Depth-averaging errors in reactive transport modeling

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[1] Depth-averaged reactive transport models are commonly used to represent field-scale contamination in groundwater aquifers. These models rely on simplifying the governing equations through defining a depth-averaged variable and vertically integrating the full reactive transport equation. This approach is exact provided that the governing equation is linear; however, vertically averaging a nonlinear conservation equation can introduce an error into the simplified model. We present a framework for analyzing this error so that the suitability of a depth-averaged reactive transport model can be assessed quantitatively before the model is implemented. This framework shows how the error introduced by depth-averaging reactive transport equations is governed by the parameters in the kinetic model and the geometry of the reactive transport problem.

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1. Introduction

[2] Many groundwater contamination sites are monitored and modelled using techniques that account for the vertical structure of the distribution of contamination [e.g., *Brun et al.*, 2002; *Wriedt and Rode*, 2006; *Zheng and Bennett*, 2002]. Depth-averaged approaches, which do not account for vertical variations, are also commonly used to model field-scale groundwater contamination. There are several reasons why depth-averaged approaches are used: (1) the horizontal extent of a contamination plume is typically much larger than the vertical extent; (2) in many cases full three-dimensional field data are unavailable to characterize vertical variability; and (3) the development and application of a depth-averaged reactive transport model requires less information regarding the characterization of the transport parameters and is computationally cheaper than using a full vertical reactive transport model. Regardless of the reasons for using a depth-averaged reactive transport model, these models all rely on simplifying the conservation equations by averaging in the vertical direction. In this work we explore the consequences of averaging reactive transport equations by averaging a reactive transport model for a two-dimensional vertical slice to give a simplified one-dimensional model.

[3] Averaging a conservation equation with only linear terms yields an exact simplified mathematical model. This is not true when the governing equation is nonlinear. Since field-scale reactive transport modeling often involves advection-dispersion-reaction processes with nonlinear reaction kinetics, great care ought to be exercised when applying a vertically averaged reactive transport model. However, depth-averaged reactive transport models are routinely applied by assuming that the nonlinear terms can be averaged in the same way as linear terms. In general, this approach is inexact and can introduce an error.

[4] Although depth-averaged reactive transport models are frequently used to represent groundwater contamination, the assumptions required for a depth-averaged reactive transport model to be valid are typically unstated and no attempt to quantify the suitability of using a depth-averaged model is made. For example, previous investigations have used depth-averaged models without any explicit discussion of their validity [e.g., *Atteia et al.*, 2008; *Gomez et al.*, 2008; *Ling and Rifai*, 2007; *Lu et al.*, 1999, 2005; *Ocampo et al.*, 2006]. Although some of these studies involve reactive transport through shallow aquifer material, the assumption of using a depth-averaged model is not justified quantitatively. Other studies justify the validity of a depth-averaged reactive transport model by assuming that vertical mixing processes are sufficiently fast that vertical variations in any contaminant concentration are negligible [e.g., *Singleton et al.*, 2006]. None of these approaches offer any way of quantifying the validity of this assumption.

[5] The aim of this work is to provide a framework to analyze the error introduced by depth-averaging reactive transport equations. The depth-averaging error is analyzed at three levels: (1) we use Jensen's inequality to show the error acts either as an additional source or sink in the depth-averaged equations; (2) for a simplified plume geometry we show that the magnitude of the error introduced into the governing equations can be determined a priori; and (3) solutions of a full vertical reactive transport model are compared with solutions of a depth-averaged model to investigate how closely the simplified analysis represents a system with a full plume geometry. The practical significance of this work is to help identify a source of error that can be introduced when using depth-averaged reactive transport models. This error has not been previously considered or analyzed in the literature. This analysis can help distinguish between situations where depth-averaged mod-

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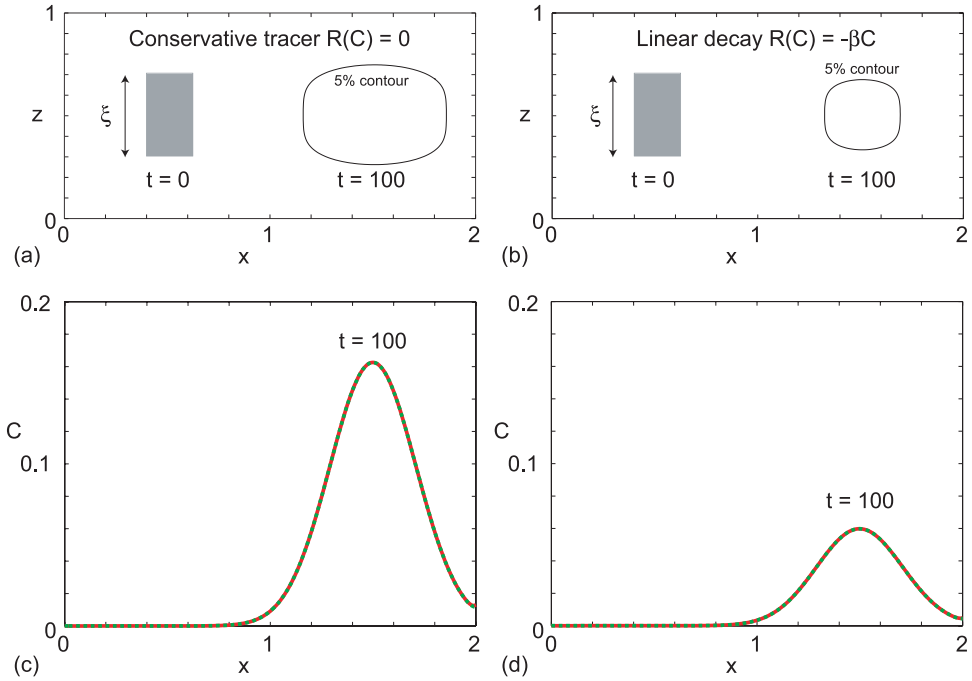

