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Taylor Dispersion

Evolution from the Initial Conditions

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Some Background...

- Taylor dispersion is an old problem; first papers in the 1940s, but made popular by Taylor (1954) and Aris (1956).

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- It is *not* a mathematically simple system! There have been literally thousands of papers on this topic, many devoted to theory.

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Some Background...

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- It is *not* a mathematically simple system! There have been literally thousands of papers on this topic, many devoted to theory.
- There are still several unresolved theoretical *challenges* with Taylor dispersion.

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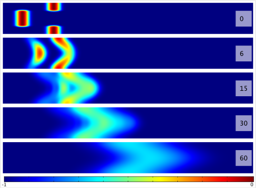
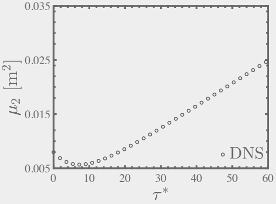
Challenges: Example 1

Example of a *challenge*: Decreasing second moments

For some initial configurations, the second moment can actually decrease in time. Does this imply that one should define a *negative* dispersion coefficient?





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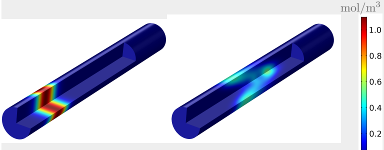
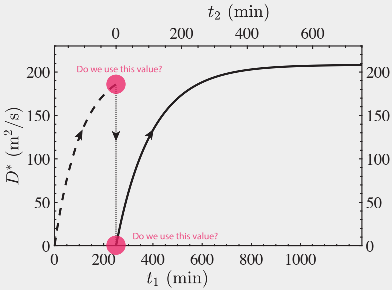
Challenges: Example 2

Example of a *challenge*: The superposition problem.

Any time-dependent process can be broken into intervals. E.g. $t_0 < t < t_{final} \Rightarrow t_0 < t < t_2 \cup t_2 < t < t_{final}$. This requires only that we know the new "initial" condition at t_2. But, what dispersion coefficient do we use for the second time interval?



$t_1 = 0$ min ($t = 0$ min) $t_2 = 0$ min ($t = 250$ min)



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To start: Some *Requirements* for a Well-Structured Dispersion Theory

1. The effective dispersion coefficient should be *positive*.
   - Avoids *inverse heat equations* (Weber, 1981)
   - Avoids incompatibility with macroscale thermodynamics (Miller *et al.*, 2018).

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3. Solutions to the effective convection-dispersion equation should be *superposable* (Taylor, 1959).

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2. The effective dispersion coefficient should be *independent* of the particular initial conditions imposed.
3. Solutions to the effective convection-dispersion equation should be *superposable* (Taylor, 1959).
4. Solutions should approach the classical asymptotic values for the dispersion coefficient.

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Our Approach.

- The details of our analysis are reported in an upcoming JFM paper ("Preasymptotic Taylor dispersion: Evolution from the initial condition")
- The approach is outlined roughly as follows.
  1. Upscaling using volume averaging theory (VAT).

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     - Closures by developing balances for perturbations.
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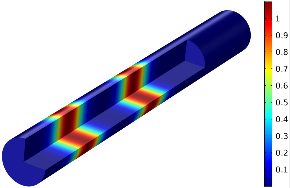
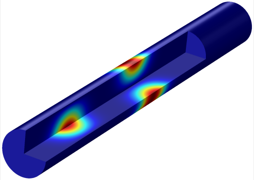
     - Closures by developing balances for perturbations.
     - Integral solutions to closure PDEs
  2. Comparisons with direct numerical solutions (DNS).

Geometry

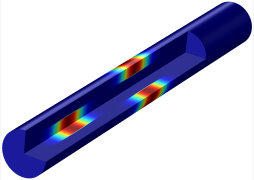
Initial conditions considered (note 1:10 aspect ration change).



