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A CENTER MANIFOLD APPROACH TO TRANSPORT IN STRATIFIED AQUIFERS

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ABSTRACT

An asymptotic description of dispersion in stratified aquifers using the center manifold theory is presented. The system is assumed to evolve slowly in time and space thus allowing the center manifold approach to be applicable. The spatial variability in the process is accounted for by using spatially variable conductivity and dispersion coefficients. The approach presented herein focuses on longitudinal dispersion in the direction of mean flow. An important advantage of the proposed approach is that higher order asymptotically correct approximations are easily obtained once the first approximation has been derived. In addition, the approach yields a one-dimensional ordinary differential equation that can be easily solved in comparison with the two-dimensional advection dispersion equation. The predictions of the center manifold equations closely match the observed spatial moments for the Cape Cod tracer experiment of Massachusetts, USA.

KEYWORDS: Contaminant Transport, Stratified Aquifers, Center Manifold Theory, Advection Dispersion Equation, Groundwater Transport.

1. INTRODUCTION

In many physical problems the system evolves quickly towards a certain state and thereafter it relaxes relatively slowly in space and time. The center manifold theory has been developed to describe the slow evolution of such systems. The theory provides a systematic approach to calculate a sequence of successive approximations to the evolution of the principle structure in space and time [1]. Roughly, the theory states that if the reference state of the system contains N zero eigenvalues and if all the other eigenvalues are negative, then the system evolves exponentially quickly towards

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an N-dimensional manifold called the center manifold. The system then relaxes relatively slowly on this center manifold according to the evolution of some dominant modes for which differential equations can be derived.

When a contaminant is first released in a porous medium, two basic mechanisms combine to distribute it in time. The contaminant is advected downstream by the average flow field, while being dispersed longitudinally and laterally by the fluctuating velocity field. These two components combine to ensure that, on average, the mean concentration distribution is relatively smooth. This distribution then evolves relatively slowly in space and will be governed by the flow field. Center manifold theory may be applied to such a situation where the slow relaxation of the system in space and time can be described.

The technique employed in this analysis is an extension of that used by [2] to describe dispersion in channels with varying flow properties. Their method is an extension and simple application of the original method proposed by [3]. Center manifold theory, as developed by [1, 3, 4] is systematic and can easily be adapted to different problems. An advantage of the center manifold theory is that successive higher order approximations are obtained easily once the first order approximation is known.

To start the analysis we assume that the dispersion occurs in a two-dimensional stratified aquifer, which has horizontally constant hydraulic conductivity and dispersion coefficients. These parameters vary only with the layers of the aquifers as they change in the vertical direction. Though the technique is employed in a two-dimensional setting, we restrict our attention to the evolution in the direction of average flow. It is assumed that the velocity is known a priori. In addition we assume that concentration (c) variations in the x direction and time are small so that terms involving ($\partial / \partial x$) and ($\partial / \partial t$) are small. This assumption is convenient for the case of a stratified aquifer where the significant variations in velocities and concentrations occur in the direction normal to the layers. In addition, only molecular diffusion and local dispersion (relative to the advective front) are affecting concentration variation along the x direction, whereas concentration variation in y-direction is strongly influenced by the different advective fronts in different layers. Therefore, variations in c in the vertical y-direction are assumed relatively large compared to those in x direction, and thus terms involving $(\partial/\partial y)$ may not be small. The assumption of a slow variation in space and time is important because it reflects the situation where center manifold theory may be applied. The governing advection dispersion equation for a stratified aquifer with stratification parallel to x direction is written as

$$\frac{\partial c}{\partial t} = -u(y)\frac{\partial c}{\partial x} + D_{xx}(y)\frac{\partial^2 c}{\partial x^2} + D_{yy}(y)\frac{\partial^2 c}{\partial y^2} \tag{1}$$

where c is the contaminant concentration defined as mass of solute per unit volume of flowing water, $u(y)$ is the groundwater velocity in the x direction, which varies only normal to the layering along y direction, D_{xx} is the longitudinal dispersion coefficient and D_{yy} is the transversal dispersion coefficient.

