Supplemental material for Technique note: Simple formulations and solutions of the dual-phase diffusive transport for biogeochemical modeling

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A Analytic solution of equation set (13)

Define $D_1 = \varepsilon_1 D_g + \alpha\theta_1 D_w$ and $D_2 = \alpha\theta_2 D_w$, and use Eq. (3), Eq. (13) is rewritten as

$$D_1 \frac{d^2 C_g}{dz^2} - \alpha Q_1 \theta_1 C_g = 0, \text{ for } 0 \le z \le z_1 \tag{A1-a}$$

$$D_2 \frac{d^2 C_g}{dz^2} + Q_2 = 0, \text{ for } z_1 < z < z_2 \tag{A1-b}$$

$$\left(D_1 \frac{dC_g}{dz}\right)_{z_1^-} = \left(D_2 \frac{dC_g}{dz}\right)_{z_1^+} \tag{A1-c}$$

$$\frac{dC_g}{dz} = 0, \text{ for } z \ge z_2 \tag{A1-d}$$

Because Q_2 is constant, then by integrating (A1-b) with respect to z twice, one finds

$$C_g = b_0 + b_1(z - z_1) - \frac{Q_2}{2D_2}(z - z_1)^2 \tag{A2}$$

Therefore, by applying Eq. (A1-d) at z_2, one obtains

$$b_1 = \frac{Q_2}{D_2}(z_2 - z_1) \tag{A3}$$

To solve Eq. (A1-b), we assume an ansatz

$$C_g = a_1 \exp(-\lambda_1 z) + a_2 \exp(\lambda_1 z) \tag{A4}$$

By substation of Eq. (A4) into Eq. (A1-b), one can show

$$\lambda_1 = \sqrt{\frac{Q_1\theta_1\alpha}{D_1}} \tag{A5}$$

To solve a_1 and a_2, one applies the top boundary condition and Eq. (A1-c), and then obtains

$$a_1 + a_2 = C_a \tag{A6-a}$$

$$\lambda_1 D_1 \left[-a_1 \exp(-\lambda_1 z_1) + a_2 \exp(\lambda_1 z_1)\right] = D_2 b_1 \tag{A6-b}$$

From which, it can be shown

$$a_1 = \frac{C_a \exp(\lambda_1 z_1) - \dfrac{D_2 b_1}{\lambda_1 D_1}}{\exp(-\lambda_1 z_1) + \exp(\lambda_1 z_1)} \tag{A7-a}$$

$$a_2 = \frac{C_a \exp(-\lambda_1 z_1) + \dfrac{D_2 b_1}{\lambda_1 D_1}}{\exp(-\lambda_1 z_1) + \exp(\lambda_1 z_1)} \tag{A7-b}$$

which, when combined with Eq. (A3) and Eq. (A5), can be rewritten as

$$a_1 = \frac{C_a \exp\left(\sqrt{\dfrac{\alpha Q_1\theta_1}{D_1}} z_1\right) - \dfrac{Q_2}{D_1}\sqrt{\dfrac{D_1}{\alpha Q_1\theta_1}}(z_2 - z_1)}{\exp\left(-\sqrt{\dfrac{\alpha Q_1\theta_1}{D_1}} z_1\right) + \exp\left(\sqrt{\dfrac{\alpha Q_1\theta_1}{D_1}} z_1\right)} \tag{A8-a}$$

$$a_2 = \frac{C_a \exp\left(-\sqrt{\dfrac{\alpha Q_1\theta_1}{D_1}} z_1\right) + \dfrac{Q_2}{D_1}\sqrt{\dfrac{D_1}{\alpha Q_1\theta_1}}(z_2 - z_1)}{\exp\left(-\sqrt{\dfrac{\alpha Q_1\theta_1}{D_1}} z_1\right) + \exp\left(\sqrt{\dfrac{\alpha Q_1\theta_1}{D_1}} z_1\right)} \tag{A8-b}$$

Therefore, by substitution of Eq. (A5) and Eq. (A8) into Eq. (A4), one obtains Eq. (14-a) in the text. Further, by applying Eq. (A2) and Eq. (A5), it is easy to show that

$$b_0 = C_g\left(z_1\right) \tag{A9}$$

with which, the solution for the region where $z \geq z_2$ can be found as

$$C_g = C_g\left(z_1\right) + \frac{Q_2}{2D_2}\left(z_2 - z_1\right)^2 \tag{A10}$$

and by merging Eqs. (2), (3) and (9), one obtains the solution for $z_1 < z < z_2$ as

$$C_g = C_g\left(z_1\right) + \frac{Q_2}{D_2}\left(z_2 - z_1\right)\left(z - z_1\right) - \frac{Q_2}{2D_2}\left(z - z_1\right)^2 \tag{A11}$$

Now we obtain the solution as indicated in Eq. (14) in the main text.