Case A



Case B



Case C

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Balance Laws

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Microscale Equations

$$\frac{\partial c_{A\gamma}}{\partial t} = \nabla \cdot (\mathscr{D}_{A\gamma} \nabla c_{A\gamma}) - \nabla \cdot (c_{A\gamma} \mathbf{v}_\gamma), \quad \mathbf{x} \in \mathscr{V}_\gamma^0$$

B.C.1 $\quad -\mathbf{n}_{\gamma\kappa} \cdot (\mathscr{D}_{A\gamma} \nabla c_{A\gamma}) = 0, \quad \mathbf{x} \in \mathscr{A}_{\gamma\kappa}^0$

B.C.2a $\quad c_{A\gamma}(\mathbf{x}, t) \Rightarrow 0, \quad \mathbf{x} \in \mathscr{A}_{\gamma e+}^0, \mathbf{x} \in \mathscr{A}_{\gamma e-}^0$

B.C.2b $\quad -\mathbf{n}_{\gamma e} \cdot (\mathscr{D}_{A\gamma} \nabla c_{A\gamma}) \Rightarrow 0, \quad \mathbf{x} \in \mathscr{A}_{\gamma e+}^0, \mathbf{x} \in \mathscr{A}_{\gamma e-}^0$

I.C.1 $\quad c_{A\gamma}(\mathbf{x}, 0) = \varphi_A(\mathbf{x}), \quad \mathbf{x} \in \mathscr{V}_\gamma^0$

$$\mathbf{v}_\gamma(r) = (0, 0, v_z(r)) = \left(0, 0,\ 2U\left(1 - \frac{r^2}{a^2}\right)\right)$$

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Upscaling

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Upscaling

Average

$$\langle \psi_\gamma \rangle^\gamma \big|_{(\boldsymbol{x},t)} = \int_{\boldsymbol{y} \in \mathscr{V}(\boldsymbol{x})} \psi_\gamma(\boldsymbol{x}+\boldsymbol{y},t) w(\boldsymbol{y}) \, dV(\boldsymbol{y})$$

Spatial Averaging Theorem

$$\langle \nabla \psi \rangle \big|_{\mathbf{x}} = \nabla \, \langle \psi \rangle \big|_{\mathbf{x}} + \int_{\boldsymbol{y} \in A_{\gamma\kappa}(\boldsymbol{x})} \boldsymbol{n}_{\gamma\kappa}(\boldsymbol{x}+\boldsymbol{y}) \psi(\boldsymbol{x}+\boldsymbol{y}) w(\boldsymbol{y}) \, dA(\boldsymbol{y})$$

Decompositons

$$c_{A\gamma}(\boldsymbol{r},t) = \langle c_{A\gamma} \rangle^\gamma \big|_{(\boldsymbol{x},t)} + \tilde{c}_{A\gamma}(\boldsymbol{r},t)$$

$$\boldsymbol{v}_\gamma(\boldsymbol{r}) = (0,0,U) + (0,0,\tilde{v}_z(r)) \quad \Rightarrow \quad \tilde{v}_z(r) = 2U\left(\frac{1}{2} - \frac{r^2}{a^2}\right)$$

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Upscaling

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Upscaled Balance Equation: Unclosed

$$\left.\frac{\partial \langle c_{A\gamma}\rangle^{\gamma}}{\partial t}\right|_{(\mathbf{x},t)} = \nabla \cdot \left(\mathscr{D}_{A\gamma} \nabla \left. \langle c_{A\gamma}\rangle^{\gamma}\right|_{(\mathbf{x},t)} \right) - \mathbf{U} \cdot \left. \langle c_{A\gamma}\rangle^{\gamma}\right|_{(\mathbf{x},t)} \underbrace{- \nabla \cdot \left. \langle \tilde{c}_{A\gamma} \tilde{\mathbf{v}}_{\gamma}\rangle^{\gamma}\right|_{(\mathbf{x},t)}}_{\textit{unclosed}}$$

B.C. 1a $\left. \langle c_{A\gamma}\rangle^{\gamma}\right|_{(\mathbf{x},t)} = 0, \quad \mathbf{x} \in \mathscr{A}^{0}_{\gamma e+}, \ \mathbf{x} \in \mathscr{A}^{0}_{\gamma e-}$