2. EXISTENCE OF THE CENTER MANIFOLD

To show the existence of the center manifold we follow the path laid out by [2] for dispersion in channels. Taking the space Fourier transform of Eq. (1) with respect to x, we have

$$\frac{\partial \hat{c}}{\partial t} = \Im\hat{c} - uik\hat{c} - D_{xx}k^2\hat{c} \tag{2}$$

where $i = \sqrt{-1}$, k is the wave number coordinate in Fourier space, $\hat{c}$ is the Fourier transform of the concentration c, and the operator $\Im$ is defined as

$$\Im\hat{c} = D_{yy}\frac{\partial^2 \hat{c}}{\partial y^2} \tag{3}$$

As we are interested in the slow evolution of the system in space, only small values of the wave number k are relevant. Following standard analysis of bifurcation using center manifold theory (e.g., [5], Sec. 1.5) we adjoin the equation

$$\frac{\partial k}{\partial t} = 0 \tag{4}$$

to Eq. (2). By doing this one can consider the last two terms on the right hand side of Eq. (2) as nonlinear terms and consider the first term as the only linear term in the system of Eqs. (2) and (4). The linearity of the first term is attributed to the fact that the wave number k is a small parameter, and hence, only linear relations expressing $\hat{c}$ in terms of k are significant. Equations (2) and (4) can now be written in the form

$$\frac{d(\boldsymbol{X})}{dt} = \boldsymbol{AX} + \boldsymbol{F}(\boldsymbol{X}) \tag{5}$$

where $\boldsymbol{X} = (k, \hat{c})^T$ is the unknown vector, $\boldsymbol{A}$ is a matrix linear operator defined as

$$\boldsymbol{A} = \begin{bmatrix} 0 & 0 \\ 0 & \Im \end{bmatrix} \tag{6}$$

and $\boldsymbol{F}(\boldsymbol{X})$ contains the nonlinear terms. The linear operator $\boldsymbol{A}$ has two zero eigenvalues corresponding to the eigenvectors $(1, 0)^T$ and $(0, 1)^T$. All the other eigenvalues are strictly negative. If the two nonlinear terms did not exist, the system would thus decay exponentially quickly onto the space spanned by the two vectors $(1, 0)^T$ and $(0, 1)^T$. However, center manifold theory asserts that in the presence of the nonlinear terms this is still qualitatively true; it is just that the system approaches a curved manifold rather than a flat vector space [2].

3. CENTER MANIFOLD PARAMETERIZATION

To apply the center manifold technique to this problem we invoke a formal procedure described in detail in [1]. We assume the large time variation of the contaminant may be described in terms of a certain mode function as well as its spatial derivatives with respect to the direction of the mean flow (x direction). The basic idea here is to define a mode function that remains constant in the y direction so as to facilitate the mathematical manipulations involved. Define the relevant mode function

$$M(x) = \int_{-b}^{b} \int_{x-\delta/2}^{x+\delta/2} nc(x, y)\,dx\,dy \tag{7}$$

where n is the effective porosity. This function represents the average mass of contaminant contained in a small strip of width δ around point x in an aquifer of width $2b$ (see Fig. 1). It is assumed that δ is sufficiently small that the concentration $c(x, y)$ does not change horizontally within δ, and as such, $\boldsymbol{M}(x)$ can be rewritten as

$$M(x) = \delta \int_{-b}^{b} nc(x,y)dy \tag{8}$$

Assuming that the head gradient, J, across the medium in the x direction is constant, one can write the velocity as $u(y)=(K_{xx}(y)/n)\,J$. Further, the dispersion coefficients can be written as $D_1(y)=D_{xx}(y)=\alpha_L\, u(y)$ and $D_2(y)=D_{yy}(y)=\alpha_T\, u(y)$, with α_L and α_T being the longitudinal and transverse dispersivity, respectively.

