ANZIAM Conference 2021
31 January-5 February 2021 (Virtual)

New semi-analytical solutions for advection-diffusion-reaction equations in layered media

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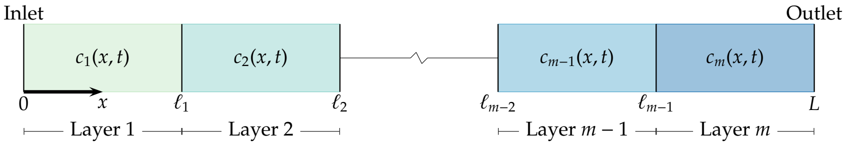


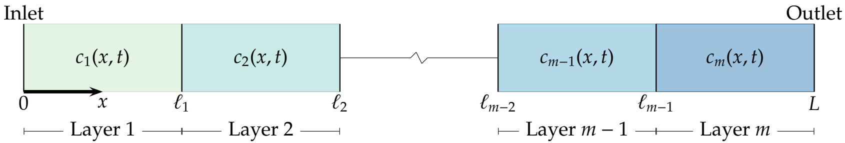
$$R(x)\frac{\partial c}{\partial t} = \frac{\partial}{\partial x}\left(D(x)\frac{\partial c}{\partial x} - v(x)c\right) - \mu(x)c + \gamma(x).$$

$$R(x), D(x), v(x), \mu(x), \gamma(x) = \begin{cases} R_1, D_1, v_1, \mu_1, \gamma_1, & 0 < x < \ell_1, \\ R_2, D_2, v_2, \mu_2, \gamma_2, & \ell_1 < x < \ell_2, \\ \vdots & \vdots \\ R_m, D_m, v_m, \mu_m, \gamma_m, & \ell_{m-1} < x < L. \end{cases}$$

Layered media arise in natural environments such as stratified soils and manufactured environments such as composite landfill liners.

Advection-diffusion-reaction in layered media

Governing equations



- Governing equations (Guerrero et al., 2013; van Genuchten and Alves, 1982):

$$R_i \frac{\partial c_i}{\partial t} = D_i \frac{\partial^2 c_i}{\partial x^2} - v_i \frac{\partial c_i}{\partial x} - \mu_i c_i + \gamma_i, \qquad i = 1, \ldots, m,$$

$$c_i(x,0) = f_i,$$

$$c_i(\ell_i, t) = c_{i+1}(\ell_i, t), \quad \theta_i D_i \frac{\partial c_i}{\partial x}(\ell_i, t) = \theta_{i+1} D_{i+1} \frac{\partial c_{i+1}}{\partial x}(\ell_i, t),$$

where $v_i \theta_i = v_{i+1}\theta_{i+1}$.

- General boundary conditions:

$$a_0 c_1(0,t) - b_0 \frac{\partial c_1}{\partial x}(0,t) = g_0(t), \qquad a_L c_m(L,t) + b_L \frac{\partial c_m}{\partial x}(L,t) = g_L(t).$$

- Classical eigenfunction expansion solution:

$$c_i(x,t) = \sum_{n=1}^{\infty} a_n T_n(t;\lambda_n) X_n(x;\lambda_n).$$

- Eigenvalues (λ_n, $n \in \mathbb{N}^+$) identified by substituting eigenfunctions into the boundary and interface conditions and enforcing a non-trivial solution.

- Yields a nonlinear transcendental equation for the eigenvalues:

$$f(\lambda) = 0,$$

$$\text{where} \quad f(\lambda) := \det(\mathbf{A}(\lambda)), \qquad \mathbf{A} \in \mathbb{R}^{2m\times 2m}.$$

- For many layers (large m) evaluating $f(\lambda)$ is numerically unstable.

- Solutions tend to breakdown for $m > 10$ layers (Carr and Turner, 2016).

- Previous solutions given by Liu et al. (1998) (advection-diffusion only) and Guerrero et al. (2013) (advection-diffusion-decay only) restricted to a moderate number of layers and specific boundary conditions.

- Idea: reformulate the model into m isolated single layer problems (Carr and Turner, 2016; Rodrigo and Worthy, 2016; Zimmerman et al., 2016).