B.C. 1b $-\mathbf{n}_{\gamma\kappa} \cdot \left(\mathscr{D}_{A\gamma} \nabla \left. \langle c_{A\gamma}\rangle^{\gamma}\right|_{(\mathbf{x},t)} \right) = 0, \quad \mathbf{x} \in \mathscr{A}^{0}_{\gamma e+}, \ \mathbf{x} \in \mathscr{A}^{0}_{\gamma e-}$

I.C.1 $\left. \langle c_{A\gamma}\rangle^{\gamma}\right|_{(\mathbf{x},0)} = \left. \langle \varphi_{A}\rangle^{\gamma}\right|_{\mathbf{x}}, \quad \mathbf{x} \in \mathscr{V}^{0}_{\gamma}$

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Upscaling

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Closure

To complete the upscaling of the problem, one needs to develop a way of expressing $\tilde{c}_{A\gamma}$ in terms of the averaged concentration. This is known as *closure*.

Process:

- A balance (a PDE) for the unclosed quantity is developed.

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- This solution is substituted into the averaged balance equation to eliminate $\tilde{c}_{A\gamma}$.

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- A balance (a PDE) for the unclosed quantity is developed.
- A solution to the problem is developed.
- This solution is substituted into the averaged balance equation to eliminate $\tilde{c}_{A\gamma}$.
- *Effective* macroscale properties often arise in this process.

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Closure: Simplified Problem (Cylindrical Coordinates)

$$\frac{\partial \tilde{c}_{A\gamma}}{\partial t} = \frac{1}{r}\frac{\partial}{\partial r}\left(r\mathscr{D}_{A\gamma}\frac{\partial \tilde{c}_{A\gamma}}{\partial r}\right) + \mathscr{D}_{A\gamma}\frac{\partial^2 \tilde{c}_{A\gamma}}{\partial z^2} - U\frac{\partial \tilde{c}_{A\gamma}}{\partial z} - \tilde{v}_z\frac{\partial \tilde{c}_{A\gamma}}{\partial z} - \underbrace{\tilde{v}_z \left.\frac{\partial \langle c_{A\gamma}\rangle^\gamma}{\partial z}\right|_{(r,z,t)}}_{\text{source}}$$

B.C.1 $$-\mathscr{D}_{A\gamma}\left.\frac{\partial \tilde{c}_{A\gamma}}{\partial r}\right|_{(r,z)} = 0$$

B.C.2b $$\tilde{c}_{A\gamma}(r,z) = 0$$

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Closure: Integral Solutions via Green's Functions

After some simplification (primarily a separation of length scales such that $a \ll L_0$, where L_0 is the length of the IC)

$$\tilde{c}_{A\gamma}(r,z,t) = b_A(r,t)\frac{\partial \langle c_{A\gamma}\rangle^{\gamma}}{\partial z} + \Phi_{A\gamma}(r,z,t)$$

$b_{A\gamma}$ and $\Phi_{A\gamma}$ are known as *closure variables*. These functions are defined by

$$b_A(r,t) = -\int_{\tau=0}^{\tau=t}\int_{\zeta=-\infty}^{\zeta=\infty}\int_{\rho=0}^{\rho=a} G_A(r,\rho,z,\zeta,t-\tau)\tilde{v}_z(\rho)\rho d\rho d\zeta d\tau$$

$$\Phi_{A\gamma}(r,z,t) = \int_{\zeta=-\infty}^{\zeta=\infty}\int_{\rho=0}^{\rho=a} G_A(r,\rho,z,\zeta,t-\tau)\tilde{\varphi}_A(\rho,\zeta)\rho d\rho d\zeta$$

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Closed Macroscale Balance

$$\underbrace{\left.\frac{\partial\langle c_{A\gamma}\rangle^{\gamma}}{\partial t}\right|_{(z,t)}}_{\text{accumulation}} = \underbrace{D^{*}_{A\gamma}(t)\left.\frac{\partial^{2}\langle c_{A\gamma}\rangle^{\gamma}}{\partial z^{2}}\right|_{(z,t)}}_{\text{diffusive transport}} - \underbrace{U\left.\frac{\partial\langle c_{A\gamma}\rangle^{\gamma}}{\partial z}\right|_{(z,t)}}_{\text{convective transport}} - \underbrace{s^{*}_{A\gamma}(z,t)}_{\text{non-conventional source}}$$

+B.C.'s and I.C.