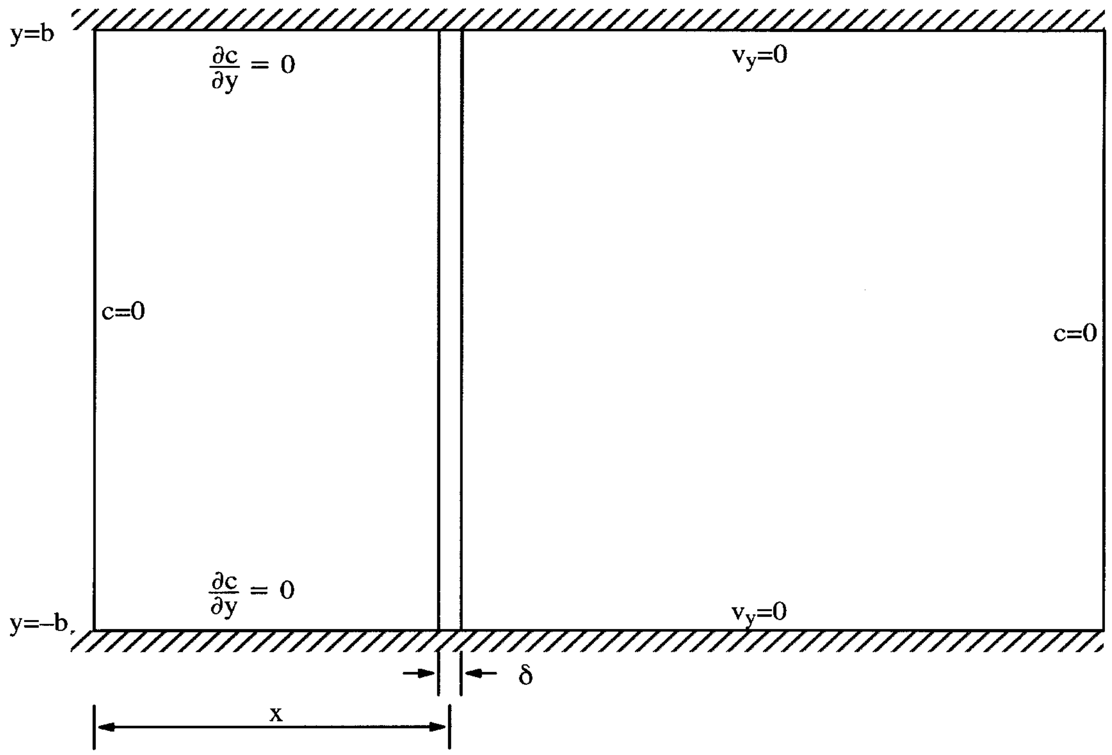

Fig. 1. Domain setting and boundary conditions.

The center manifold may be parameterized by the mode function $\boldsymbol{M}(x)$ so that on the center manifold the concentration takes the form

$$c(x,y,t) = V[y,M;x] \tag{9}$$

with evolution governed by

$$\frac{\partial M}{\partial t} = G[M;x] \tag{10}$$

where V and G are the unknown functions that need to be derived. The square brackets represent a functional dependence (in x) upon not only the argument M, but also on its derivatives with respect to x. For example $V[M; x]$ means that V depends upon M, $\partial M / \partial x$, $\partial^2 M / \partial x^2$, etc. Henceforth, we will use partials to denote total derivative with respect to a given variable, while a subscript will denote a partial derivative with respect to that subscripted symbol. Therefore we can now write

$$\begin{aligned}\frac{\partial c}{\partial t} &= V_t + \frac{\partial V}{\partial M}\frac{\partial M}{\partial t} + \frac{\partial V}{\partial M_x}\frac{\partial M_x}{\partial t} + \dots \\ &= V_t + V_M G + V_{M_x} G_x + \dots\end{aligned} \tag{11}$$

Again we invoke the assumption that the variations in the x direction and time are small, ($\partial c / \partial x, \partial c / \partial t$ are small quantities) and seek an asymptotic approximation for the center manifold of the form

$$c = V[y,M;x] \cong \sum_{l=0}^{\infty} V^l [y,m;x] \tag{12}$$

on which the evolution of the mode $M(x)$ takes place according to the equation

$$\frac{\partial M}{\partial t} = G[M;x] \cong \sum_{l=0}^{\infty} G^l [M;x] \tag{13}$$

