

Realizable entropic lattice Boltzmann method for high-Péclet scalar transport

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We present a realizable entropic lattice Boltzmann method (RELBM) for scalar transport at high Péclet (Pe) number. The method combines an ADE-tailored entropic relaxation with a nonorthogonality correction to ghost-mode damping and a strictly conservative population-space realizability limiter activated only when required to enforce positivity. Comprehensive benchmarks including deformational mixing, Graetz transport, and Taylor dispersion up to $Pe = 2 \times 10^5$, demonstrating suppression of spurious oscillations and quantitative agreement with theory. Furthermore, pore-scale simulations in a homogeneous geometry up to $Pe = 10^4$ resolve scalar-dissipation dynamics consistent with intermediate lamellar and late-time Fickian scalings. These results establish the method's robustness and physical fidelity for multiscale advection-diffusion dynamics across diverse systems.

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Scalar transport underpins a wide range of natural and engineered systems, including atmospheric aerosols [1], oceanic salinity [2], porous media mixing [3,4], turbulent mixing [5,6], electrochemical storage [7], and thermal convection [8]. High Péclet numbers are commonly encountered in these processes, making it essential to understand scalar transport behavior in the advection-dominated regime.

In the high-Péclet number regime, scalar transport becomes a singularly perturbed problem: the scalar field is continuously stretched and folded into thin filaments, while diffusion regularizes sharp gradients only over vanishingly small length scales [9]. Accurately capturing the resulting filamentary dynamics and associated transport scalings therefore requires numerical schemes with low and well-controlled artificial dissipation [10]. However, pushing dissipation too low introduces a fundamental risk: without sufficient damping, numerical solutions can easily violate physical constraints, leading to negative concentrations or instabilities particularly near sharp gradients [11,12]. This creates a critical need for a transport framework that can reconcile these opposing requirements: it must possess the fidelity to accurately capture the multiscale transport dynamics, yet simultaneously enforce strict conservation and positivity to ensure physical realism across all regimes [12–14].

The lattice Boltzmann method (LBM) provides an appealing kinetic description of transport, inherently guaranteeing strict conservation and locality [15,16]. Among its variants, entropic LBM (ELBM) leverages a convex H functional to enforce a discrete H theorem [17]. While this parameter-free stabilization has proven robust in turbulence [18,19], supersonic flow [20], multiphase flow [21,22], and conjugate heat transfer [23], extending it to the advection-diffusion equation is nontrivial: although the convex H functional is simply the negative of a kinetic entropy and thus a Lyapunov functional, its entropic relaxation must be aligned with the advection-diffusion closure to strictly control scalar relaxation. Existing stabilized advection-diffusion equation lattice Boltzmann (ADE-LBM) strategies all act, in one form or another, on the higher-order nonequilibrium sector of the populations. Multiple-relaxation-time (MRT) and two-relaxation-time (TRT) formulations prescribe the relaxation rates for the corresponding moments *a priori* [24–26], so the damping is fixed once the model parameters are chosen. Regularized schemes instead reconstruct or modify the nonequilibrium contribution before collision, typically from lower-order or macroscopic information [27]. In RELBM, the higher-order nonequilibrium sector is represented by the ghost component and is relaxed collectively through a local entropy condition written for the ADE, so the damping is determined adaptively at each lattice site. Positivity is enforced, when required, by conservatively rescaling that same collision increment [12,28]. Concretely, RELBM constructs an ADE-specific collision increment in which the higher-order nonequilibrium sector is damped through a locally determined entropic parameter, and then rescales that same increment only when needed to keep all populations realizable. The

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update therefore preserves the transported scalar, restores positivity, and confines additional dissipation to locations where realizability would otherwise fail.