Effective Parameters:

$$s^{*}_{A\gamma}(z,t) = \left\langle \tilde{v}_z \frac{\partial \Phi_A}{\partial z} \right\rangle^{\gamma}$$

$$D^{*}_{A\gamma}(t) = \mathscr{D}_{A\gamma} - \langle \tilde{v}_z b_A \rangle^{\gamma}$$

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Closure Solutions

Closure: Solutions– Straightforward but tedious

- The problem now is to determine the functions $s^*_{A\gamma}(z,t)$ and $D^*_{A\gamma}(t)$

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- This really means finding the fields b_A and Φ_A.

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Closure: Solutions– Straightforward but tedious

- The problem now is to determine the functions $s^*_{A\gamma}(z,t)$ and $D^*_{A\gamma}(t)$
- This really means finding the fields b_A and Φ_A.
- This can be done by substituting

$$\tilde{c}_{A\gamma}(r,z,t) = b_A(r,t)\frac{\partial \langle c_{A\gamma}\rangle^\gamma}{\partial z} + \Phi_{A\gamma}(r,z,t)$$

back into the balance for the deviations.

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Closure Solutions

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back into the balance for the deviations.

- The result is a set of two linear PDEs.

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Solutions for b_A and D_A^*

Recall:

$$D^*_{A\gamma}(t) = \mathscr{D}_{A\gamma} - \langle \tilde{v}_z b_A \rangle^\gamma$$

$$\frac{D^*_{A\gamma}(t)}{\mathscr{D}_{A\gamma}} = \left(1 + \frac{1}{48}\frac{U^2 a^2}{\mathscr{D}^2_{A\gamma}}\right)\mathscr{H}(t) - 4\frac{U^2 a^2}{\mathscr{D}^2_{A\gamma}}\sum_{n=1}^{\infty}\left(\frac{J_3(\lambda_n)}{\lambda_n^2 J_0(\lambda_n)}\right)^2 \exp\left(-\lambda_n^2 \frac{\mathscr{D}_{A\gamma}}{a^2} t\right)$$

$$J_1(\lambda_n) = 0, \; n = 1, 2, 3, ..$$

Does not depend upon initial condition!

$$D^*_{A\gamma}(t \to \infty) = \mathscr{D}_{A\gamma} + \frac{U^2 a^2}{48\mathscr{D}_A}$$

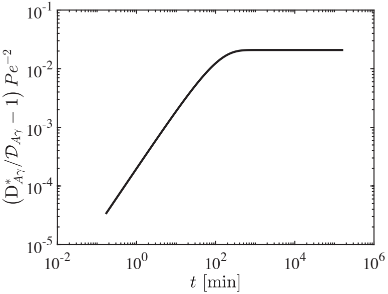

Figure: Analytical solution for dispersion tensor.

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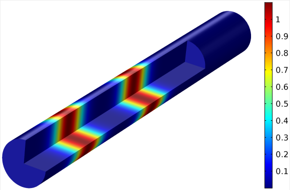
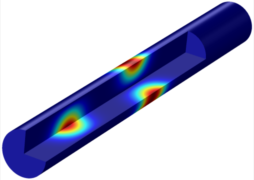
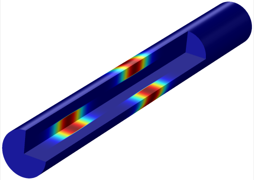
Solutions for Φ_A and s_A^*: Initial conditions



Case A



Case B



Case C

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Closure Solutions

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Solutions for Φ_A and s_A^*: Initial condition C