where the superscript l denotes the order of each term. Note that the terms of order l contain precisely l space and time derivatives. For example the terms of order 3 may be of the form $\frac{\partial^3 M}{\partial x^3}$, $[\frac{\partial M}{\partial x}]^3$, $\frac{\partial^2 M}{\partial x^2}\frac{\partial u}{\partial x}$, etc. One can obtain the equation of the center manifold which expresses the concentration distribution in terms of the mode function $M(x)$ and its evolution in space. This equation will have the form

$$c(x,y,t) = f_0(y)M + f_1(y)M_x + f_2(y)M_{xx} + f_3(y)M_{xxx} + \dots \tag{14}$$

where the functions $f_0(y)$, $f_1(y)$, $f_2(y)$, $f_3(y)$, ... vary with y and are functions of the known parameters of the flow field as well as the hydraulic and transport parameters of the porous medium. Here the subscripts on M denote space derivatives with respect to x. The evolution of the mode $M(x)$ in time may also be obtained in the form

$$\frac{\partial M}{\partial t} = g_1 M_x + g_2 M_{xx} + g_3 M_{xxx} + \dots \tag{15}$$

Again the functions g_1, g_2, g_3, … will be dependent on the known data of the problem. It should be mentioned here that the actual forms of the relations expressing the center manifold and the evolution on it may be different than those given above if we assume that the horizontal velocity u changes in x. For instance, one may have a second order term for the center manifold equation of the form ($f_2\, u_x\, M_x$) with or without the term involving M_{xx}.

Substituting the above relations into the governing Eq. (1) one can write

$$\Im V = \frac{\partial V}{\partial t} + u\frac{\partial V}{\partial x} \tag{16}$$

where $\Im$ is now defined as

$$\Im = \Im_1 + \Im_2 = D_1\frac{\partial^2}{\partial x^2} + D_2\frac{\partial^2}{\partial y^2} \tag{17}$$

Expressing V as an asymptotic sum and utilizing Eq. (11), the governing equation becomes

$$\begin{aligned}\Im[\sum_{l=0}^{\infty} V^l] = [\sum_{l=0}^{\infty} V^l]_t + [\sum_{l=0}^{\infty} V^l]_M [\sum_{l=0}^{\infty} G^l] + [\sum_{l=0}^{\infty} V^l]_{M_x} [\sum_{l=0}^{\infty} G^l]_x \\ + \dots + u\frac{\partial}{\partial x}[\sum_{l=0}^{\infty} V^l]\end{aligned} \tag{18}$$

Note that the operator $\Im_1$ contains a second derivative with respect to x and therefore, when acting on any term, it will increase its order by a factor of 2. On the other hand the operator $\Im_2$, which contains a second derivative with respect to y, does not change the order of its operand since only variations in x are considered small. The above equation is now written in expanded form as

$$
\begin{aligned}
&\Im[V^0+V^1+V^2+V^3+\dots]=[V_t^0+V_t^1+V_t^2+V_t^3+\dots]\\
&+[V_M^0+V_M^1+V_M^2+V_M^3+\dots][G^0+G^1+G^2+G^3+\dots]\\
&+[V_{M_x}^0+V_{M_x}^1+V_{M_x}^2+V_{M_x}^3+\dots][G_x^0+G_x^1+G_x^2+G_x^3+\dots]\\
&+[V_{M_{xx}}^0+V_{M_{xx}}^1+V_{M_{xx}}^2+V_{M_{xx}}^3+\dots][G_{xx}^0+G_{xx}^1+G_{xx}^2+G_{xx}^3+\dots]\\
&+\dots+u[V_x^0+V_x^1+V_x^2+V_x^3+\dots]
\end{aligned}
\tag{19}
$$

Equating terms of like order on both sides of (19) gives the following system of equations:

For terms of order 0

$$\Im_2 V^0 = V_M^0 G^0 \tag{20}$$

For terms of order 1

$$\Im_2 V^1 = V_t^0 + V_M^0 G^1 + V_M^1 G^0 + V_M^1 G_x^0 + uV_x^0 \tag{21}$$

For terms of order 2

$$
\begin{aligned}
&\Im_2 V^2 + \Im_1 V^0 = V_t^1 + V_M^0 G^2 + V_M^1 G^1 + V_M^2 G^0\\
&+V_M^1 G_x^1 + V_{M_x}^2 G_x^0 + V_{M_{xx}}^2 G_{xx}^0 + uV_x^1
\end{aligned}
\tag{22}
$$

or generally, for terms of order *l*

$$\Im_2 V^1 + \Im_1 V^{1-2} = V_t^{l-1} + \sum_{j=0}^{l} V_M^{l-j} G^j + \sum_{j=0}^{l-1}\sum_{p=1}^{l-j} V_{M^{(p)}}^{l-j} \frac{\partial^p G^j}{\partial x^p} + uV_x^{l-1} \tag{23}$$