We formulate a realizable entropic collision model for scalar lattice Boltzmann transport in terms of populations $\{g_i\}$ associated with lattice velocities $\{c_i\}$ and weights $\{W_i\}$. The transported scalar is defined as $C = \sum_i g_i$, while the advective flux satisfies $\sum_i c_i g_i^{\text{eq}} = C\mathbf{u}$. Stability is enforced through Boltzmann's H theorem by introducing the strictly convex entropy functional

$$H[g] = \sum_i g_i \ln\left(\frac{g_i}{W_i}\right). \quad (1)$$

The collision acts on the nonequilibrium deviations $g_i^{\text{neq}} = g_i - g_i^{\text{eq}}$. To separate physical transport from purely kinetic artifacts, we decompose g_i^{neq} into a flux-carrying component Δs_i and a higher-order kinetic remainder Δh_i (ghost modes) by projecting onto the first-order moment subspace spanned by c_i :

$$\Delta s_i = \frac{W_i}{c_s^2} \left(c_i \cdot \sum_j c_j g_j^{\text{neq}} \right), \quad \Delta h_i = g_i^{\text{neq}} - \Delta s_i, \quad (2)$$

with lattice sound speed c_s . By construction,

$$\begin{aligned} \sum_i \Delta s_i &= \sum_i \Delta h_i = 0, \quad \sum_i c_i \Delta h_i = \mathbf{0}, \\ \sum_i c_i \Delta s_i &= \sum_i c_i g_i^{\text{neq}} \equiv \mathbf{j}. \end{aligned} \quad (3)$$

Thus, Δs_i recovers the macroscopic diffusive flux $\mathbf{j}$ while Δh_i contains the higher-order nonequilibrium contribution, i.e., the ghost sector. The collision operator then relaxes these two contributions at distinct rates,

$$\Omega_i = -\beta(2\Delta s_i + \gamma\Delta h_i). \quad (4)$$

The parameter β is determined from the target diffusivity $D = c_s^2(\tau - \frac{1}{2})\Delta t$ through $\beta = (2\tau)^{-1}$. The ghost-mode relaxation parameter γ is determined locally from a discrete entropy condition associated with (1). Introducing the entropic scalar product

$$\langle x|y \rangle_H = \sum_i \frac{x_i y_i}{g_i^{\text{eq}}}, \quad (5)$$

the entropic stabilizer admits the explicit closed form [29]

$$\gamma_{\text{std}} = \frac{1}{\beta} - \left(2 - \frac{1}{\beta}\right) \frac{\langle \Delta h | \Delta s \rangle_H}{\langle \Delta h | \Delta h \rangle_H}. \quad (6)$$

For the advection-diffusion equation, the nonorthogonality of equilibrium moments requires an additional correction to the standard expression. Enforcing the resulting discrete entropy condition yields [30]

$$\gamma = \gamma_{\text{std}} + \frac{C}{\beta \langle \Delta h | \Delta h \rangle_H}, \quad C = \sum_i \Delta h_i \ln\left(\frac{g_i^{\text{eq}}}{W_i}\right). \quad (7)$$

For scalar transport on the two-dimensional nine-velocity (D2Q9) lattice, the ADE equilibrium is not orthogonal to the ghost subspace. The term C in Eq. (7) accounts for that projection, so the ghost-sector damping parameter follows

from an ADE-specific local entropy condition and is not prescribed *a priori*. This construction selectively damps high-wavenumber kinetic instabilities through Δh_i while leaving the transport physics encoded in Δs_i unchanged. Additional lattice-structure details, including the D2Q9/D2Q5 comparison [31], are given in the Supplemental Material [30].

Entropic stabilization alone does not strictly preclude negative populations near shocklike fronts. We therefore augment the collision step with a hard realizability constraint by under-relaxing along the collision increment,

$$g_i^{\text{new}} = g_i + \alpha \Omega_i, \quad \alpha \in [0, 1], \quad (8)$$

where the step length is chosen as the maximal realizable value ensuring $g_i^{\text{new}} \geq \epsilon$ for all i ,

$$\alpha = \min\left(1, \min_{i:\Omega_i < 0} \frac{g_i - \epsilon}{-\Omega_i}\right), \quad (9)$$

with $\epsilon > 0$ a small safety threshold. Since $\sum_i \Omega_i = 0$, scaling by α preserves the zeroth moment and exactly conserves C . Moreover, by convexity of H , any under-relaxed update $g + \alpha\Omega$ with $\alpha \in [0, 1]$ is H -nonincreasing, i.e. $H(g + \alpha\Omega) \leq H(g)$, so realizability control is compatible with entropic stability. Accordingly, the realizability correction is inactive in smooth regions ($\alpha = 1$) and intervenes only when the entropic update would otherwise drive some populations negative. The added diffusion is therefore localized to the small subset of cells and times where realizability is at risk.

