Truncation effect on Taylor–Aris dispersion in lattice Boltzmann schemes: Accuracy towards stability

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A B S T R A C T

The Taylor dispersion in parabolic velocity field provides a well-known benchmark for advection–diffusion (ADE) schemes and serves as a first step towards accurate modeling of the high-order non-Gaussian effects in heterogeneous flow. While applying the Lattice Boltzmann ADE two-relaxation-times (TRT) scheme for a transport with given Péclet number (Pe) one should select six free-tunable parameters, namely, (i) molecular-diffusion-scale, equilibrium parameter; (ii) three families of equilibrium weights, assigned to the terms of mass, velocity and numerical-diffusion-correction, and (iii) two relaxation rates. We analytically and numerically investigate the respective roles of all these degrees of freedom in the accuracy and stability in the evolution of a Gaussian plume. For this purpose, the third- and fourth-order transient multi-dimensional analysis of the recurrence equations of the TRT ADE scheme is extended for a spatially-variable velocity field. The key point is in the coupling of the truncation and Taylor dispersion analysis which allows us to identify the second-order numerical correction \( \delta k_f \) to Taylor dispersivity coefficient \( k_f \). The procedure is exemplified for a straight Poiseuille flow where \( \delta k_f \) is given in a closed analytical form in equilibrium and relaxation parameter spaces. The predicted longitudinal dispersivity is in excellent agreement with the numerical experiments over a wide parameter range. In relatively small Pe-range, the relative dispersion error increases with Péclet number. This deficiency reduces in the intermediate and high Pe-range where it becomes Pe-independent and velocity-amplitude independent. Eliminating \( \delta k_f \) by a proper parameter choice and employing specular reflection for zero flux condition on solid boundaries, the d2Q9 TRT ADE scheme may reproduce the Taylor–Aris result quasi-exactly, from very coarse to fine grids, and from very small to arbitrarily high Péclet numbers. Since free-tunable product of two eigenfunctions also controls stability of the model, the validity of the analytically established von Neumann stability diagram is examined in Poiseuille profile. The simplest coordinate-stencil subclass, which is the d2Q5 TRT bounce-back scheme, demonstrates the best performance and achieves the maximum accuracy for most stable relaxation parameters.

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1. Introduction

In his seminal work in 1953, G. Taylor [1] revealed the longitudinal dispersion of the soluble matter, induced by the radial variation of the velocity field in a straight circular pipe. In 1955, R. Aris [2] developed the mathematical analysis of
the moments for averaged solute distributions, removed several Taylor assumptions, such as zero molecular diffusion in the longitudinal direction, and extended it for arbitrary-shaped pipes. His results showed that the rate of growth of the variance is proportional to the apparent diffusion coefficient, a sum of the molecular diffusion coefficient $D_0$ and Taylor dispersion coefficient $D_T$. Later, Brenner [3] introduced the generalized approach to predict dispersion in porous flow, where this phenomena is of fundamental importance because of the disordered structure, [4,5]. The work by Salles et al. [6] applied the Brenner method for numerical computation of the hydrodynamic dispersion tensor [7] in prescribed periodic microscopic velocity fields. Following an alternative numerical approach, dispersion coefficients were estimated from random-walk particle-tracking simulations in micro-porous flow, e.g., modeled with the Lattice Boltzmann hydrodynamic schemes [8,9]. The perturbation analysis [10,11] predicted dispersion coefficients due to variation of the superficial (phase averaged) flow in homogeneous and heterogeneous packed tubes. Similar analysis has been applied in the description of hydraulic dispersion in wetlands [12]. The recently proposed extended momentum method (EMM) [13] restores any-order moments, either for the resident-time-distribution approach [14] or for the spread of initially narrow concentration pulse, in any-scale stationary periodic velocity field over the impermeable or permeable obstacles. The advection–diffusion two-relaxation-times (TRT) Lattice Boltzmann schemes [15–18] have been also extended in work [13] to simulate solute transport in heterogeneous porous media specified by discontinuous porosity distribution. The EMM analytical predictions and the TRT direct numerical computations validated one other for several benchmark cases. In particular, in stratified porous layers, the EMM required up to nine moments to obtain the perfect agreement with the TRT results obtained with the five-speed d2QS scheme, while overall, the dispersivity, skewness and kurtosis were found sufficient to predict the principal distribution shape. The isotropic/anisotropic one-two-three dimensional TRT ADE schemes are all supported by stability and truncation analysis developed in constant-velocity field [17,19] and further extended for porous flow [13]. However, the most stable schemes are not expected to be the most accurate, and vice versa, because both truncation accuracy and stability intrinsically depend on the same free-tunable product $\Lambda$ of two eigenfunctions [19]. The observations [13] of the $\Lambda$-dependency in second, third, and fourth-order moments motivated the present work on the search of the optimal model parameters for the Taylor dispersivity coefficient.