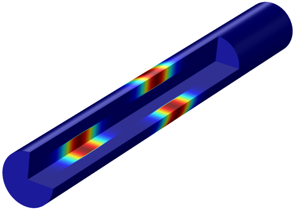
$$\varphi_A(r,z) = c_0 R_1(r) Z_1(z) + c_0 R_2(r) Z_2(z)$$

$$Z_1(z) = \alpha_1 \exp\left(-\frac{(z-\beta_1)^2}{\sigma_1^2}\right)$$

$$Z_2(z) = \alpha_2 \exp\left(-\frac{(z-\beta_2)^2}{\sigma_2^2}\right)$$

$$R_1(r) = \begin{cases} 1, & 0 \le r \le \frac{a}{2} \\ 0, & \frac{a}{2} < r \le a \end{cases}$$

$$R_2(r) = \begin{cases} 0, & 0 \le r \le \frac{a}{2} \\ 1, & \frac{a}{2} < r \le a \end{cases}$$



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Solutions for Φ_A and s_A^*: Initial condition C

Recall: $s^*_{A\gamma}(z,t) = \left\langle \tilde{v}_z \frac{\partial \Phi_A}{\partial z} \right\rangle^\gamma$

$$s_A^*(z,t) = -4c_0 U \left[\frac{\sigma_1 \alpha_1 (z - \Xi_1(t) - \beta_1)}{(\sigma_1^2 + 4\mathscr{D}_A t)^{\frac{3}{2}}} \exp\left(-\frac{(z - \Xi_1(t) - \beta_1)^2}{\sigma_1^2 + 4\mathscr{D}_A t} \right) \right.$$
$$\left. - \frac{\sigma_2 \alpha_2 (z - \Xi_2(t) - \beta_2)}{(\sigma_2^2 + 4\mathscr{D}_A t)^{\frac{3}{2}}} \exp\left(-\frac{(z - \Xi_2(t) - \beta_2)^2}{\sigma_2^2 + 4\mathscr{D}_A t} \right) \right]$$
$$\times \sum_{n=1}^{\infty} \frac{J_1(\lambda_n/2) J_3(\lambda_n)}{\lambda_n^2 J_0^2(\lambda_n)} \exp\left(-\frac{\lambda_n^2 \mathscr{D}_A}{a^2} t \right)$$

$$\Xi_1(t) = \begin{cases} \frac{7}{4} U t - \frac{1}{2} U \frac{t^{\frac{3}{2}}}{\sqrt{t_d^*}}, & \text{for } t < t_d^*, \\ \Xi_1(t_d^*) + U(t - t_d^*), & \text{for } t \geq t_d^* \end{cases} \quad \left(t_d^* = \frac{a^2}{4\mathscr{D}_{A\gamma}} \right)$$

$$\Xi_2(t) = \begin{cases} \frac{3}{4} U t + \frac{1}{6} U \frac{t^{\frac{3}{2}}}{\sqrt{t_d^*}}, & \text{for } t < t_d^* \\ \Xi_2(t_d^*) + U(t - t_d^*), & \text{for } t \geq t_d^* \end{cases}$$

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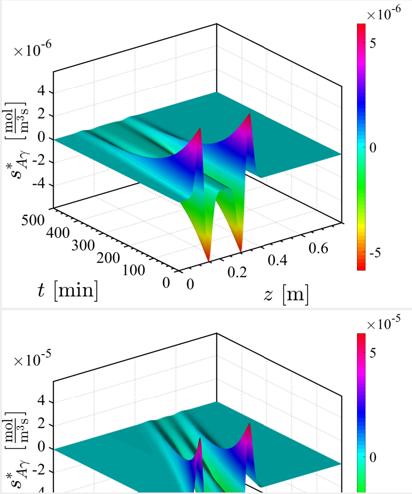
Solutions for s_A^*: Initial condition C



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Applications 1: Strictly positive dispersion coefficient