To rigorously evaluate the scheme's robustness in the limit of vanishing diffusivity, we simulate the time-reversing deformational flow with period T [32] on a grid of $N = 256 \times 256$. The velocity amplitude $u_0 = 0.01$ and molecular diffusivity $D = 10^{-5}$ correspond to a grid Péclet number $\text{Pe}_g = u_0 \Delta x / D = 1000$ (global $\text{Pe} = 2.56 \times 10^5$). In this under-resolved regime, where numerical stability is notoriously difficult to maintain, the unconstrained entropic formulation successfully maintains convergence, as shown in Fig. 1(a) (left). However, this stability comes at the cost of physical consistency: conspicuous Gibbs oscillations ripple outward from the sharp filaments, driving the minimum concentration to unphysical negative values ($C_{\min} \approx -0.03$), as quantified in Fig. 1(b). In contrast, the RELBM [Fig. 1(a), right] completely suppresses these artifacts, strictly enforcing positivity ($C \geq 0$) throughout the evolution [12].

The mechanism underlying this correction is further illuminated by the effective diffusivity diagnostic $\Delta_D = D_{\text{eff}}/D - 1$ shown in Fig. 1(c), where D_{eff} is the instantaneous effective diffusivity derived from the scalar variance decay rate [33]. It is revealing that even the unconstrained entropic scheme generates a peak effective diffusivity of $D_{\text{eff}} \approx 1.51D$ ($\Delta_D \approx 0.5$). This shows that the entropic stabilizer already contributes a modest amount of adaptive numerical dissipation in this under-resolved benchmark [18]. This baseline dissipation helps maintain stable evolution, but it does not by itself guarantee positivity of the populations. The restoration of realizability in RELBM increases this peak only moderately to $D_{\text{eff}} \approx 1.83D$ ($\Delta_D \approx 0.8$). The additional increase of about $0.3D$ is introduced by the realizability limiter, which supplies a further conservative correction when positivity would otherwise be lost. Together with the limiter-activity statistics

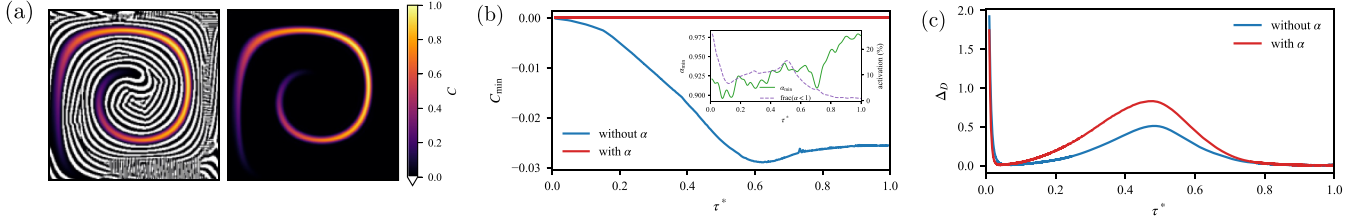


FIG. 1. Restoration of realizability in time-reversing deformational flow ($Pe = 2.56 \times 10^5$). (a) Scalar fields at maximum deformation ($\tau^* = t/T = 0.6$). The unconstrained ELBM (left) exhibits Gibbs oscillations near sharp gradients, whereas RELBM (right) maintains a strictly positive, oscillation-free profile. (b) Time evolution of the domain minimum concentration $C_{\min}$. RELBM (red) strictly enforces positivity compared to the unconstrained baseline (blue). Inset: Geometric limiter statistics. The minimum scaling factor $\alpha_{\min}$ (green) and sparse activation fraction (purple) quantify the local, perturbative nature of the correction. (c) Evolution of the excess effective diffusivity $\Delta_D = D_{\text{eff}}/D - 1$.