The measurement of Taylor dispersion coefficient $D_T = D_0k_T$ in straight channel (where $k_T$ increases as $Pe^2/210$ with Péclet number $Pe = U/H/D_0$) has been considered as the benchmark in the LBE modeling since the pioneering works [20, 21]. The results [21] confirmed the linear increase of $D_T$ with the square of the averaged velocity $U$, up to $Pe \approx 12$ using the 24-speed FCHC matrix model and channel width $H = 16$. (The suggested there) deterioration of the Taylor assumptions as the $Pe$ increases was used as a justification of small $k_T$-underestimate. The nine-speed d2QS scheme [22], based on the single-rate BGK collision [23] and bounce-back boundary rule, achieved better agreement with the Taylor prediction (within few percents) for smaller molecular diffusion coefficient $D_0 \propto (\tau_D - \frac{1}{2})$ (where $\tau_D$ is prescribed relaxation rate), as long as $\tau_D/H < 0.08$ with $\tau_D \in [0.7, 10]$ and especially, when $\tau_D = 1$. Using heuristic arguments the authors related this dependency to the Knudsen number of the tracer flow. By employing the seven-speed d3Q7 isotropic matrix collision [24], which is equivalent to d2QS TRT collision in this study, the $k_T$ values within one-two percents for $Pe = 50$ and $H = 32$ were reported based on the variance growth. At the same time, the TRT/BGK operators produced there rather different dispersion coefficients at fixed Péclet number, indicating their dependency on the free eigenvalue. The d2QS full-matrix-model [25] has shown improvements for $k_T$ against the d2QS MRT model with equilibrium correction [15,17], when $Pe \in [2, 32]$ with $\tau_D \in [1, 2]$. However, in one-dimensional channel flow the two models are expected to display equivalent, numerical-diffusion-free, isotropic second-order equations, also equivalent that modeled with the simplest d2QS TRT/BGK schemes. Thereby, all these recent results suggest that the truncation corrections may modify the apparent dispersion coefficient of the averaged second-order equation.

In fact, analysis of the bulk behavior of the linear LBE ADE schemes has been mostly focused on their numerical diffusion [15,25–29], extensions for anisotropy [15,24,25,30–33], stability [17,19,28,33–37] and truncation accuracy [15,19,26,38,34,39]. These four elements are indeed intrinsically interconnected [19]. Nevertheless, while a formal functional dependency of the third- and fourth-order truncation corrections on the constant advection velocity and model parameters has been derived [15,19,26,39], the associated apparent numerical dispersivity, manifested in variable velocity field, has been never predicted. We will show that the discrepancy with the Taylor result is entirely explained by the numerical dispersion, provided that numerical diffusion has been eliminated and zero-flux boundary condition is adequate. This result is interesting; the numerical dispersivity will originate from the truncation terms, nevertheless, it will modify the apparent transport coefficient of the second-order equation. This effect is perfectly detectable on the variance growth, similar to the decrease of the prescribed molecular diffusion coefficient due to (negative) numerical diffusion. Furthermore, the present work shows that these two effects are superposed.

It is appropriate to say first a few words about the numerical diffusion, already existing in constant velocity field. In “convective” scaling ($\delta t = \epsilon = x/L$), the numerical-diffusion term is automatically detected by the Chapman–Enskog analysis, e.g. [15,25,27,28], the equivalent partial differential equations [39], the recurrence equations [19] and asymptotic analysis [24]. However, since it originates from the mixed (space/time) derivatives of the advective flux, it is not detected by the asymptotic analysis [24,40] in “diffusive” scaling $\delta t = \epsilon^2$. In particular, the schemes [24,41,42] do not eliminate numerical diffusion, which features on top of the numerical dispersion in the reported results [24] for Taylor dispersion (see Table 10 in this work). Notice that the criticism developed in works [25,29] over anti-numerical-diffusion equilibrium correction [15,17] for its (partial, indeed) non-accounting of the spatial velocity variation is not applicable for channel flow because of its translational invariance (we leave this point last). But not least, we will show that in variable chan-
nel flow, the Taylor dispersion dominates the numerical diffusion for small diffusion coefficients, in agreement with the results [25], which show no difference for $\tau_D = 0.55$ between the two anti-numerical-diffusion approaches, and the scheme without any one of them.