The above equations are sequentially solved for the *V*'s and *G*'s in order to get an expression for the center manifold and the evolution on it.

4. SOLUTION

The above hierarchy of equations can be solved sequentially by employing some boundary and solvability conditions. We start with the zero order equation and set $G^0 = 0$ which is consistent with the definition of *G*. Recall that G represents the time derivative of the mode function M, and as such, G^0, the zero-derivative part of G, should be zero. Therefore, the equation for order 0 becomes

$$\frac{\partial^2 V^0}{\partial y^2} = 0 \tag{24}$$

which upon integrating once with respect to *y* becomes

$$\frac{\partial V^0}{\partial y} = a_1 \tag{25}$$

where a_1 is a constant to be determined from the boundary conditions. We assume that the domain represents a confined, stratified aquifer with impervious overlying and underlying layers. Therefore, the normal velocity and the concentration gradient across the top and the bottom boundaries are set equal to zero. In addition we assume that the horizontal extent of the domain is sufficiently large to ensure that the concentration vanishes on the left and right boundaries (see Fig. 1). Thus

$$\frac{\partial c}{\partial y} = 0, \qquad v_y = 0 \qquad\qquad y = \pm b \tag{26}$$

$$c = 0, \qquad\qquad x = 0 \,\&\, x = L \tag{27}$$

It should be mentioned here that the contaminant is assumed to be instantaneously released over a rectangular source having a uniform initial concentration. Utilizing the condition (26) in Eq. (25), one gets $a_1 = 0$. Equation (25) then yields $V = a_2$ where a_2 is the integration constant that does not change with *y*. This constant can be obtained by imposing the "solvability condition" which is usually determined from the center manifold equation.

With the definition of the mode function $M(x)$ in mind, one can write the solvability condition as

$$\int_{-b}^{b} nV^1 dy = \begin{cases} M/\delta & l = 0 \\ 0 & l > 0 \end{cases} \tag{28}$$

As mentioned above, this condition is inspired by examining the equation of the center manifold which can be expanded as

$$\begin{aligned} c(x,y) &= V[M;x] \cong V^0 + V^1 + V^2 + V^3 + \dots \\ &\cong f_0 M + f_1 M_x + f_1 M_x + f_2 M_{xx} + f_3 M_{xxx} + \dots \end{aligned} \tag{29}$$

Multiplying both sides of Eq. (29) by $n\delta$ and integrating over the aquifer thickness gives

$$M(x) = n\delta\left[\int_{-b}^{b} f_0 M dy + \int_{-b}^{b} f_1 M_x dy + \int_{-b}^{b} f_2 M_{xx} dy + \ldots\right] \tag{30}$$

As the first term is the only term that contains $M(x)$ explicitly and all the other terms contain higher order derivatives of $M(x)$, it is reasonable to assume that only the first term is significant. This gives us the solvability condition, which yields the value of V^0 as

$$V^0 = \frac{M}{2n\delta b} \tag{31}$$

Having obtained V^0, we can now proceed to solve the first order equation to obtain G^1 and V^1. At any order, the solution procedure starts by integrating the equation over the aquifer width from $y = -b$ to $y = b$. The left-hand side usually vanishes or gives a known contribution. The right hand side then yields a linear function in G^1. Substituting the known form of G^1 back into the original equation and integrating twice with respect to y we get V^1 up to two constants. The first one is to be determined form the boundary conditions, while the second constant is obtained by utilizing the solvability condition, Eq. (28). To solve the first-order equation we write it as

$$\Im_2 V^1 = V_M^0 G^1 + V_M^1 G^0 + V_{M_x}^1 G_x^0 + u V_x^0 \tag{32}$$

Substituting the known functions G^0 and V^0 into the above equation yields

$$D_2 \frac{\partial^2 V^1}{\partial y^2} = \frac{G^1}{2n\delta b} + \frac{K(y)}{n} J \frac{M_x}{2n\delta b \alpha_T} \tag{33}$$

or

$$\frac{\partial^2 V^1}{\partial y^2} = \frac{G^1}{2\delta b \alpha_T K(y) J} + \frac{M_x}{2n\delta b \alpha_T} \tag{34}$$