Figure 1. (a and b) Reactive transport with $R''(C) = 0$ involves no depth-averaging error. Two-dimensional simulations correspond to $D_x = 2 \times 10^{-4}$, $D_z = 2 \times 10^{-5}$, $v_x = 0.01$, and $\beta = 0.01$; $\partial C/\partial x = 0$, where $x = 0$ and $x = 2$, while $\partial C/\partial z = 0$, where $z = 0$ and $z = 1$. The location of the initial plume of unit concentration is indicated by the gray rectangle, and the $C = 0.05$ contours are shown at $t = 100$. (c and d) The two-dimensional concentration data at $t = 100$ in Figures 1a and 1b are vertically averaged using equation (11) (solid red line). Results from a one-dimensional depth-averaged model with the same parameters, depth-averaged initial condition, and boundary conditions are given in Figures 1c and 1d (dotted green line), showing that the depth-averaged model is exact. All numerical results are generated using $\Delta x = \Delta z = 0.01$ and $\Delta t = 0.1$.

eling is acceptable or unacceptable depending on the magnitude of the depth-averaging error.

2. Analysis

[6] Reactive transport processes of a single chemical species is governed by

$$\frac{\partial C}{\partial t} = L_n(C) + R(C), \tag{1}$$

where C is the solute concentration, $L_n(C)$ represents either the two-dimensional vertical ($n = 2$) or three-dimensional ($n = 3$) linear advection dispersion transport operator and $R(C)$ represents net production due to chemical reaction. The full conservation equation is often simplified by vertically integrating each term and rewriting the equation in terms of a depth-averaged variable

$$\overline{C} = \frac{1}{Z}\int_{z=0}^{z=Z} C\,\mathrm{d}z. \tag{2}$$

Dividing each term in equation (1) by the vertical depth Z, and integrating in the z direction gives

$$\frac{\partial \overline{C}}{\partial t} = L_{(n-1)}(\overline{C}) + \frac{1}{Z}\int_{z=0}^{z=Z} R(C)\,\mathrm{d}z. \tag{3}$$

Here we have assumed that there is no flux of solute into or out of the domain through the top and bottom boundaries [*Bentley and Pinder*, 1992]. The vertically integrated linear transport operator and the temporal derivative are written as a function of $\overline{C}$ and the subscript $(n - 1)$ indicates that the dimensions of the averaged system have been reduced by one. Since the source term may be nonlinear, it is not possible to write this term as a function of $\overline{C}$. It is common, however, to write the depth-averaged equations as

$$\frac{\partial \overline{C}}{\partial t} = L_{(n-1)}(\overline{C}) + R(\overline{C}). \tag{4}$$

For equation (4) to be valid, we require

$$R(\overline{C}) = \frac{1}{Z}\int_{z=0}^{z=Z} R(C)\,\mathrm{d}z. \tag{5}$$

Throughout this note we will refer to this condition as the "depth-averaging assumption." For an arbitrary plume geometry, equation (5) is only true if $R''(C) = \frac{\mathrm{d}^2 R}{\mathrm{d}C^2} = 0$.

[7] In general,

$$R(\overline{C}) \geq \frac{1}{Z}\int_{z=0}^{z=Z} R(C)\,\mathrm{d}z \tag{6}$$

if $R(C)$ is concave down so $R''(C) < 0$. Alternatively,

$$R(\overline{C}) \leq \frac{1}{Z}\int_{z=0}^{z=Z} R(C)\,\mathrm{d}z \tag{7}$$

if $R(C)$ is concave up so $R''(C) > 0$. Together, equations (6) and (7) are known as Jensen's inequality [*Rudin*, 1987].