A quasi-exact validation of the numerical diffusion and dispersion in d2Q9 scheme becomes possible in the present work by adopting the mirror specular reflection, where the particles are reflected on the wall like a light ray. Drazer and Koplik [43] made a very important contribution by numerically quantifying the decrease in apparent diffusion coefficient $D^{(num)}$ due to the bounce-back boundary rule in d3Q19 model and concluded that $D_T \approx D^{(num)} Pe^2/210$, considering very small $Pe$, $Pe < 2$. At the same time, they discovered that the “bounce-forward” (specular) reflection produces the desired Taylor result properly; the “mirror-image” method has also been proposed for impermeable wall [44]. Further boundary analysis [45] has shown that the bounce-back drawback originates in its restriction of the tangential boundary flux, handled in hydrodynamic velocity sets by their diagonal links. In the accompanying work [46], we exactly quantify the difference in mean advection velocity and diffusion/dispersion for the specular reflection and bounce-back, in plug and parabolic flows. It has also been noted [45] that the specular reflection delivered identical solutions with the periodic condition on the straight solid wall in plug flow. This property appears to be retained in Poiseuille profile allowing us to validate the bulk truncation analysis for d2Q5/d2Q9 schemes in the absence of spurious boundary effects.

In the minimal d2Q5/d3Q7 schemes, which are, respectively, the d2Q9/d3Q15 – d3Q19 equilibrium subclasses for zero diagonal-weight value, the (non-local) specular reflection reduces to local bounce-back rule. The “optimal-advection” d2Q5 BGK scheme [15,19] was successfully applied for dissolution and precipitation [47], and the d2Q5 TRT scheme with “optimal-diffusion” $\Lambda$-choice [15,19,39] was applied to produce solutions of “benchmark quality” in thermal convective flows [41,42]. The diffusion of a non-reactive solute in liquid phase of unsaturated porous media was modeled using the d3Q7 TRT scheme with $\Lambda = 1/32$, by combining it with the d2Q9 TRT scheme with $\Lambda = 3/16$ for two-phase flow. [48]. Full diffusion tensors in the (positive-definiteness) anisotropic limit were matched more accurately with the d2Q5 full-matrix-model [24] against the d2Q9 MRT anisotropic collision, but less accurately than with the d2Q9 TRT model based on the anisotropic equilibrium, [28]. The rational behind is that the anisotropic equilibrium reduces the dispersivity of the collision eigenvalue spectrum. Recently, the d2Q9 TRT scheme was found adequate for a transient (24 h) large scale oil spill modeling in kilometric-scale hydrodynamic velocity field generated by the sub-regional model, [49]. In this last work, the d2Q9 hydrodynamic stencil was preferred to the d2Q5 due to its better isotropy, in agreement with the truncation results [19], and for (rather modest) improvement of the accuracy in long-time evolution of the Gaussian plume. The computations have been performed with different time steps in two schemes, but for the same computational time. It should be borne in mind that the d2Q5 and d2Q9, and especially the d3Q7 and d3Q19, have different stable parameter range: the hydrodynamic stencils are able to reach larger advection velocities for proper weights and relaxation rates [17,19]. In present computations, the peak velocity amplitude will be systematically increased up to the two-dimensional necessary stability bound of the isotropic d2Q5 scheme, predicted to be sufficient for “optimal-stability” collision number $\Lambda = \frac{1}{16}$ [17]. The results will show that the maximum accuracy and stability can be achieved in dispersion-dominated problems with the d2Q5 scheme, by vanishing its numerical dispersion for $\Lambda = \frac{1}{2}$ in straight channel.

The paper is organized as follows. Section 2 recalls the Taylor dispersion analysis and the TRT ADE scheme. In particular, the d2Q5, “rotated” d2Q5 and “standard” hydrodynamic d2Q9 equilibrium stencils are exemplified. Section 3 builds fourth-order effective advection-diffusion equation of the TRT scheme from its recurrence equations [50] and then derives the closed-form expression for the apparent coefficient of the numerical dispersivity. Those third- and fourth-order space-time-dependent truncation corrections are identified for this purpose, which, by acting together in a space-variable velocity field, either directly alter the Taylor dispersion coefficient or numerically modify the Taylor Ansatz [1,2]. As a practical result, this analysis provides “optimal-dispersion” parameter sub-space (where numerical dispersivity vanishes) for d2Q5 and d2Q9 models, applicable for any Péclet range. Section 4 compares the numerical results for variance measurements to the theoretical predictions from both d2Q5 and d2Q9 schemes, with a particular attention to stability at high Péclet numbers. Section 5 concludes the paper. The truncation analysis of the TRT operator is extended from the constant to space-variable flow in Appendix A.