Integrating the above equation over the width of the domain and utilizing the boundary conditions give

$$0 = \frac{G^1}{2\delta b \alpha_T J} \int_{-b}^{b} \frac{1}{K(y)} dy + \frac{M_x}{n\delta\alpha_T} \tag{35}$$

from which G^1 is obtained as

$$G^1 = -\frac{2bJ}{nK_{av}^{-1}} M_x = B_1 M_x \tag{36}$$

It is interesting to notice that G^1 is of advective form; the fraction has the form of a velocity and M_x is the gradient of the mode function $M(x)$. Now by substituting Eq. (36) into Eq. (35) and integrating once with respect to y, one obtains

$$\frac{\partial V^1}{\partial y} = -\frac{M_x}{n\delta\alpha_T K_{av}^{-1}} \int \frac{1}{K(y)} dy + \frac{M_x}{2n\delta b\alpha_T} y + a_1 \tag{37}$$

where the integration constant a_1 can be determined through the boundary conditions. To do so, the integral on the right-hand side of (37) needs to be evaluated with the form of the hydraulic conductivity distribution known (e.g., from fitting to field measurements). In the next section, we hypothesize a form for the hydraulic conductivity, $K(y)$, for the Cape Cod site located in Massachusetts, USA, where there is a large set of tracer test data which will be used to validate the results of our approach.

5. APPLICATION TO CAPE COD TRACER DATA

Data from the Cape Cod experiment is used to test the applicability of the assumptions employed in developing the center manifold approach. Specifically, the predictions of the one-dimensional evolution Eq. (15) with terms up to the third order are compared to the field observations. In order evaluate the integral on the right hand side of Eq. (32) assume the form $K^{-1}(y) = R(1 + y^2)$, for $F(y)$ where y is normalized with respect to the domain width. The parameter R is determined from the field values of conductivity, porosity and hydraulic gradient at Cape Cod. The mean hydraulic conductivity for this site is about 110 m/day and the effective porosity, n, is about 0.39 [6]. The hydraulic gradient, J, at the site varies between 0.0014 and 0.0018.

Therefore, if we take n = 0.39, J = 0.0016, and R = 0.0138, we get an average conductivity of 108.38 m/day and an average flow velocity of 0.44 m/day.

The bromide concentration at 13 days after the tracer is injected is used as the initial condition for the center manifold evolution equation. The initial $M(x)$ is calculated using Eq. (8) and then the evolution equation is solved using an implicit finite difference scheme. Figure 2 compares $M(x)$ calculated from the experimental data at Cape Cod with the center manifold solution. The theory fits the field data better as time progresses. The first and second longitudinal moments obtained through the center manifold theory may also be compared to those obtained from the field data [7]. This comparison is shown in Fig. 3, and the prediction is quite good.

6. CONCLUSIONS

The equations resulting from the center manifold approach are easier to solve than the original advection dispersion equation. We need only solve a one-dimensional ordinary differential equation of the form (16) to obtain $M(x)$ and predict the longitudinal spatial moments for the moving tracer. Results indicate that the theory adequately predicts the center of mass and second longitudinal moment at Cape Cod. The procedure for computing more accurate higher order approximations is purely mechanistic once the first approximation is obtained.