2.1. Model Solution

[8] To investigate the implications of invoking the depth-averaging assumption, we examine a suite of solutions for various reactive transport problems in a two-dimensional (vertical) Cartesian domain $\Omega = \{(x, y): 0 \leq x \leq 2, 0 \leq y \leq 1\}$. For this problem the flow is uniform in the x (horizontal) direction and there is no flow in the z (vertical) direction. We consider a vertical slice through the aquifer in the $x - z$ plane. Numerical solutions of

$$\frac{\partial C}{\partial t} = D_x\frac{\partial^2 C}{\partial x^2} + D_z\frac{\partial^2 C}{\partial z^2} - v_x\frac{\partial C}{\partial x} + R(C), \tag{8}$$

with various $R(C)$ will be considered. The two-dimensional solution profiles will then be averaged along the z coordinate, giving a one-dimensional vertically averaged profile along the x coordinate. These depth-averaged profiles will be considered "exact" in the sense that the solution of the full governing equation has been used to construct the average.

[9] These exact depth-averaged results will be compared to solutions of an approximate one-dimensional depth-averaged model

$$\frac{\partial \overline{C}}{\partial t} = D_x\frac{\partial^2 \overline{C}}{\partial x^2} - v_x\frac{\partial \overline{C}}{\partial x} + R(\overline{C}). \tag{9}$$

Numerical solutions of equations (8) and (9) are obtained by solving the transport part of the equations using a standard finite difference discretization, with central differences for the advection term [*Zheng and Bennett*, 2002]. The domain is discretized with constant grid spacing Δx and Δz. The temporal derivative associated with the transport terms are approximated with a Crank-Nicolson method. The reaction terms are solved using a standard fourth-order Runge-Kutta method. The transport and reaction terms are coupled using the $\mathcal{O}[(\Delta t)^2]$ Strang (alternating) splitting method [*Simpson and Landman*, 2007]. All discretizations (Δx, Δz, Δt) are sufficiently small so that the numerical solutions are grid-independent.

3. Analysis of Depth-Averaging Error: $R''(C) = 0$

[10] First we confirm a key result implied by Jensen's inequality, that there is no depth-averaging error when $R''(C) = 0$. Two cases are considered: (1) a conservative system with $R(C) = 0$ and (2) a system undergoing linear decay with $R(C) = -\beta C$.

[11] For the two-dimensional simulations we use the initial condition

$$C(x, z, 0) = \begin{cases} 1, & 0.4 < x < 0.6 \text{ and } 0.3 < z < 0.7 \\ 0, & \text{elsewhere in } \Omega. \end{cases} \tag{10}$$

Results in Figures 1a and 1b show the initial concentration distribution and the two-dimensional contours of $C = 0.05$ at $t = 100$ for $R(C) = 0$ (Figure 1a) and $R(C) = -\beta C$ (Figure 1b). Next, both these two-dimensional profiles are averaged along each column in the finite difference grid using a discrete analogue of equation (2) given by

$$\overline{C}(x_i, t) = \frac{1}{\mathrm{NZ}}\sum_{j=1}^{j=\mathrm{NZ}} C(x_i, z_j, t), \quad \forall i = 1, 2, 3 \ldots \mathrm{NX}, \tag{11}$$

where NZ and NX are the number of nodes in the vertical and horizontal directions in the finite difference grid respectively, $C(x_i, z_j, t)$ are discrete values of the two-dimensional concentration profile in the ith column and jth row of the finite difference grid and $\overline{C}(x_i, t)$ is the depth-averaged concentration in the ith column of the finite difference grid. The resulting depth-averaged profiles are given in Figure 1c for $R(C) = 0$ and Figure 1d for $R(C) = -\beta C$.

[12] To compare the two-dimensional depth-averaged profiles with the prediction of a one-dimensional depth-averaged model, the two-dimensional initial condition (equation (10)) is averaged in the vertical direction giving

$$\overline{C}(x, 0) = \begin{cases} 0, & 0 < x < 0.4 \\ 0.4, & 0.4 < x < 0.6 \\ 0, & 0.6 < x < 2. \end{cases} \tag{12}$$

The depth-averaged one-dimensional model (equation (9)) is solved using the initial condition given by equation (12) and the same reaction and transport parameters used in the two-dimensional simulations (Figures 1a and 1b). The solutions of equation (9) are indistinguishable from the two-dimensional depth-averaged profiles (Figures 1c and 1d) confirming that equation (5) is valid when $R''(C) = 0$. Further simulations with different reaction and transport parameters and different initial conditions confirm that there is no depth-averaging error provided that $R''(C) = 0$.

4. Analysis of Depth-Averaging Error: $R''(C) \neq 0$

[13] The depth-averaging assumption is invalid when $R(C)$ is nonlinear and $R''(C) \neq 0$. To explore the consequence of this condition we consider the ubiquitous Monod model

$$R(C) = -\frac{\alpha C}{K + C}. \tag{13}$$

In this case $R(C)$ is concave up with $R''(C) = 2\alpha K/[(K + C)^3] > 0$. Consequently Jensen's inequality implies that the solution of equation (9) will always underestimate the true depth-averaged concentration.