- Introduce unknown functions of time, $g_i(t)$ $(i = 1, \ldots, m-1)$, at the layer interfaces (Carr and Turner, 2016; Rodrigo and Worthy, 2016):

$$g_i(t) := \theta_i D_i \frac{\partial c_i}{\partial x}(\ell_i, t).$$

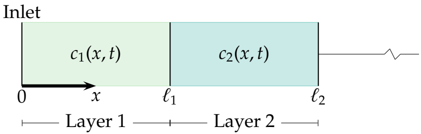
- Yields isolated single layer problems e.g. in the first layer:

$$R_1 \frac{\partial c_1}{\partial t} = D_1 \frac{\partial^2 c_1}{\partial x^2} - v_1 \frac{\partial c_1}{\partial x} - \mu_1 c_1 + \gamma_1,$$

$$c_1(x, 0) = f_1,$$

$$a_0 c_1(0, t) - b_0 \frac{\partial c_1}{\partial x}(0, t) = g_0(t),$$

$$\theta_1 D_1 \frac{\partial c_1}{\partial x}(\ell_1, t) = g_1(t).$$



- Each problem coupled together by imposing continuity of concentration at the interfaces.

Advection-diffusion-reaction in layered media
Analytical solution via Laplace transform

- Solve and express the solution in terms of the unknown interface functions.

- Taking Laplace transforms yields boundary value problems e.g. in the first layer:

$$D_1 \frac{\mathrm{d}^2 C_1}{\mathrm{d}x^2} - v_1 \frac{\mathrm{d}C_1}{\mathrm{d}x} - (\mu_1 + R_1 s) C_1 = -R_1 f_1 - \frac{\gamma_1}{s},$$

$$a_0 C_1(0,s) - b_0 \frac{\mathrm{d}C_1}{\mathrm{d}x}(0,s) = G_0(s),$$

$$\theta_1 D_1 \frac{\mathrm{d}C_1}{\mathrm{d}x}(\ell_1, s) = G_1(s),$$

where $C_i(x,s) = \mathcal{L}\{c_i(x,t)\}$ denotes the Laplace transform of $c_i(x,t)$ with transformation variable $s \in \mathbb{C}$ and $G_i(s) = \mathcal{L}\{g_i(t)\}$ for $i = 1, \ldots, m-1$.

- Laplace transforms of the boundary functions:

$$G_0(s) = \mathcal{L}\{g_0(t)\},$$
$$G_L(s) = \mathcal{L}\{g_L(t)\},$$

are assumed to be able to be found analytically.

Advection-diffusion-reaction in layered media

Analytical solution via Laplace transform

- Boundary value problems: second-order constant-coefficient differential equations.
- Solving using standard techniques in the Laplace domain:

$$\begin{aligned} C_1(x,s) &= A_1(x,s)G_0(s) + B_1(x,s)G_1(s) + P_1(x,s), \\ C_i(x,s) &= A_i(x,s)G_{i-1}(s) + B_i(x,s)G_i(s) + P_i(x,s), \quad i = 2,\ldots,m-1, \\ C_m(x,s) &= A_m(x,s)G_{m-1}(s) + B_m(x,s)G_L(s) + P_m(x,s), \end{aligned}$$

  where the functions P_i, A_i and B_i ($i = 1,\ldots,m$) are known functions.
- To determine $G_1(s),\ldots,G_{m-1}(s)$, the Laplace transformations of the unknown interface functions $g_1(t),\ldots,g_{m-1}(t)$, enforce

$$C_i(\ell_i,s) = C_{i+1}(\ell_i,s), \quad i = 1,\ldots,m-1.$$

- Yields a tridiagonal system of linear equations:

$$\mathbf{A}\mathbf{x} = \mathbf{b},$$

  where $\mathbf{x} = (G_1(s),\ldots,G_{m-1}(s))^T$.
- Summary: Concentration can be evaluated at any x and s in the Laplace domain.

- Inversion of the Laplace transform is carried out numerically.
- Hence, our solution method is *semi*-analytical.
- Trefethen et al. (2006) defines the following numerical approximation:

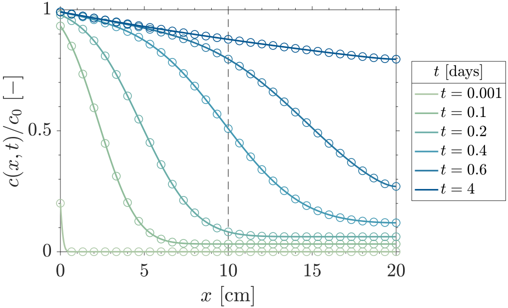
$$c_i(x,t) = \mathcal{L}^{-1}\left\{C_i(x,s)\right\} \approx -\frac{2}{t}\Re\left\{\sum_{k\in O_N} w_k C_i\left(x,s_k\right)\right\},$$

where $s_k = z_k/t$, O_N is the set of positive integers less than N and $w_k, z_k \in \mathbb{C}$ are the residues and poles of the best (N,N) rational approximation to e^z on the negative real line.