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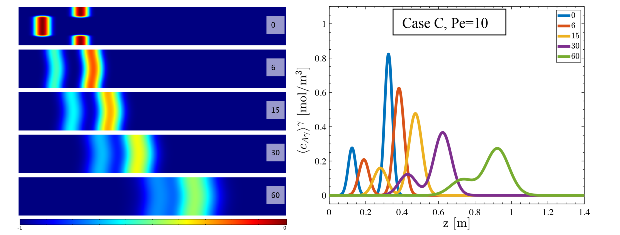
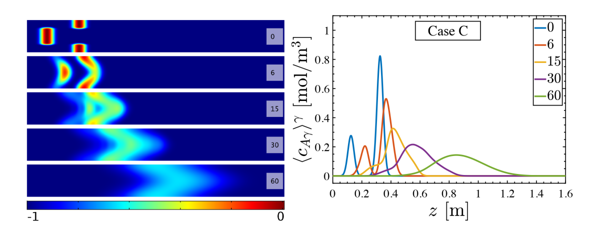
Microscale Solutions from DNS: Initial condition C





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Applications 1: Strictly positive dispersion coefficient

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Comparison: DNS versus Upscaled Averaged Concentrations

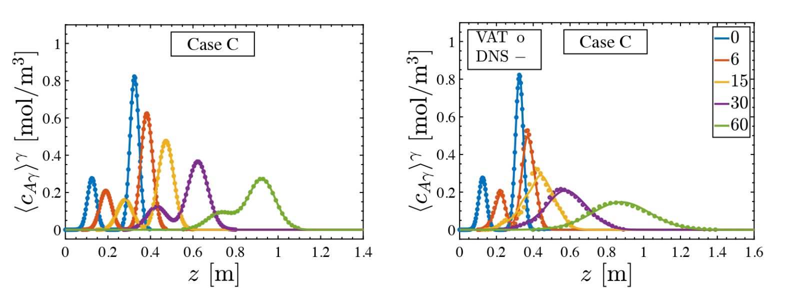

Figure: $Pe = 10$ (left) and $Pe = 100$ (right). Errors are $\leq 7\%$ for worst case ($Pe = 100$).

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Applications 1: Strictly positive dispersion coefficient

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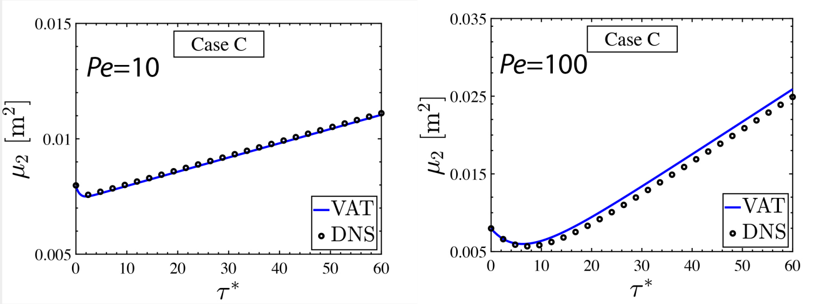
Comparison: Second Centered Moment



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Applications 2: Superposition

A Two Step Problem (Superposition)

[Regarding the] Eulerian diffusion equation in which the diffusion coeffcient varied with the time since the diffusing material had been concentrated. It seems to me that this is an illogical conception. The one thing that seems to be agreed, whatever theory one may have about diffusion, is that diffusing distributions are superposable. If therefore you attempt to analyse the distribution of concentration from two sources which started at different times by this method, it would be necessary to assume, in places where the distributions overlapped, that the diffusion constant had two different values at the same time and at the same point in space.

–Taylor (1959)

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Applications 2: Superposition

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A Two Step Problem (Superposition)

$$S_1: \quad 0 < t_1 < t_M$$
$$S_2: \quad 0 < t_2 < t_F - t_M$$

Problem 1: $0 < t_1 < 250$ min

$$\frac{\partial \langle c_{A\gamma} \rangle^\gamma}{\partial t} = D^*_{A\gamma}(t) \frac{\partial^2 \langle c_{A\gamma} \rangle^\gamma}{\partial z^2} - U \frac{\partial \langle c_{A\gamma} \rangle^\gamma}{\partial z} - s^*_{A\gamma}$$