[14] Two measures of the depth-averaging error will be introduced. The absolute error is defined as

$$\mathrm{E_{abs}} = \frac{1}{Z}\int_{z=0}^{z=Z} R(C)\,\mathrm{d}z - R(\overline{C}). \tag{14}$$

For the Monod kinetic model $\mathrm{E_{abs}} \geq 0$. We assume that a plume of uniform concentration $C = \widehat{C}$ is present in an aquifer with an arbitrary depth Z. Furthermore, we assume

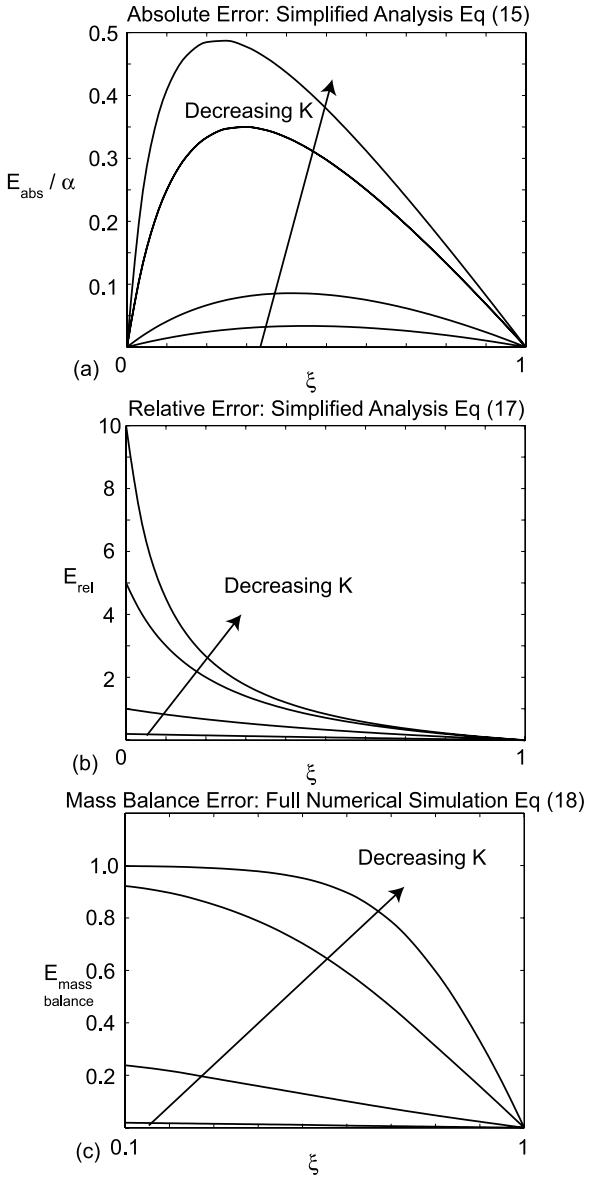

Figure 2. Error analysis with $R(C) = -\alpha C/(K + C)$. (a) Absolute error given by equation (15) with $\widehat{C} = 1$, indicating that the absolute error increases with α and decreases with K. Values of E_{abs}/α are given for $K = 0.1$, 0.2, 1, 5. (b) Relative error given by equation (17), showing that the relative error decreases with K. Profiles are shown for $K = 0.1$, 0.2, 1, 5. (c) Relative mass balance error for the numerical solutions with $\alpha = 0.1$ at $t = 10$ for $K = 0.1$, 0.2, 1, 5.

that the plume occupies a fraction of the vertical depth $\xi \in [0, 1]$. To evaluate E_{abs}, the details of where this fraction is located are unimportant. For example, if $\xi = 1/2$, it is unimportant whether the plume is located in the top half, the bottom half, or some other configuration. Under these conditions the absolute error (equation (14)) simplifies to

$$\frac{E_{abs}}{\alpha} = \frac{\widehat{C}^2 \xi(1-\xi)}{(K+\widehat{C})(K+\xi\widehat{C})}. \tag{15}$$

Several limiting cases of the absolute error expression confirm our intuitive expectations about invoking the depth-averaging assumption. When $\xi = 1$ the plume of constant concentration occupies the full vertical extent of the domain and there is no depth-averaging error [*Simpson et al.*, 2009]. Similarly when $\xi = 0$ or $\widehat{C} = 0$ there is no plume and no depth-averaging error.