## 2. Basis equations

### 2.1. Taylor dispersion in straight channel

Assume that the concentration field $C(x, y, t)$ obeys the two-dimensional advection-diffusion equation with molecular diffusion coefficient $D_0$ in straight Poiseuille flow $u(x,y) = \frac{\partial \bar{H}}{\partial y} y(\bar{H} - y)$:

$$\partial_t C + u_x(y) \partial_x C = \tilde{D}_0 (\partial_y^2 C + \partial_x^2 C) ,$$

subject to zero-flux condition on the two solid plates distanced by $\bar{H}$:

$$\partial_y C|_{y=0} = 0 , \quad \partial_y C|_{y=\bar{H}} = 0 .$$

Let us decompose $C(x, y, t)$ and $u(x,y)$ around their cell-averaged values $\bar{C}(x,t)$ and $\bar{u}$, respectively.
\[ C = \tilde{C}(x, t) + C'(x, y, t) \cdot \tilde{C}(x, t) = \langle C(x, y, t) \rangle = \frac{\hat{H}}{0} \int C(x, y, t)dy \cdot \frac{\partial y C}{y=0, \hat{H} = 0}. \]

\[ u_x(y) = \bar{U} + u'(y) \cdot \bar{U} = \langle u_x(y) \rangle = \frac{\bar{u}_0 \bar{H}^2}{12}, \bar{u}_0 = -\nabla_x P \mu. \]  

(3)

The averaged concentration \( \bar{C}(x, t) \) obeys the one-dimensional advection-diffusion equation in the averaged velocity field \( \bar{U} \), where \( \bar{D}_0 \) obtains Taylor dispersion correction \( D_T = \bar{D}_0 k_T \):

\[ \partial_t \bar{C} + \bar{U} \partial_y \bar{C} = \tilde{D}_0 (1 + k_T) \partial_y^2 \bar{C}, \quad k_T = \frac{P \epsilon^2}{210}, \quad P e = \frac{\bar{U} \bar{H}}{\bar{D}_0}. \]  

(4)

The averaged Eq. (4) can be obtained as following. One first applies the averaging to Eq. (1) taking into account that, (i) \( \langle u' \rangle = 0, \langle C' \rangle = 0 \), then \( \langle u'(\bar{C}) \rangle = 0, \langle \bar{U}' C \rangle = 0 \), then \( u_y(y) C = \langle \bar{U}' \bar{C} \rangle \) + \( \langle u' C \rangle \) and (ii), \( \langle \partial_y^2 C \rangle \) vanishes due to no-flux boundary condition, as a result the averaged Eq. (1) reads:

\[ \partial_t \bar{C} + \bar{U} \partial_y \bar{C} + \partial_x (u'C) = \tilde{D}_0 \partial_x^2 \bar{C} . \]  

(5)

The key point is the following relation, referred hereafter as the Taylor Ansatz:

\[ \tilde{D}_0 \partial_x^2 C' \approx u'(y) \partial_y \bar{C} . \]  

(6)

By applying zero-flux boundary condition, it gives: \( C'(x, y, t) = \tilde{D}_0^{-1} \alpha(y) \partial_y \bar{C}(x, t), \alpha(y) = \int_0^y \int_0^y u'(y')dy' \ 1/210, \quad \tilde{D}_0 = \bar{D}_0 \), and this term produces correction \( k_T \tilde{D}_0 \) to diffusion coefficient \( \bar{D}_0 \) in Eq. (4), with

\[ k_T = -\tilde{D}_0^{-2} (u'(y) \alpha(y)) = -\tilde{U}^2 \tilde{H}^2 \ 1/210 \tilde{D}_0 = \bar{D}_0. \]  

(7)

The Taylor Ansatz assumes that the faster diffusion process happens in the transverse direction, and it can be established applying the perturbation technique using \( x' = \epsilon(x - \bar{U}t), t' = \epsilon^2 t, C = \bar{C} + C' \), Eq. (1) reads in moving coordinate frame:

\[ \epsilon^2 \partial_t \bar{C} + \epsilon^3 \partial_t C'' + \epsilon^2 u' \partial_t C'' + \epsilon u' \partial_y \bar{C} = \tilde{D}_0 (\epsilon^2 \partial_x^2 C + \epsilon \partial_x^2 C') \].  

(8)

Equating the leading order terms, one gets \( \epsilon u' \partial_t \bar{C} = \epsilon \tilde{D}_0 \partial_x^2 C' \) which gives Eq. (6). Our purpose is to examine if the truncation corrections may modify the Taylor Ansatz (6) and/or dispersive coefficient \( k_T \) given by Eq. (7).