I.C.1 $\langle c_{A\gamma} \rangle^\gamma |_{(z,0)} = c_0 Z_1(z)$

Problem 2: $0 < t_2 < 750$ min

$$\frac{\partial \langle c_{A\gamma} \rangle^\gamma}{\partial t} = D^*_{A\gamma}(t) \frac{\partial^2 \langle c_{A\gamma} \rangle^\gamma}{\partial z^2} - U \frac{\partial \langle c_{A\gamma} \rangle^\gamma}{\partial z} - s^*_{A\gamma}$$

I.C.1 $\langle c_{A\gamma} \rangle^\gamma |_{(z,0)} = S_1(z, 250)$

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Applications 2: Superposition

A Two Step Problem (Superposition)- Initial Conditions

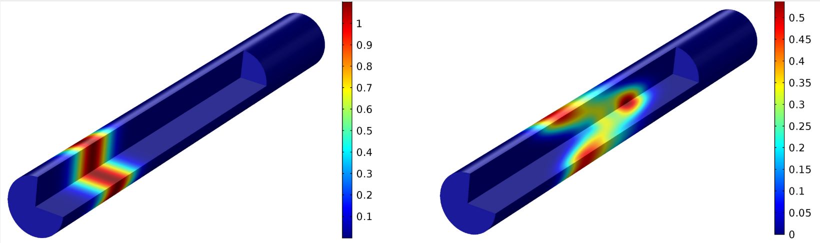

Figure: Initial conditions. First step (left). Second step ($t_2 = 0,\ t = 250$), Right.

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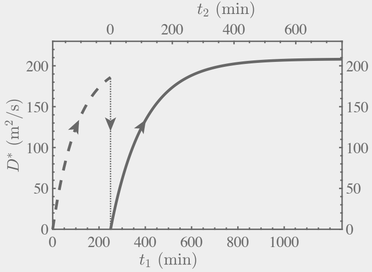
Applications 2: Superposition

A Two Step Problem (Superposition)- $D_A^*(t)$ and $s_A^*(z,t)$ Fields



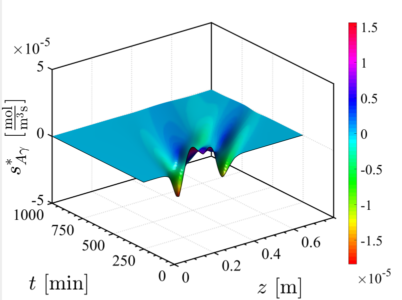


Figure: Two step fields. $D_A^*(t)$ (left). $s_A^*(z,t)$ (right).

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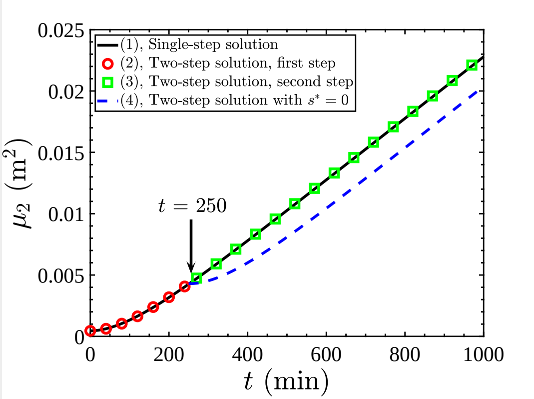
Applications 2: Superposition

A Two Step Problem (Superposition)- Second Moment



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Conclusions

- We presented a new method for handling Taylor dispersion near the early time relaxation.

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  1. *Positive*.
  2. *Independent* of initial conditions.
  3. *Superposable*.
  4. Gives classical asymptotic values.

Conclusions

- We presented a new method for handling Taylor dispersion near the early time relaxation.
- Our approach directly addressed the four desirable properties for a dispersion theory
  1. *Positive*.
  2. *Independent* of initial conditions.
  3. *Superposable*.
  4. Gives classical asymptotic values.
- There was good correspondence between DNS and the 1-dimensional effective theory.

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Questions?