[15] For intermediate values of ξ, Figure 2a shows how the absolute depth-averaging error behaves under a range of conditions. This is a key result giving us insight into the influence of the depth-averaging error and how the error varies with the parameters in the model and the geometry of the problem. For example, the analysis shows exactly how the absolute error increases with α and decreases with K. The analysis also shows that for each choice of α and K, the absolute error has a maximum for some intermediate value of ξ. Therefore, before performing any simulations we know that if α is small and K is large then the depth-averaging error may be negligible. Conversely, if α is large and K is small, then the depth-averaging error may be significant. This kind of quantitative tool gives us greater insight into the implications of using a depth-averaged model compared to other approaches where the validity of depth averaging is not examined. We now have a rational and quantitative method to explore the relationships between the depth-averaging error, the geometry of the problem and the parameters in the reactive transport model.

[16] We also define a relative error

$$E_{rel} = \left| \frac{\frac{1}{Z}\int_{z=0}^{z=Z} R(C)\,dz - R(\overline{C})}{\frac{1}{Z}\int_{z=0}^{z=Z} R(C)\,dz} \right|. \tag{16}$$

The relative error is defined with an absolute value since the numerator of the expression in equation (16) is positive whereas the denominator is negative for the Monod kinetic model. The relative error expression simplifies to

$$E_{rel} = \frac{\widehat{C}(1-\xi)}{(K+\widehat{C}\xi)} \tag{17}$$

for a plume of constant concentration $C = \widehat{C}$, that occupies a fraction of the vertical depth of the aquifer, ξ. The relative error is independent of α and decreases with K. This relationship is shown graphically in Figure 2b.

[17] The error expressions given by equations (15) and (17) measure the difference in the magnitude of the source terms in the two-dimensional vertical model (equation (8)) and the depth-averaged model (equation (9)), for a simplified plume geometry. To examine how this analysis predicts the accuracy of depth-averaged simulations for a more realistic plume geometry, we repeat the numerical simulations in Figure 1 with $R(C) = -\alpha C/(K + C)$. These simulations use the same initial condition, boundary conditions and transport parameters that were used for the problems in Figure 1. Representative results in Figures 3a and 3b illustrate that the depth-averaging error that manifests in the solution of the reactive transport equations behaves similarly to the simplified analysis given in Figures 2a and 2b.

[18] Results in Figure 3a are for large K and show that the depth-averaged model is a very good approximation to the

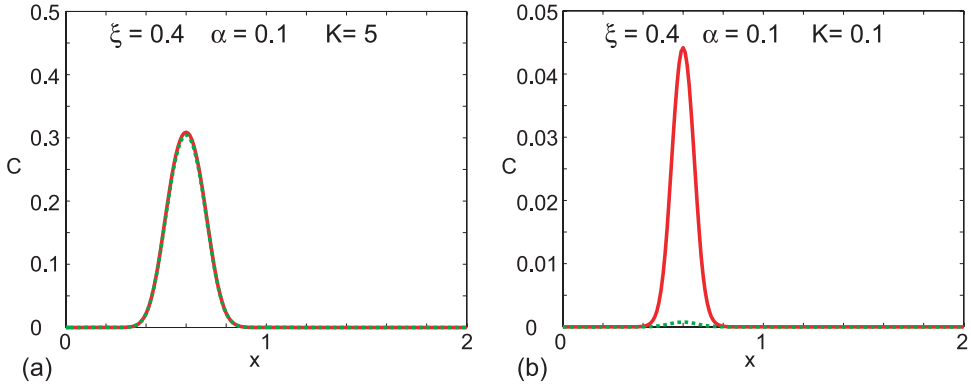

Figure 3. Reactive transport with $R(C) = -\alpha C/(K + C)$ introduces a depth-averaging error. Two-dimensional simulation data with the same initial condition, boundary conditions, and transport parameters used in Figures 1a and 1b are presented for $R(C) = -\alpha C/(K + C)$ and $\alpha = 0.1$. Two-dimensional data at $t = 10$ are depth-averaged using equation (11), giving the profiles (solid red line) for (a) $K = 5$ and (b) $K = 0.1$. Results from a one-dimensional depth-averaged simulation with the same parameters, depth-averaged initial condition, and boundary conditions are superimposed (dotted green line), showing that the accuracy of the depth-averaged model is very sensitive to the kinetic parameters.

full vertical model even though the vertical distribution of the solute is not uniform. Alternative results in Figure 3b with small K show that the depth-averaged model is a very poor approximation of the full vertical model. In this case, the results from the depth-averaged model are barely discernable at the scale shown in Figure 3b. For all values of the parameters the depth-averaged model underestimates the exact data since $R(C)$ is concave up.

[19] In summary, comparing the solutions of the full vertical reactive transport model with the solutions of the depth-averaged reactive transport model confirm that the depth-averaging error depends strongly on the parameters of the kinetic model. Furthermore, the simplified analysis captures the main features of the error behavior illustrated by the numerical solutions. This is because the differences in the model solutions reflect the differences in the source terms of the governing equations which are described by the simplified analysis.