reported in the Supplemental Material [30], this shows that the added dissipation remains localized and activation dependent, concentrated near the sharpest fronts [17]. Furthermore, as the flow reverses and gradients relax ($t > T/2$), the numerical dissipation in both schemes rapidly decays to zero, recovering the intrinsic physical diffusivity in well-resolved regions. Despite the increased effective dissipation, the RELBM achieves a lower global reconstruction error [30] ($E_{L2} \approx 7.27 \times 10^{-2}$) compared to the unconstrained baseline (8.31×10^{-2}). The limiter thus effectively filters out irreversible grid-scale artifacts, preserving the global structure better than the ostensibly lower-dissipation entropic scheme.

We next consider the classical two-dimensional Graetz problem between isothermal parallel plates, a standard entrance-region test for wall-bounded laminar heat or mass transfer [34]. This configuration combines convection-dominated scalar transport with a steady shear profile, cold walls, and an open downstream boundary, providing a practically relevant assessment of the method in confined channel flow. Details of the numerical setup, the reference solution, and the error definitions are provided in the Supplemental Material [30]. There, the reference is defined from the standard high-Pe Graetz approximation with axial diffusion neglected and is evaluated as a streamwise initial-value problem on the same transverse grid used by the RELBM calculation. Figure 2 reports the steady cross-sectional mean temperature $\langle \theta \rangle_y(x)$ for a 1002×256 lattice with $u_b = 0.02$ and $Pe \in \{100, 1000, 10000\}$. The RELBM results remain stable and nonoscillatory throughout and closely follow the expected entrance-region decay over the full streamwise extent. At $Pe = 10^4$, the RELBM mean-profile error is $E_{L2}^{\text{mean}} = 3.99 \times 10^{-4}$, comparable to that of an independent finite-volume scheme with a total-variation-diminishing flux limiter (FVM + TVD), 3.15×10^{-4} , while the RELBM/FVM difference remains below 1% in relative L_2 norm. These results show that the realizable entropic closure preserves high accuracy in a genuinely wall-bounded convection-dominated channel-flow setting.

We further consider the classical Taylor dispersion of a passive scalar between parallel plates. This problem assesses the scheme's ability to capture shear-enhanced longitudinal spreading over long times, governed jointly by transverse diffusion and streamwise shear. The domain is periodic in

the streamwise direction and bounded by no-flux walls in the transverse direction, with a full channel width of $N_y = 32$. A Poiseuille velocity profile with mean speed $u_{\text{avg}} = 0.02$ is imposed, and the molecular diffusivity is varied to scan global Péclet numbers $Pe = u_{\text{avg}}H/D$ from 20 to 2×10^5 .

Figure 3(a) presents the results for the low-to-moderate regime ($20 \leq Pe \leq 2000$). The normalized effective diffusivity coefficient is plotted against the dimensionless diffusive time $\tau_D^* = Dt/H^2$. The simulation data (symbols) show excellent agreement with the analytical time-dependent