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References

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Error Analysis

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Estimate of Errors: Closure Error

$$\mathbf{O}\left(\mathscr{D}_{A\gamma}\boldsymbol{\nabla}\tilde{c}_{A\gamma} - \boldsymbol{U}\tilde{c}_{A\gamma} - \tilde{\boldsymbol{v}}_{\gamma}\langle c_{A\gamma}\rangle^{\gamma}\right) \gg \mathbf{O}\left(-\tilde{\boldsymbol{v}}_{\gamma}\tilde{c}_{A\gamma} + \langle\tilde{\boldsymbol{v}}_{\gamma}\tilde{c}_{A\gamma}\rangle^{\gamma}\right)$$

$$\epsilon_1(z,t) = \left(\frac{\left\langle\left|\tilde{v}_z\tilde{c}_{A\gamma} - \left\langle\tilde{v}_z\tilde{c}_{A\gamma}\right\rangle^{\gamma}\right|\right\rangle^{\gamma}}{\left\langle\left|U\tilde{c}_{A\gamma}\right| + \left|\mathscr{D}_{A\gamma}\frac{\partial\tilde{c}_{A\gamma}}{\partial z}\right| + \left|\mathscr{D}_{A\gamma}\frac{\partial\tilde{c}_{A\gamma}}{\partial r}\right| + \left|\tilde{v}_z\langle c_{A\gamma}\rangle^{\gamma}\right|\right\rangle^{\gamma} + \epsilon_0} \times 100\right)$$

$$\epsilon_{\text{closure}}(t) = \frac{1}{A_\epsilon(t)}\int_{z=0}^{z=L}\frac{1}{2}\epsilon_1^2(z,t)dz$$

$$A_\epsilon(t) = \int_{z=0}^{z=L}\epsilon_1(z,t)dz$$

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Error Analysis

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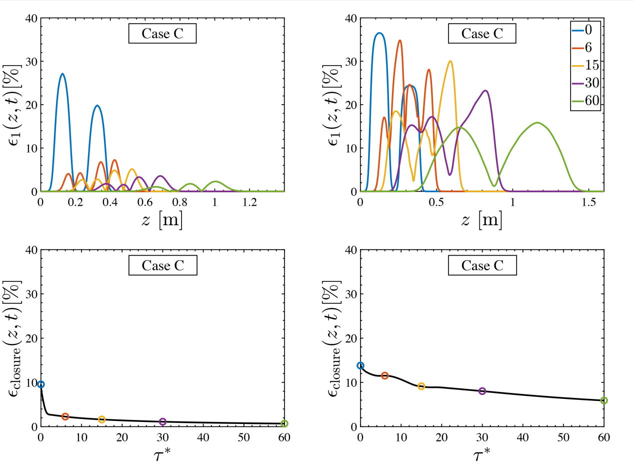
Estimate of Errors: Closure Errors



Error Analysis

Estimate of Errors: Observed Model Error

$$\epsilon_{\mathrm{model}}(t) = \max_{z} \left(\frac{\left| \langle c_{A\gamma} \rangle^{\gamma}_{\mathrm{DNS}} - \langle c_{A\gamma} \rangle^{\gamma}_{\mathrm{VAT}} \right|}{\max_{z} \left(\langle c_{A\gamma} \rangle^{\gamma}_{\mathrm{DNS}} \right)} \times 100 \right)$$

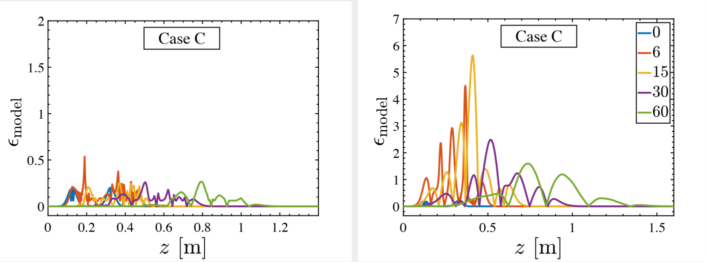


Figure: Observed model error. $Pe = 10$ (left). $Pe = 100$ (right).

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Applications

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Comparison: Skewness at Long Times (DNS)