Comment on "Taylor Dispersion with Absorbing Boundaries: A Stochastic Approach"

Recently, Biswas and Sen analyzed the Taylor-Aris dispersion of point-sized solutes entrained in a Poiseuille flow between two reactive plates, where the solute is depleted via a first-order reaction on the plates [1]. They argue that classical Taylor-Aris dispersion methods fail to properly describe the long-time transport process, and claim to present, for the first time, the correct stochastic description.

Generalized Taylor-Aris dispersion theory [2] has long since been properly modified to describe reactive transport processes [3,4]. Not only have the specific problems of reactive flow in a tube [3] and between a reactive and an inert plate [4] been examined, but the general approach has also been extended to arbitrary continuous systems with first-order surface and bulk reactions [3,4], time-periodic systems [5], spatially periodic systems [6] and mixtures of reacting species [7]. The extant theoretical framework [2–7] extends far beyond the simple problem considered in Ref. [1] and leads to nontrivial concepts, such as the fictitious initial condition, that are not addressed by Biswas and Sen.

In the generic continuous Taylor-Aris dispersion paradigm [2], the physical space is decomposed into an unbounded global space $\mathbf{Q}$, where the transport properties are independent of position in $\mathbf{Q}$-space, and a bounded local-space $\mathbf{q}$, where these properties may depend functionally on position in $\mathbf{q}$-space. For example, the problem of reactive plates located at $y = \pm h$ furnishes $\mathbf{Q} = x$ and $\mathbf{q} = y$.

The reactive probability density $P_r(\mathbf{Q}, \mathbf{q}, t|\mathbf{q}')$ of locating a reactive particle at position $(\mathbf{Q}, \mathbf{q})$ at time t, given its introduction at $(\mathbf{0}, \mathbf{q}')$ at time $t = 0$, can be mapped to the nonreactive probability density $P(\mathbf{Q}, \mathbf{q}, t|\mathbf{q}')$ via [4]

$$P(\mathbf{Q}, \mathbf{q}, t|\mathbf{q}') \equiv \frac{\exp(\bar{K}t)}{A(\mathbf{q})} P_r(\mathbf{Q}, \mathbf{q}, t|\mathbf{q}'). \qquad (1)$$

To apply the moment matching scheme for P, it is necessary that $\int P d\mathbf{Q} d\mathbf{q} = 1$. Substituting Eq. (1) into the governing convection-diffusion-reaction equation and (possibly reactive) boundary conditions governing P_r, and then imposing the latter normalization condition, leads to a self-adjoint eigenvalue problem for $\bar{K}$ and $A(\mathbf{q})$ [4]. The eigenvalue $\bar{K}$ with the smallest real part is the net reaction rate $\bar{K}^*$, and its corresponding $\mathbf{q}$-space eigenfunction $A(\mathbf{q})$ is the normalizing function required for Eq. (1) and subsequent calculations of the mean velocity vector $\mathbf{U}^*$ and dispersivity dyadic $\mathbf{D}^*$ [4]. Upon making this transformation, the standard Taylor-Aris moment matching scheme can be applied to P and then mapped back to the reactive probability density P_r, ultimately resulting in a macrotransport equation

$$\frac{\partial \bar{P}_r}{\partial t} + \bar{\mathbf{U}}^* \cdot \nabla \bar{P}_r - \bar{\mathbf{D}}^* : \nabla \nabla \bar{P}_r + \bar{K}^* \bar{P}_r = A(\mathbf{q}') \delta(\mathbf{Q}) \delta(t) \qquad (2)$$

for the long-time, local-space averaged probability density $\bar{P}_r(\mathbf{Q}, t|\mathbf{q}')$ governing a solute introduced at local position $\mathbf{q}'$. This represents a complete asymptotic description of the problem [3], the higher-order moments not being needed for long times, in agreement with [1]. It is crucial to note that the effective description (2) requires a $\mathbf{q}'$-dependent "fictitious" initial condition, a point which was not addressed in [1]. In simple cases like flow in a surface-reactive tube [3], the nonintuititve behavior noted in [1] is observed.

In conclusion, the correct stochastic description is not only known, but has been widely applied and extended [2–7]. This problem has also been addressed by a number of other coarse-graining methods [8].

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