2.2. The TRT advection–diffusion scheme

2.2.1. The TRT operator

We consider advection–diffusion two-relaxation-times (TRT) schemes [15,16] in the form [17,19,28] restricting them to the modeling of isotropic diffusion tensor. The discrete, \( d \)-dimensional velocity set consists of zero vector \( \bar{c}_0 \) and \( Q_m = Q - 1 \) vectors \( \bar{c}_q \) connecting grid nodes \( \bar{r} \). This velocity set is anti-symmetric, that is each vector \( \bar{c}_q \) has the opposite one \( \bar{c}_{-q} \), hereafter \( \bar{c}_q = -\bar{c}_{-q} \). Two local equilibrium values \( e_q' (\bar{r}, t) \) for each couple of the opposite velocities, with \( e_q^+ = e_q^- \) and \( e_q^- = -e_q^+ \). The primary variable of the scheme is the vector \( \{ f_q(\bar{r}, t) \} \) composed of \( Q \) “populations”. The TRT scheme updates them with the help of the two relaxation parameters \( s^\pm(\bar{r}, t) \) restricted to the linear stability interval \( [0, 2] \):

\[ f_q(\bar{r} + c_q, t + 1) = f_q(\bar{r}, t) + g_q^+ + g_q^-, q = 0, \ldots, \frac{Q_m}{2}, \]

\[ f_q(\bar{r} - c_q, t + 1) = f_q(\bar{r}, t) + g_q^+ - g_q^-, q = 1, \ldots, \frac{Q_m}{2}, \]  

with

\[ g_q^\pm = -s^\pm(f_q^\pm - e_q^\pm), \quad g_q^+ = -2 \sum_{q=1}^{Q_m/2} g_q^+, \quad g_q^- = 0, \quad f_q = f_q^+ + f_q^- \]  

(9)

Solution for concentration field \( C(\bar{r}, t) \) is set equal to the local mass (sum) of populations:

\[ \bar{C}(\bar{r}, t) = \sum_{q=0}^{Q_m/2} f_q = f_0 + 2 \sum_{q=1}^{Q_m/2} f_q^+ . \]  

(10)

The relaxation rates enter the second-order macroscopic equations and their truncation corrections only via the positive eigenfunctions \( \Lambda^+ \) and their product \( \Lambda^2 \).
\[
\lambda^\pm = \frac{1}{s^\pm} - \frac{1}{2}, \quad \Lambda = \Lambda^+ \Lambda^-.
\] (11)

A special role for stability of TRT ADE schemes is played by the particular value [17]:
\[
\Lambda = \frac{1}{4} \quad \text{then} \quad \frac{s^+ + s^-}{2} = 1, \quad \forall \ s^\pm \in [0, 2].
\] (12)

including the BGK subclass [23] where \(s^+ = s^- = 1/\tau\) for one particular value \(\tau = 1\). The choice \(\Lambda = \frac{1}{4}\) determines the so-called “optimal-stability” TRT subclass where the necessary von Neumann stability conditions may become sufficient for any Péclet-range.

It is important to say that the steady-state non-dimensional TRT solutions are set by the non-dimensional numbers of the problem only when the spatial grid-distribution of \(\Lambda\) remains fixed for any altering of the transport coefficient [50]. In particular, those numerical solutions of ADE are set by Péclet number for any value of the diffusion eigenfunction \(\Lambda^-\) only provided that \(\Lambda^+ = \Lambda/\Lambda^-\) varies inversely to \(\Lambda^-\). Yet, the obtained solutions depend on \(\Lambda\). This truncation dependency is commonly expected to be beyond the second-order in bulk. However, we will derive the analytical dependency of the numerical dispersion on \(\Lambda\) in d2Q9 model. This result will show, first, that the apparent dispersion coefficient of the second-order equation depends on \(\Lambda\). Second, the choice (12) will appear as the most accurate, as well as the most stable, for moderate and high Péclet numbers with the d2Q5 velocity set.

2.2.2. Advection-diffusion equilibrium

Consider linear equilibrium distribution \(e^+_q(\vec{r}, t) = E^+_q(\vec{r})C(\vec{r}, t)\) where \(E^+_q(\vec{r})\) has the following form:

\[
E^+_q = E^{(m)}_q c_e + E^{(a)}_q (\vec{U}), \quad E^-_q = -E^{(a)}_q (\vec{U} \cdot \vec{c}_q), \quad q = 1, \ldots, M, \quad E^+_0 = 1 - 2 \sum_{q=1}^Q E^+_q, \\
E^{(a)}_q = t^{(a)}_q \vec{U} \bar{U} + \frac{1}{2} |\vec{c}_q|^2 \sum_{a=1}^D (U_a^2 - \bar{U}^2) c^2_{q,a} + \sum_{a \neq b} U_a U_b c_{q,a} c_{q,b} + \sum_{q' \neq q, a \neq b} c_{q,a} c_{q',b}, \quad \bar{U}^2 = \frac{U^2}{d}, \quad U^2 = \sum_{a=1}^D U_a^2.
\] (13)

This equilibrium applies with the “minimal” velocity sets dQ2(2D + 1), as d1Q3, d2Q5 and d3Q7, and the “full” schemes as d2Q9/d3Q15, for modeling of the advection–diffusion equation in prescribed velocity field \(\vec{U}(\vec{r}, t)\) with the isotropic diffusion tensor \(D_0 \delta_{\alpha\beta}\), where molecular diffusion coefficient \(D_0\) reads (in lattice units):

\[
D_0 = c_e \Lambda^-.
\] (14)