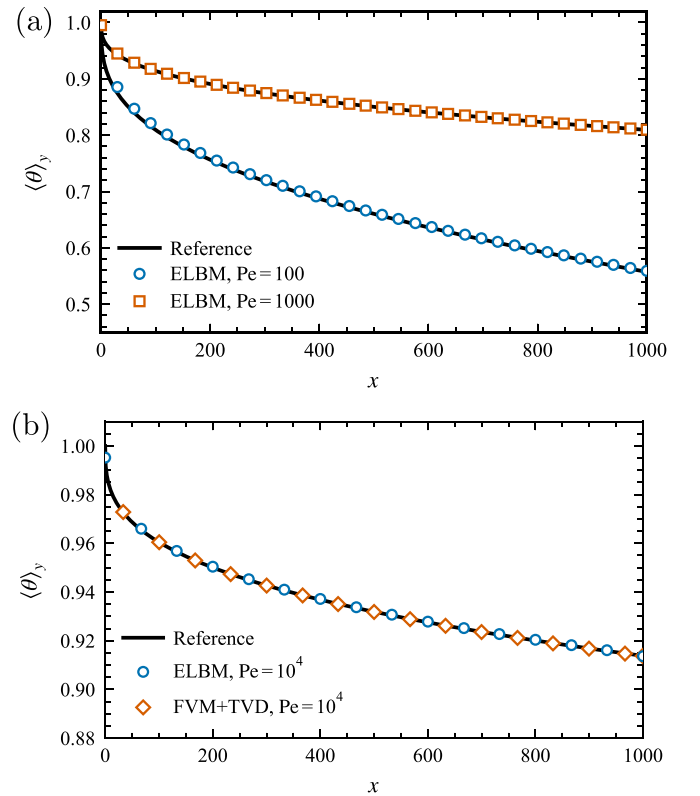


FIG. 2. Steady Graetz transport between parallel plates. The cross-sectional mean temperature $\langle \theta \rangle_y$ is plotted against streamwise distance x ; solid curves denote the high-Pe semianalytical reference. (a) RELBM results at $Pe = 100$ and 1000 . (b) RELBM and FVM+TVD results at $Pe = 10^4$.

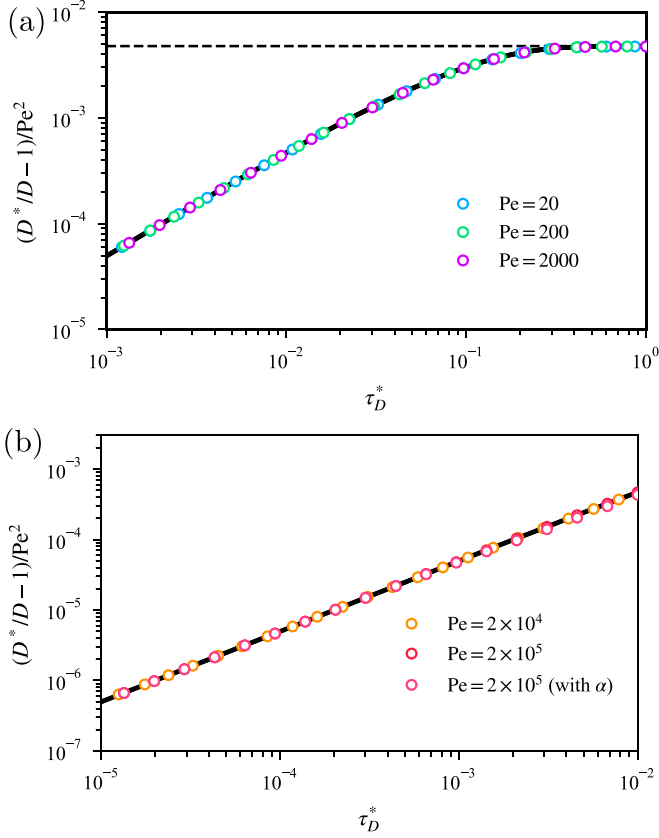


FIG. 3. Validation of transient Taylor dispersion across Péclet numbers $Pe \in [20, 2 \times 10^5]$. The normalized dispersion coefficient $(D^*/D - 1)/Pe^2$ is plotted against dimensionless diffusive time $\tau_D^* = Dt/H^2$. Solid curves represent the analytical solution of Eq. (10). (a) Relaxation to the asymptotic Taylor-Aris limit ($1/210$, dashed line). (b) The high-Pe regime. The solver captures the preasymptotic advective scaling ($D^* \propto t$) even at the extreme case of $Pe = 2 \times 10^5$.

solution [35]:

$$\frac{D^*/D - 1}{Pe^2} = \frac{9}{2\pi^6} \sum_{m=1}^{\infty} \frac{1 - e^{-4m^2\pi^2\tau_D^*}}{m^6}. \quad (10)$$

Equation (10) captures the complete relaxation process, transitioning from the initial advection-dominated scaling to the classic Taylor-Aris asymptotic limit of $(D^*/D - 1)/Pe^2 \rightarrow 1/210$ as $t \rightarrow \infty$ [30]. This perfect match confirms that the entropic framework correctly recovers the subtle interplay between transverse diffusion and streamwise shear.