- Summary: Concentration can be evaluated at any x and t in the time domain.
- Attractiveness is that the solution is completely explicit. Unlike eigenfunction expansion solutions that require a nonlinear algebraic equation to be solved for the eigenvalues:

$$f(\lambda) = 0,$$

$$\text{where} \quad f(\lambda) := \det(\mathbf{A}(\lambda)), \qquad \mathbf{A} \in \mathbb{R}^{2m\times 2m}.$$

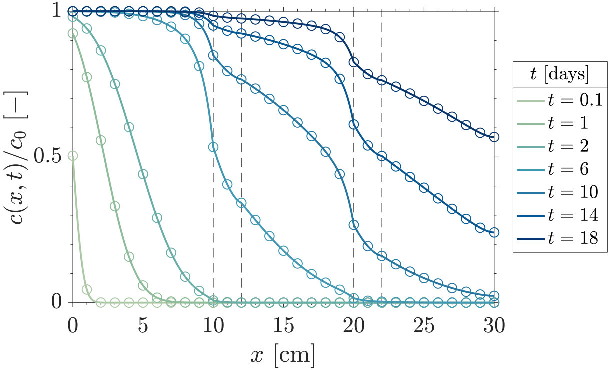


$$\text{BCs}: \qquad v_1 c_1(0,t) - D_1 \frac{\partial c_1}{\partial x}(0,t) = v_1 c_0, \qquad \frac{\partial c_2}{\partial x}(20,t) = 0.$$

Benchmarked against single-layer analytical solutions (van Genuchten and Alves, 1982).

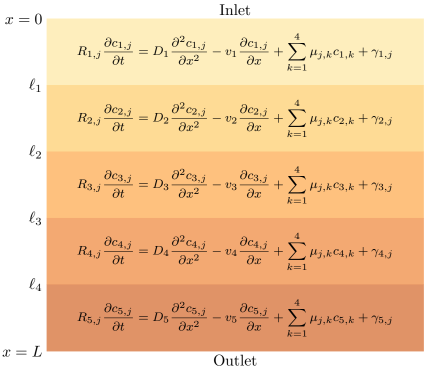
Absolute errors

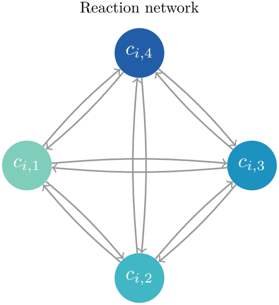
$t = 10^{-3}$	$t = 0.1$	$t = 0.2$	$t = 0.4$	$t = 0.6$	$t = 4$
4.11×10^{-14}	5.53×10^{-10}	8.69×10^{-9}	1.24×10^{-9}	5.84×10^{-8}	6.10×10^{-10}



$$\text{BCs}: \qquad v_1 c_1(0,t) - D_1 \frac{\partial c_1}{\partial x}(0,t) = v_1 c_0, \qquad \frac{\partial c_5}{\partial x}(30,t) = 0.$$

Agrees with solutions tabulated by Liu et al. (1998) and Guerrero et al. (2013)





$$R_i\frac{\partial \mathbf{c}_i}{\partial t} = D_i\frac{\partial^2 \mathbf{c}_i}{\partial x^2} - v_i\frac{\partial \mathbf{c}_i}{\partial x} + \mathbf{M}\mathbf{c}_i + \boldsymbol{\gamma}_i, \qquad \mathbf{c}_i = (c_{i,1},\ldots,c_{i,n})^T.$$

Coupled multispecies equations can be decoupled using the eigenvalue decomposition of **M** (Clement, 2001) yielding **standard decoupled multi-layer problems for each species**.

Single-species problem (arxiv.org/abs/2001.08387) (github.com/elliotcarr/Carr2020a):

Transport in Porous Media (2020) 135:39–58
https://doi.org/10.1007/s11242-020-01468-z

Check for updates

New Semi-Analytical Solutions for Advection–Dispersion Equations in Multilayer Porous Media

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Received: 1 July 2020 / Accepted: 12 August 2020 / Published online: 1 September 2020

Multi-species problem (arxiv.org/abs/2006.15793) (github.com/elliotcarr/Carr2021a):

Applied Mathematical Modelling 94 (2021) 87–97

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Contents lists available at ScienceDirect

Applied Mathematical Modelling

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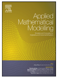

Generalized semi-analytical solution for coupled multispecies advection-dispersion equations in multilayer porous media

Check for updates

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