Giving the characteristic length and mean velocity, in physical and lattice units as \(\bar{H}, \bar{U}\) and \(H, U\), respectively, the numerical value of \(D_0\) is adjusted to fit the prescribed Péclet number:

\[
Pe = \frac{\bar{U} \bar{H}}{D_0} = \frac{uH}{D_0}.
\] (15)

The diffusion–scale equilibrium parameter \(c_e \in [0, 1]\) can be freely selected inside its stability interval which depends on the mass-weights \(t^{(m)}_q\) [17,19]. The three families of weights \(t^{(m)}_q\), \(t^{(a)}_q\) and \(t^{(d)}_q\) are all restricted to one (isotropic) constraint:

\[
2 \sum_{q=1}^M t^{(d)}_q c_{q,a} c_{q,b} = \delta_{\alpha\beta}, \quad t^{(d)}_q = [t^{(m)}_q, t^{(a)}_q, t^{(d)}_q], \quad t^{(d)}_q \geq 0.
\] (16)

The purpose of the anisotropic equilibrium correction \(E^{(a)}_q\) is to remove the second-order tensor of numerical diffusion. In constant velocity field, it has the form of the anisotropic tensor \(D^{(num)}_{\alpha\beta} = -\Lambda^- U_{\alpha} U_{\beta}\), and \(E^{(a)}_q\) is able to remove it with the d2Q9/d3Q15 velocity sets. The d2Q5 TRT scheme cannot remove the cross-diagonal elements \(-\Lambda^- U_{\alpha} U_{\beta}\) but they vanish for axis-aligned flow. We will show that \(E^{(a)}_q\) is also able to remove \(D^{(num)}_{\alpha\beta}\) in channel flow, as \(\vec{U} = U_{\alpha}(y)\), and therefore, not only the d2Q9 but also the d2Q5 applies in Poiseuille profile without numerical diffusion.

Further remarks. The extension of the “weighted” equilibrium form (13) to d3Q19 and to full anisotropic tensors in the frame of the TRT scheme can be find in work [28]. This form also applies with the isotropic/anisotropic MRT schemes assigned in standard hydrodynamic basis [15,28,39]. It was applied by dropping \(E^{(a)}_q\)-term with the so-called link-wise L-collision [15,28,32] and matrix models [24,40]. We point out that in absence of the off-diagonal diffusion entries, the MRT, matrix and L-collision coincide on the coordinate stencils for the most natural, equal choice of free eigenvalues assigned for all symmetric modes. This applies for MRT dDQ(2D + 1) models [39,41,42] and matrix models [24,40]. The work [28] also proves that the one-rate for all symmetric modes has quite adequate stability properties for mass conservation equation. In the isotropic case, all these models then reduce to the TRT operator, as exemplified in Section 4.2.5 for model [24]. Finally,
the $E_{q}^{(u)}$-term removes numerical diffusion in plug or channel flow, at least, from either the isotropic/anisotropic TRT/MRT schemes or their equivalents, [28].

The only principal restriction of the minimal d2Q5/d3Q7 models is that they cannot model the cross-diffusion entries in the frame of the BGK/TRT/L-MRT operators, [15,32]. However, they may combine the coordinate-stencil for the principal equilibrium (mass and advection) terms either with the cross-diffusion diagonal links (similar to last $U_{x}U_{y}$-term in Eq. (13)) or with the finite-difference “pseudo-velocities” [26]. They may also create the cross-diffusion locally with the full-matrix collision [24,31] or, equivalently, in “rotated velocity basis” [28]. Furthermore, the d1Q3/d2Q5/d3Q7 schemes with $E_{q}^{(u)} = 0$, isotropic and full anisotropic matrix-collisions, may vanish their numerical diffusion with the help of velocity-dependent eigenfunctions, [28]. Finally a specific combination, consisting of the matrix-entry correction for cross-diagonal numerical diffusion and $E_{q}^{(u)}$-correction for its diagonal (coordinate) entries, was found most appealing (see Eqs. (56) and (59) in work [28]), because it allows to increase the velocity stability bound of the matrix scheme towards the TRT bound and, most important, to reduce the dispersivity of its spectrum. This last problem was also encountered in the recent work [40] where the anisotropic coordinate grid transformation was applied for Taylor dispersion in channel. Earlier, the stretched physical grids were already modeled with the help of two techniques [45]: (i) anisotropic equilibrium and (ii) anisotropic relaxation rates, then extended for non-uniform refining in work [51]. It should be born in mind that the full and minimal stencils, as well as the two alternative, matrix and equilibrium, anisotropic approaches, have different stable anisotropic parameter range, [17,19,28]. All in all, the works [28,32,45,51] give preference to the TRT collision with the anisotropic equilibrium for its advanced accuracy in reaching very high anisotropic ratios, made possible for suitable choice of $\Lambda$. At the same time, the anisotropic and/or space-variable relaxation rates are advantageous in heterogeneous problems, where they allow to maintain continuous equilibrium over the grid.