[20] The depth-averaging error in the solutions of the governing equations can be quantified in many ways. We chose to use a measure of the relative mass balance error

$$\mathrm{E}_{\text{mass balance}} = \left| \frac{M(t)_{\mathrm{n}} - M(t)_{(\mathrm{n}-1)}}{M(t)_{\mathrm{n}}} \right|, \tag{18}$$

where $M(t)$ is the total mass of contaminant in the domain at time t and the subscript n is associated with the full vertical model whereas the subscript $(n - 1)$ is associated with the depth-averaged model.

[21] These masses are evaluated by spatially integrating the concentration profile

$$\begin{aligned} M(t)_{\mathrm{n}} &= \int_{x=0}^{x=X} \overline{C}(x,t)_{\mathrm{n}}\, \mathrm{d}x, \\ M(t)_{(\mathrm{n}-1)} &= \int_{x=0}^{x=X} \overline{C}(x,t)_{(\mathrm{n}-1)}\, \mathrm{d}x, \end{aligned} \tag{19}$$

where X is the total length of the domain, $\overline{C}(x, t)_{\mathrm{n}}$ is the depth-averaged profile obtained from the two-dimensional vertical model equation (8), and $\overline{C}(x, t)_{(\mathrm{n}-1)}$ is the profile obtained from the simplified depth-averaged one-dimensional model equation (9). For all results presented here, the integrals in equation (19) are approximated using a trapezoid rule with panel width Δx. Results in Figure 2c are presented for a suite of simulations with the same boundary conditions and transport parameters as those results given in Figure 3. For the vertical model simulations in this set of results we used the initial condition

$$C(x,z,0) = \begin{cases} 1, & 0.4 < x < 0.6 \quad \text{and} \quad 0 < z < \xi \\ 0, & \text{elsewhere in} \quad \Omega. \end{cases} \tag{20}$$

To perform depth-averaged simulations, we average the two-dimensional initial condition given by equation (20), to give the depth-averaged initial condition

$$\overline{C}(x,0) = \begin{cases} 0, & 0 < x < 0.4 \\ \xi, & 0.4 < x < 0.6 \\ 0, & 0.6 < x < 2. \end{cases} \tag{21}$$

Numerical data in Figure 2c show how the error given by equation (18) varies with plume geometry ξ and the kinetic parameter K. This data confirms that the trends established in the simplified error analysis (Figures 2a and 2b) are reflected by the errors in simulations with a more realistic plume geometry.

5. Analysis of Depth-Averaging Error: Multicomponent Reactive Transport

[22] To demonstrate the generality of this analysis we now discuss coupled multicomponent reactive transport by considering a two-component system,

$$\begin{aligned} \frac{\partial C_1}{\partial t} &= L_{\mathrm{n}}(C_1) + R_1(C_1, C_2), \\ \frac{\partial C_2}{\partial t} &= L_{\mathrm{n}}(C_2) + R_2(C_1, C_2), \end{aligned} \tag{22}$$

where $R_1(C_1, C_2)$ and $R_2(C_1, C_2)$ represent arbitrary coupling kinetics. Following the approach in section 2, we define depth-averaged variables and integrate the coupled system

$$\frac{\partial \overline{C_1}}{\partial t} = L_{(n-1)}(\overline{C_1}) + \frac{1}{Z}\int_{z=0}^{z=Z} R_1(C_1, C_2)\,dz,$$
$$\frac{\partial \overline{C_2}}{\partial t} = L_{(n-1)}(\overline{C_2}) + \frac{1}{Z}\int_{z=0}^{z=Z} R_2(C_1, C_2)\,dz. \quad (23)$$

We now analyze the difference between equation (23) and the simplified system given by

$$\frac{\partial \overline{C_1}}{\partial t} = L_{(n-1)}(\overline{C_1}) + R_1(\overline{C_1}, \overline{C_2}),$$
$$\frac{\partial \overline{C_2}}{\partial t} = L_{(n-1)}(\overline{C_2}) + R_2(\overline{C_1}, \overline{C_2}). \quad (24)$$

Absolute and relative error expressions can be defined in the same way as in section 2, for example the absolute error expressions are

$$\mathrm{E1_{abs}} = \frac{1}{Z}\int_{z=0}^{z=Z} R_1(C_1, C_2)\,dz - R_1(\overline{C_1}, \overline{C_2}),$$
$$\mathrm{E2_{abs}} = \frac{1}{Z}\int_{z=0}^{z=Z} R_2(C_1, C_2)\,dz - R_2(\overline{C_1}, \overline{C_2}). \quad (25)$$

The absolute error expressions are zero for linear coupling kinetics, this was confirmed with simulation data (not shown). For a more interesting case we consider a multiple Monod problem with

$$R_1(C_1, C_2) = \frac{-\alpha_1 C_1 C_2}{(K_2 + C_1)(K_2 + C_2)},$$
$$R_2(C_2, C_2) = \frac{-\alpha_2 C_1 C_2}{(K_1 + C_1)(K_2 + C_2)}. \quad (26)$$