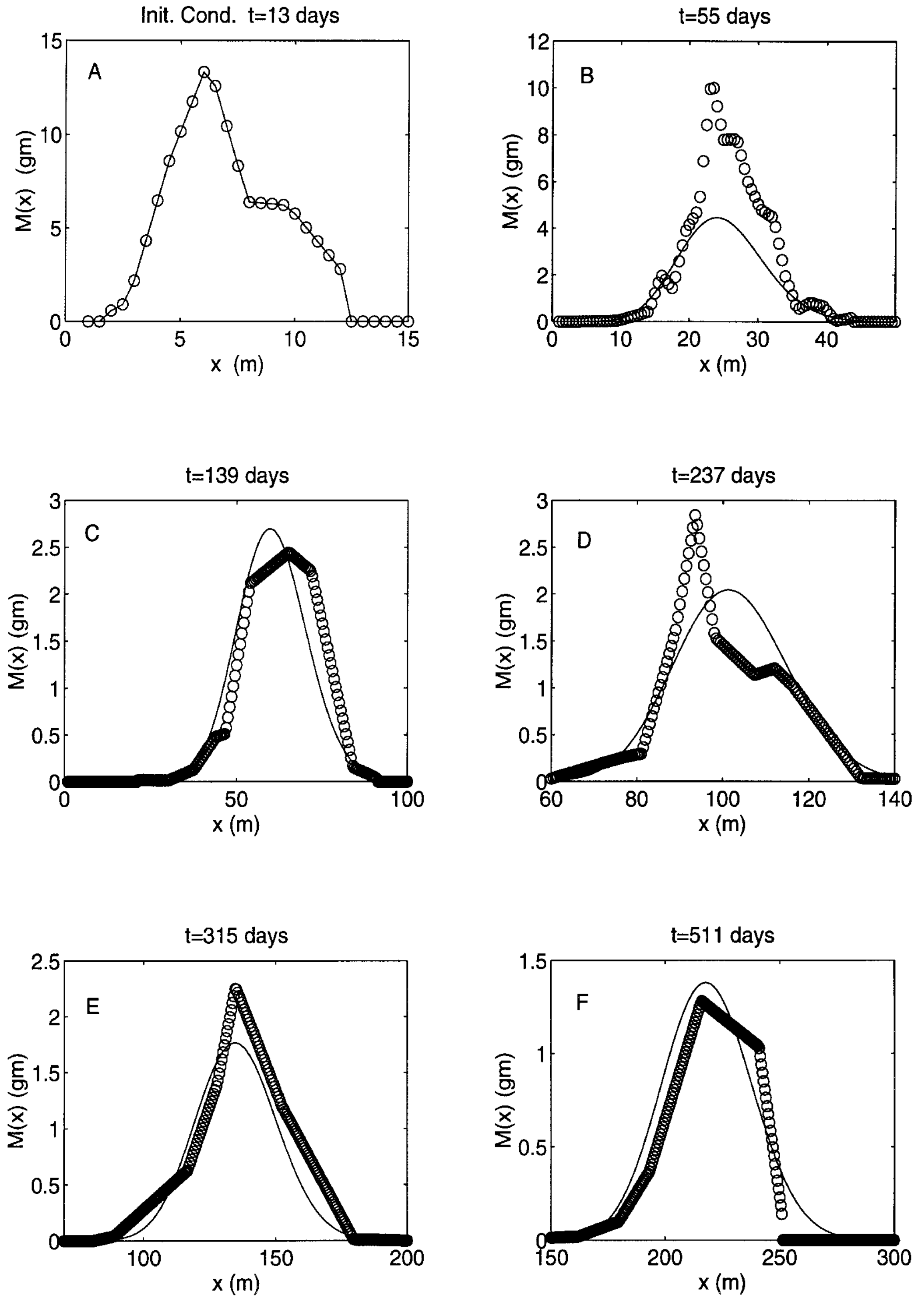

Fig. 2. Simulated and observed mode function at different times for a vertical Bromide concentration distribution. Solid line is the center manifold approach and circles are for actual Cape Cod data.