2.2.3. Two-dimensional schemes

We consider the eight moving velocities of d2Q9 scheme such that the first four discrete-velocity vectors $\tilde{c}_{q}$ have the components $c_{x} = \{1, 0, 1, -1\}$ and $c_{y} = \{0, 1, 1, 1\}$, then Eq. (13) reads (see Fig. 1):

\[
\begin{align*}
E_{1}^{+} &= t_{c}^{(m)}c_{e} + t_{c}^{(u)}U^{2} + \frac{(U_{x}^{2} - U_{y}^{2})}{4},
E_{1}^{-} &= t_{c}^{(a)}U_{x}, \\
E_{2}^{+} &= t_{c}^{(m)}c_{e} + t_{c}^{(u)}U^{2} - \frac{(U_{x}^{2} - U_{y}^{2})}{4},
E_{2}^{-} &= t_{c}^{(a)}U_{y}, \\
E_{3}^{+} &= t_{d}^{(m)}c_{e} + t_{d}^{(a)}U^{2} + \frac{U_{x}U_{y}}{4},
E_{3}^{-} &= t_{d}^{(a)}(U_{x} + U_{y}), \\
E_{4}^{+} &= t_{d}^{(m)}c_{e} + t_{d}^{(a)}U^{2} - \frac{U_{x}U_{y}}{4},
E_{4}^{-} &= t_{d}^{(a)}(U_{x} - U_{y}), \\
E_{0}^{+} &= 1 - 2\sum_{q=1}^{9n}t_{q}^{(m)}c_{e} - 2\sum_{q=1}^{9n}t_{q}^{(a)}U^{2},
E_{0}^{-} &= 0, U^{2} = \frac{1}{2}(U_{x}^{2} + U_{y}^{2}).
\end{align*}
\] (17)

The diagonal weights $t_{d}^{(q)}$ and the coordinates weights $t_{c}^{(q)}$ are linked through Eq. (16):

\[
\begin{align*}
t_{d}^{(m)} &= \frac{1 - 2t_{c}^{(m)}}{4},
&= \frac{1 - 2t_{c}^{(a)}}{4},
&= \frac{1 - 2t_{c}^{(a)}}{4}.
\end{align*}
\] (18)

The weights can be selected independently for each of three families. The “standard” d2Q9 equilibrium, borrowed from the Navier–Stokes model [23], yields $t_{c}^{(m)} = t_{c}^{(a)} = \frac{1}{2}, t_{d}^{(m)} = t_{d}^{(a)} = \frac{1}{4}, t_{c}^{(a)} = \frac{1}{6}$ (cf. also Eq. (18) and Eqs. (28)–(30) in work [17]). One of the most stable choices [17,19] is $t_{c}^{(a)} = t_{c}^{(m)} = t_{c}^{(a)} = \frac{1}{4}$. The d2Q5 scheme is recovered when $t_{c}^{(m)} = t_{c}^{(a)} = t_{c}^{(a)} = \frac{1}{2}, E_{3} = E_{4} = 0$.

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**Fig. 1.** Sketch for equilibrium notations in Eq. (13) for d2Q9 scheme (17)–(20).
2.2.4. BGK scheme

In particular, the BGK subclass yields $\Lambda^+ = \Lambda^- = \sqrt{3}$. The BGK subclass yields $\Lambda^+ = \Lambda^- = \sqrt{3}$. It has been also proved [17] that in constant velocity field, the sufficient BGK-stability bound is determined by the entire set of equilibrium non-negativity conditions: $|E^+_q + E^-_q| \geq 0, \forall q = 0, \ldots, \frac{Qm}{2}$. In particular, the non-negativity conditions yield in dQ5:

$$|U| \leq |U|^{\text{max}}(c_e) = \begin{cases} \sqrt{2c_e}, & c_e \in [0, \frac{1}{2}], \\ \sqrt{1-2c_e}, & c_e \in [\frac{1}{2}, 1], \end{cases} \quad \max(|U|) = |U|^{\text{max}}(c_e = \frac{1}{4}) = \frac{\sqrt{2}}{2}. \quad (22)$$