Supplemental figures

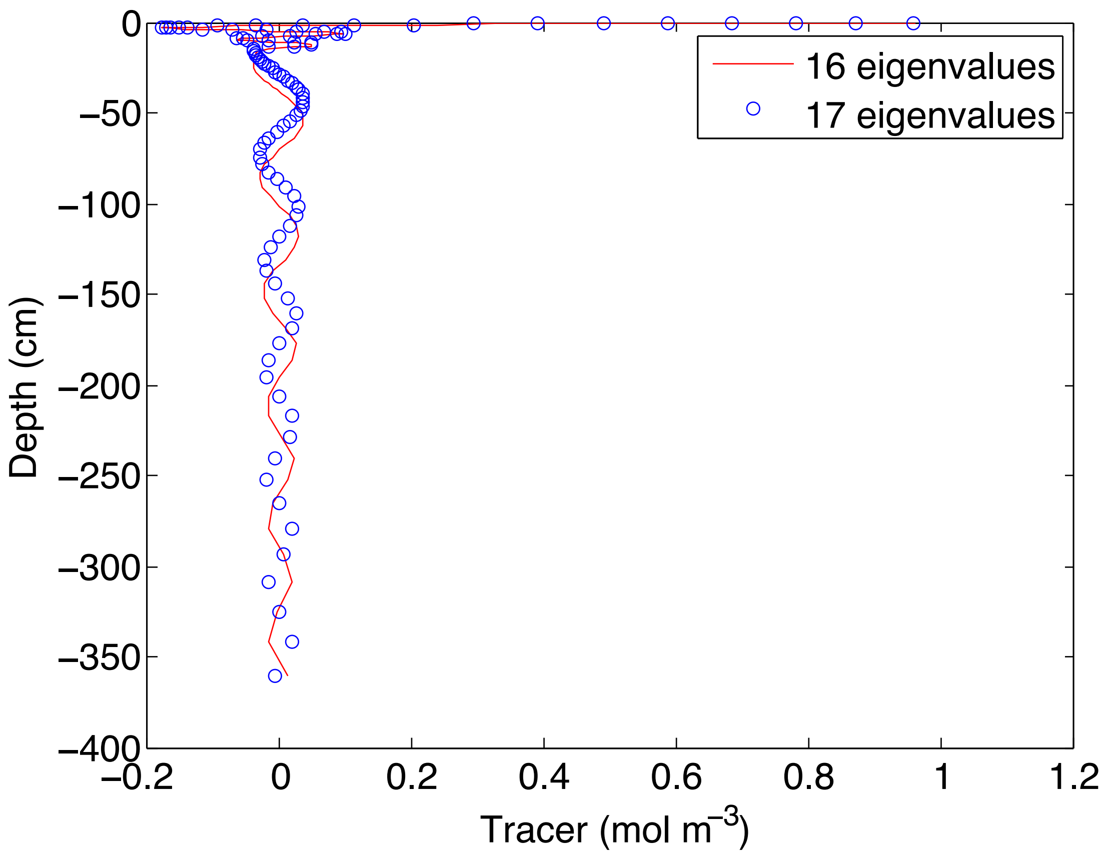

Figure S1. Tracer profiles at time zero obtained by numerical evaluation of the analytic solution Eq. (16). Ideally, the initial tracer profile should be zero everywhere except at the top boundary. Because of the limited numerical precision in MATLAB, the eigenvalues are not exact in the sense of making Eq. (16-c) equal to zero. When this is further combined with the series summation in Eqs. (16-a) and (16-b), the numerical evaluation does not give exact solution as it is supposed to. However, the error diminishes with time to zero as the system approaches the steady state.