In this problem C_1 represents a decaying contaminant and the decay of C_1 is coupled to the uptake of an indigenous background component C_2. This kind of multiple Monod formulation is commonly used to represent complex biodegradation processes [*Zheng and Bennett*, 2002]. To evaluate equation (25) we consider a plume of uniform concentration $C_1 = \widehat{C_1}$ occupying a fraction $\xi \in [0, 1]$ of the total depth Z. We also suppose that the indigenous background component has a uniform concentration $C_2 = \widehat{C_2}$ distributed evenly across the vertical depth. Under these conditions we obtain

$$\frac{\mathrm{E1_{abs}}}{\alpha_1} = \frac{\mathrm{E2_{abs}}}{\alpha_2} = \frac{\widehat{C_1}^2 \widehat{C_2}\xi(1-\xi)}{(K_1 + \widehat{C_1})(K_2 + \widehat{C_2})(K_1 + \xi\widehat{C_1})}. \quad (27)$$

As for the single species analysis, the error expression for the coupled problem shows explicitly how the depth-averaging error varies with the model parameters and the geometry of the problem. For this particular problem we plot equation (27) for $\widehat{C_1} = \widehat{C_2} = 1$ in Figure 4a showing that $\mathrm{E1_{abs}}$ and $\mathrm{E2_{abs}}$ increase as values of K_1 and K_2 decrease. Furthermore the analysis shows that the depth-averaging error is more sensitive to reductions in K_1 than K_2.

[23] Full numerical solutions of the multicomponent problem are given to illustrate how the simplified error analysis applies to the full problem. For simplicity and brevity we present results for the C_1 profile only, and note that similar trends are evident in the C_2 profile. Simulation data in Figure 4b for $K_1 = K_2 = 1$ show that the solution of the depth-averaged model underestimates the exact profile. Further results in Figures 4b and 4c confirm that the depth-averaging error increases as K_1 and K_2 decrease, as well as confirming that the depth-averaging error is more sensitive to reductions in K_1 than K_2.

[24] In summary, we have shown that the basic analysis in section 2 can be extended to more complex kinds of reactive transport. Other types of kinetic reactions for systems with an arbitrary number of components can be analyzed in this way.

6. Limitations of Analysis

[25] This analysis ignores particular details which may be important in certain applications. For instance we have not explicitly dealt with spatial heterogeneity. If a three-dimensional (x, y, z) transport operator is vertically averaged to give a depth-averaged transport operator in the (x, y) plane, the analysis presented here is valid when the transport coefficients are spatially variable in the (x, y) plane. If the transport coefficients are spatially variable in the vertical direction, then we must replace the vertically varying coefficients with depth-averaged transport coefficients. This additional averaging introduces a new source of error. We do not explicitly consider this new source of error here, as a depth-averaged model is unlikely to be used in the situation where the vertical variation in the transport coefficients are explicitly known. This does not lessen the practical significance of this analysis as many reactive transport studies are conducted without detailed knowledge of the vertical variation of the transport coefficients [e.g., *Atteia et al.*, 2008; *Ling and Rifai*, 2007; *Lu et al.*, 1999; *Ocampo et al.*, 2006].

[26] This work also ignores advective transport in the vertical direction by setting $v_z = 0$. This assumption has often been made in practical reactive transport modeling case studies and there are several reasons why vertical advective transport is often ignored. For example, (1) it may be sufficient to approximate the advective transport using a one-dimensional uniform flow approximation [*Clement et al.*, 2002; *Ocampo et al.*, 2006], or (2) it may be sufficient to obtain a depth-averaged advective velocity field by using a depth-averaged groundwater flow model, such as using MODFLOW with a single layer of cells [*Clement et al.*, 2000; *Lu et al.*, 1999, 2005; *Ling and Rifai*, 2007]. Further complications, such as considering multiphase reactive transport or transport involving cross diffusion are not explicitly considered as a part of this work.

[27] In summary, it is often necessary to introduce certain idealizations before a particular problem can be mathematically analyzed. In this section we acknowledge the idealizations that have been necessary for us to investigate this