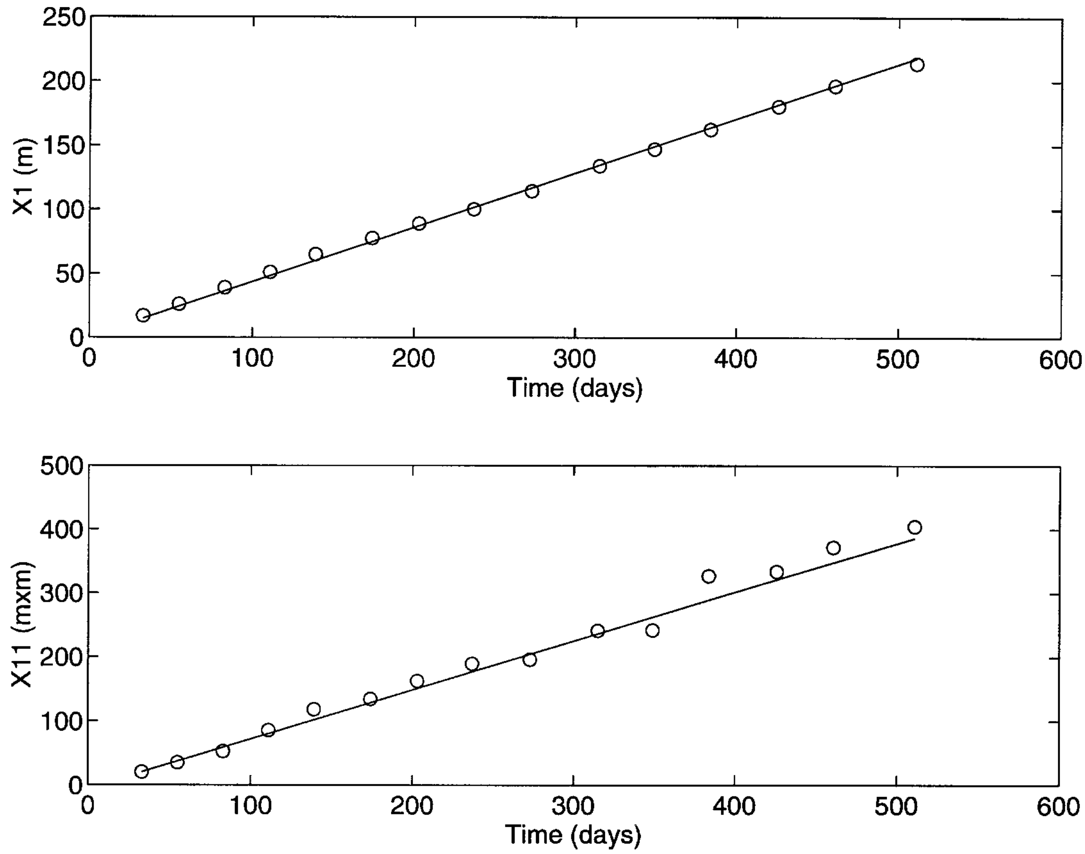

Fig. 3. Simulated longitudinal first and second spatial moments for the Cape Cod experiment with vertical cross sectional simulation. Solid line is the center manifold approach and circles show actual spatial moments of bromide from [7].

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تطبيق طريقة المشعب المركزي على انتشار الملوثات في الخزانات الطبقية

يقدم البحث وصفاً لانتشار الملوثات في الخزانات الطبقية باستخدام طريقة المشعب المركزي، ويفترض أن عملية الانتشار تتطور ببطء مع الزمن والمسافة مما يسمح بتطبيق نظرية المشعب المركزي، وقد تم اخذ التباين المكاني لخواص النظام في الاعتبار باستخدام معاملات متغيرة لخواص الخزان مثل معامل النفاذية ومعامل الانتشار، والطريقة المقدمة في هذه الدراسة تركز على الانتشار في الاتجاه الطولي الموازي لحركة المياه الجوفية، ومن أهم مميزات هذه الطريقة أن الحلول الأعلى دقة يمكن الحصول عليها بسهولة بمجرد الحصول على الحل من الدرجة الأولى وبالإضافة إلى هذا فإن هذه الطريقة تؤدي إلى معادلة تفاضلية في بعد واحد يمكن حلها بسهولة أكثر من معادلة الانتشار الأصلية في بعدين، وقد وجد أن حل معادلة الانتشار باستخدام هذه الطريقة يؤدي إلى نتائج قريبة الى حد كبير من معدلات الانتشار المقاسة في الطبيعة عندما تم تطبيق هذه الطريقة على تجارب الانتشار في منطقة "كيب كود" الواقعة في ولاية "ماساتشوتس" بالولايات المتحدة الأمريكية.