In the high Pe regime shown in Fig. 3(b), we vary the diffusivity to achieve $Pe = 2 \times 10^4$ and 2×10^5 . For the latter case, the grid Péclet number reaches an extreme value of $Pe_g = Pe/N_y \approx 6250$. Despite this, the RELBM remains stable and accurately resolves the early-time scaling ($D^* \propto t$), where dispersion is dominated by pure advection [36]. Notably, unlike the shock-dominated case in Fig. 1, the geometric limiter here leaves the effective diffusivity invariant. Since the scalar field in Taylor dispersion remains smooth (free of Gibbs oscillations), the realizability condition is naturally satisfied, and the limiter α remains effectively inactive ($\alpha = 1$). In this smooth-flow benchmark, the limiter remains dormant and the scheme reduces to the entropic update.

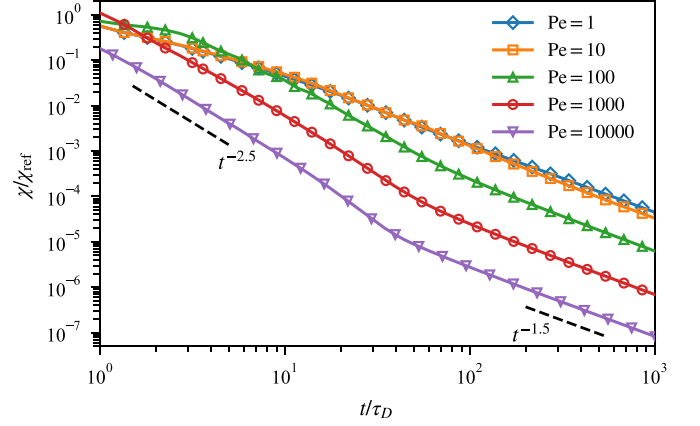


FIG. 4. Scalar dissipation rate $\chi(t)/\chi_{\text{ref}}$ versus t/τ_D for $Pe = 1$ – $10\,000$, where $\tau_D = \Delta x^2/D$ (with $\Delta x = 1$ in lattice units) and $\chi_{\text{ref}} \equiv \chi_{\text{ana}}(\tau_D)$ with $\chi_{\text{ana}}(t) = \frac{c_0^2 L_y}{8\sqrt{2\pi}D} t^{-1.5}$ and $c_0 = m_0/L_y$. Black Dashed lines: lamellar (shear-diffusion) mixing limit $\chi \propto t^{-2.5}$ and late-time Fickian scaling $\chi \propto t^{-1.5}$. Intermediate-time fits give $\chi \propto t^{-2.05}$ ($Pe = 100$), $t^{-2.35}$ ($Pe = 1000$), and $t^{-2.51}$ ($Pe = 10\,000$).

To isolate pore-scale mixing dynamics in the high-Péclet limit, we simulate passive-scalar transport through a deterministic periodic granular array (particle diameter $d_p = 20$, throat size $l \approx 15$ [30]). The geometry is macroscopically homogeneous, so pore-scale advection competes primarily with transverse diffusion and shear-driven stretching [37–39]. In contrast to previous pore-scale LBM studies that mainly addressed reactive and nonequilibrium transport in evolving or nanoporous media [40–42], the present setup is nonreactive and remains within the continuum advection-diffusion regime. Excluding reaction, rarefaction, and pore-structure evolution therefore allows the temporal scaling of scalar dissipation to be attributed directly to pore-scale advection, shear-driven stretching, and transverse diffusion. Mixing is quantified by the scalar dissipation rate [43]

$$\chi(t) \equiv \kappa \int_{\Omega} |\nabla c|^2 d\Omega = -\frac{1}{2} \frac{dM}{dt}, \quad (11)$$