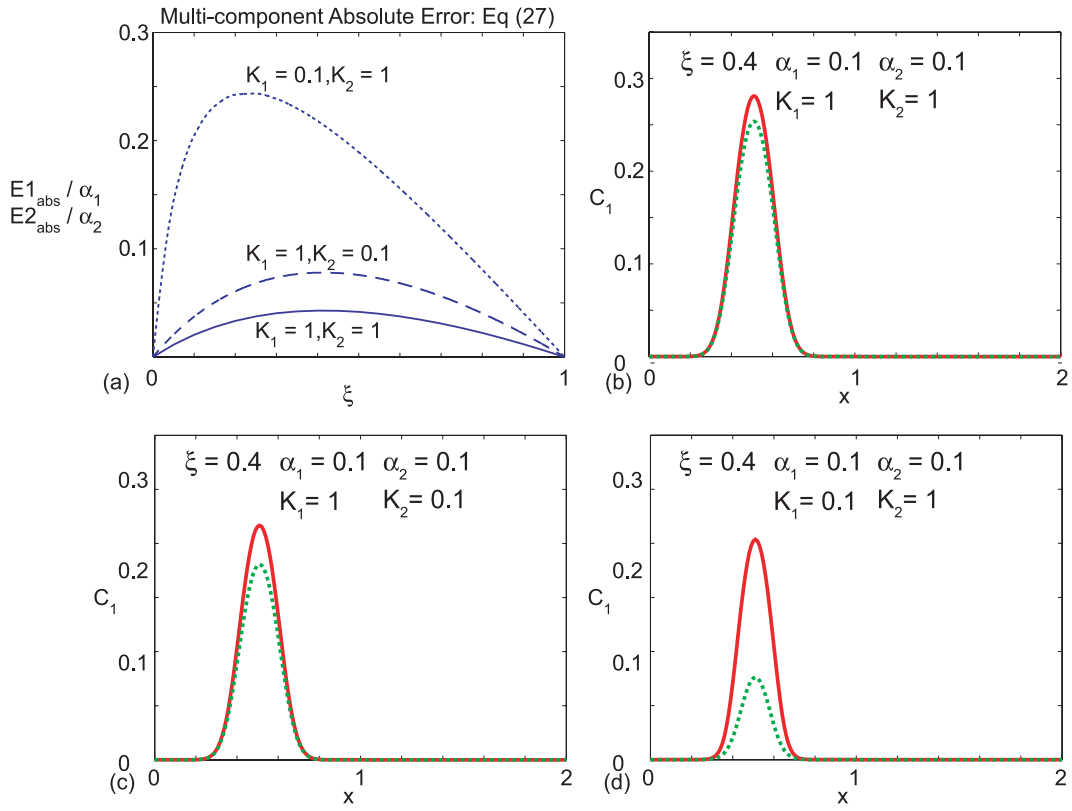

Figure 4. Multicomponent reactive transport with $R_1(C_1, C_2) = -\alpha_1 C_1 C_2/[(K_1 + C_1)(K_2 + C_2)]$ and $R_2(C_1, C_2) = -\alpha_2 C_1 C_2/[(K_1 + C_1)(K_2 + C_2)]$ introduces a depth-averaging error. (a) The absolute error expression (equation (27)) with $\widehat{C_1} = \widehat{C_2} = 1$ shows how the depth-averaging error varies with ξ, K_1 and K_2. (b–d) Two-dimensional simulation data with the same initial condition, boundary conditions, and transport parameters used in Figures 1c–1d at $t = 10$ are depth averaged. Results from the vertical model (solid red line) are compared with results from the depth-averaged model (dotted green line).

fundamental mathematical modeling issue which has not been addressed previously. Regardless of these simplifying assumptions, this analysis remains valid as many of the assumptions made here are also made in practice.

7. Summary and Conclusions

[28] Depth-averaged reactive transport models are commonly used to represent field-scale contamination; however, the assumptions enabling the full governing equations to be depth averaged are often unstated and untested. In many cases the use of a depth-averaged reactive transport model introduces an error associated with averaging nonlinear reaction terms. To help evaluate the validity of using a depth-averaged model we present a framework for quantifying the magnitude of the depth-averaging error. This analysis shows that the depth-averaging error only occurs when the source term is nonlinear and that the error acts either as an additional source or sink depending on whether the source term is concave up or concave down. For a simplified plume geometry, we explore how the magnitude of the depth-averaging error varies with (1) the parameters in an example reaction model and (2) the geometry of the plume. This analysis can be used to investigate whether the depth-averaging error is likely to compromise the accuracy of a depth-averaged model relative to a full vertical model.

[29] Without any analysis, the magnitude of the depth-averaging error in a particular application of a depth-averaged model to replicate field data would be difficult to detect. This is because field-scale reactive transport modeling usually involves some model calibration procedure where the reaction and/or transport parameters are adjusted so that the model predictions match the observed data [*Zheng and Bennett*, 2002]. If present, the depth-averaging error would be hidden by this calibration step. In contrast, the development of a rational method to analyze and quantify the depth-averaging error is preferable to simply accepting that model calibration will mask the depth-averaging error.

[30] The analysis presented here is very general and can be adapted in several ways. While detailed results were presented for the single and multiple Monod kinetic models, the analysis can be performed for any reaction terms. Similarly, the analysis can be applied to reactive transport problems in other coordinate systems such as cylindrical coordinates. If detailed information about the vertical struc-

ture of the plume is available, it is possible to evaluate the integral expressions in equations (14) and (16) and state the depth-averaging error for that particular plume geometry.

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