and temporally.

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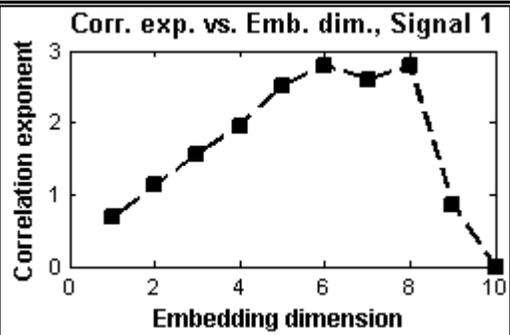
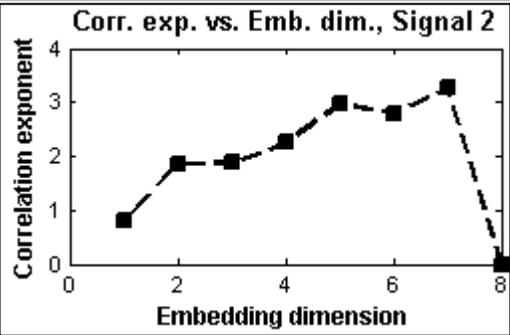
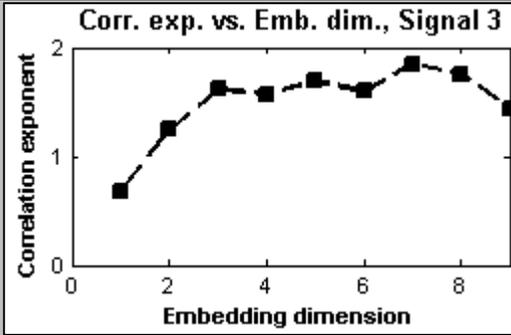
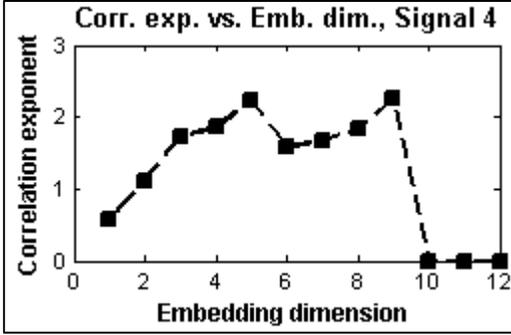
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Appendix

The results for the 62 ST signals are encapsulated in the table below. E_m refers to the value of EM until which computed correlation exponent could be considered as valid. Class refers to stable/instable saturation followed by the value(s) of correlation dimension.

Table 3. Classified results of 62 solute transport signals.

Signal	Delay, τ	E_m	Results	Class
1	7	8		SS-3
2	9	7		IS-3, 4
3	8	9		SS-2
4	6	9		IS-2, 3