with $M(t) = \int_{\Omega} c^2 d\Omega$ the scalar variance [44]. The boundary contributions vanish as specified in the Supplemental Material [30], yielding the identity $\chi = -\frac{1}{2} dM/dt$. For power-law regimes $M \sim t^q$ we thus have $\chi \sim t^{q-1} \equiv t^{-p}$ with $p = 1 - q$. Figure 4 shows that for $Pe \leq 10$ the dissipation rate rapidly approaches the classical Fickian dispersion scaling $\chi \sim t^{-1.5}$ [43]. Moreover, for all Pe we observe the same asymptotic decay at late times ($t \gg \tau_D$), consistent with a self-similar effective 1D diffusive regime in which transverse diffusion homogenizes the plume cross section [38,43]. In this limit the longitudinal spread obeys $\sigma \sim t^{0.5}$, implying $M(t) = \int c^2 d\Omega \sim \sigma^{-1} \sim t^{-0.5}$ and therefore $\chi \sim -\frac{1}{2} dM/dt \sim t^{-1.5}$ [43]. A fit over the late-time window $t/\tau_D \in [100, 1000]$ yields $q \simeq -0.50$ – -0.53 , corresponding to $p \simeq 1.50$ – 1.53 (theoretical $p = 1.5$).

At intermediate times, advection-dominated nonequilibrium mixing produces a distinct non-Fickian dissipation regime for $Pe \geq 100$. Over $t/\tau_D \in [4, 40]$ at $Pe = 100$ we obtain $q = -1.05 \pm 0.004$, i.e., $\chi \sim t^{-2.05}$, indicating a modestly accelerated decay compared with the late-time Fickian

regime. As Pe increases, this intermediate decay steepens and approaches the classical lamellar (shear-diffusion) prediction: for $Pe = 1000$ over $t/\tau_D \in [1, 20]$ we measure $q = -1.35 \pm 0.006$ (i.e., $\chi \sim t^{-2.35}$), while for $Pe = 10000$ over the same window we obtain $q = -1.51 \pm 0.001$, giving $\chi \sim t^{-2.51}$, essentially indistinguishable from the canonical $t^{-2.5}$ scaling.

The $p \approx 2.5$ is the hallmark of shear-diffusion (lamellar) kinematics. In the homogeneous media, persistent pore-scale shear and velocity gradients stretch the plume ballistically along its principal axis ($\ell \sim t$), while diffusion controls the lamellar thickness ($w \sim t^{0.5}$) [37,38,45].

In our 2D pore-resolved setting, the lamella area scales as ℓw [45]. Assuming approximate mass conservation within a lamella, $c \sim (\ell w)^{-1}$, and that the dominant gradients are transverse to the lamella so that $|\nabla c| \sim c/w$, we obtain

$$\chi \sim \kappa (\ell w) \frac{c^2}{w^2} \sim \kappa (\ell w) \frac{(\ell w)^{-2}}{w^2} \sim \frac{\kappa}{\ell w^3} \sim t^{-2.5}. \quad (12)$$

Importantly, the emergence of the $t^{-2.5}$ regime here does not require structural disorder or strong macroscopic heterogeneity: it arises already in a strictly homogeneous, deterministic array through shear-driven stretching and transverse diffusion.

At the same time, we do not claim universality across arbitrary porous media: in strongly heterogeneous formations with broad residence-time statistics, trapping/intermittency can modify or obscure this intermediate lamellar window and lead to different effective decay exponents.

In summary, the RELBM framework combines entropic stability with strict realizability by enforcing a convex H theorem alongside a geometric limiter. This ensures non-negativity and conservation even in shocklike, under-resolved regimes, while introducing only localized and moderate additional numerical dissipation when the realizability correction is activated. By accurately capturing key transport scalings in high-Péclet flows, the method offers a robust and general framework for simulating advection-dominated transport across a wide range of systems, including turbulent mixing, geophysical and environmental scalar transport, and reactive flows in complex geometries.

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Data availability. The data supporting the findings of this study are available in Ref. [46].

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