It has been proved [17] that, in periodic domain, these necessary conditions are sufficient in the dQ5 with $\Lambda = \frac{1}{4}$, for any $\Lambda^-$. Otherwise, when $\Lambda \neq \frac{1}{4}$, the effective stability in the interval $c_e \in [0, \frac{1}{2}]$ depends, in a very complex way, on the two relaxation rates $\Lambda^+$ separately [37]. The BGK subclass yields $\Lambda^- = \Lambda^+ = \sqrt{3}$. It has been also proved [17] that in constant velocity field, the sufficient BGK-stability bound is determined by the entire set of equilibrium non-negativity conditions: $|E^+_q + E^-_q| \geq 0, \forall q = 0, \ldots, \frac{Qm}{2}$. In particular, the non-negativity conditions yield in dQ5:

$$|U| \leq |U|^{\text{max}}(c_e) = \begin{cases} \frac{1-\sqrt{4c_e}}{2}, & c_e \in [0, \frac{1}{4}], \\ \frac{1}{1-2c_e}, & c_e \in [\frac{1}{4}, \frac{1}{2}], \end{cases} \quad \max(|U|) = |U|^{\text{max}}(c_e = \frac{1}{4}) = \frac{\sqrt{2}}{2}. \quad (23)$$

The necessary stability conditions (22) and non-negativity conditions (23) are illustrated in Fig. 2 (the reader can find their closed-form expressions for different velocity sets in work [17]). The non-negativity conditions become necessary for the BGK scheme only when $\Lambda \to 0$, [37]. However, their left (advection-dominant) branch is either much too restrictive, e.g., for $\Lambda = \frac{1}{4}$ (see Fig. 2) or insufficient in TRT, depending together on $\Lambda$ and $\Lambda^-$. The dQ9 model has mass-weight-dependent diffusion constraint which reads (cf. Eqs. (3.17)–(3.19) in [19] for isotropic case $a_{\nu} = 0$):

$$U^2 \leq U^2_0 = \min\{1 - c_e, \frac{1 - 4\ell^{(m)}_c c_e}{2\ell^{(m)}_c}, c_e \leq \min\{1, \frac{1}{4\ell^{(m)}_c}\}. \quad (24)$$
When \( c_e \in [\frac{1}{4}, \frac{1}{2}] \), the diffusion condition \( U^2 \leq U_d^2 = 1 - 2c_e \) of the d2Q5 model is sufficient to guarantee Eq. (24). In principle, when \( \Lambda = \frac{1}{4} \), the advection line \( U_d^2 = 2c_e \) can be relaxed in the d2Q9 for hydrodynamic weights, and it vanishes for uniform weights \( t_c^0 = \frac{1}{2} \) (see Fig. 12 in [17], Figs. 8–10 in [19]). This is opposed to case when \( t_c^0 = 0 \) or \( t_c^0 = 0 \), as in Eq. (20), where this advection line is not expected to be sufficient.

As previously, the focus is put on the most interesting choices, such as (i) the “optimal-stability” with \( \Lambda = \frac{1}{4} \), \( \forall \Lambda^− \); (ii) the “optimal-advection” with \( \Lambda = \frac{1}{6} \) and (iii), the “optimal diffusion” with \( \Lambda = \frac{1}{5} \) (we discuss them in next section). The two last choices are especially interesting with \( (\Lambda^−)^2 = \frac{1}{12} \). The choice \( \Lambda = \frac{1}{12} \) suffers from a drop in stable velocity amplitude when \( \Lambda^− \rightarrow 0 \) (see [37]) or \( c_e \rightarrow 0 \) (Figs. 8–9 in [19]); \( \Lambda = \frac{1}{6} \) is expected to behave much better, [19]. In this work, we will increase the maximum (peak) velocity amplitude in Poiseuille profile up to d2Q5 stability line (22) and examine its validity in a wide range of equilibrium and relaxation parameters.

3. Numerical dispersion of the TRT scheme

The isotropic and anisotropic multi-dimensional TRT ADE schemes have been supported by the fourth-order truncation analysis [15,19] developed in constant velocity field and extended [13] for block-wise porosity-dependent Darcy’s flow. The spatial truncation components in advection and diffusion forms vanish, respectively, with \( \Lambda = \frac{1}{12} \) and \( \Lambda = \frac{1}{6} \). These two choices are equilibrium-independent and they also annihilate the third- and fourth-order coefficients, respectively, in steady state Chapman–Enskog expansion for hydrodynamic solutions, [50,52]. However, with these choices, either the advection or diffusion truncation form is entirely eliminated only for particular diffusion eigenfunction: \( (\Lambda^−)^2 = 1/12 \), in agreement with the simulated waves and evolution of slugs, [15,19,39]. Therefore, even if, for example the d2Q5 scheme is able to annihilate the entire third- and fourth-order corrections for one fixed-amplitude velocity [13], the two corrections cannot be removed simultaneously in general case, and the most stable choice \( \Lambda = \frac{1}{4} \) is not expected to be most accurate, [19]. Similar conclusion has been drawn with respect to the equilibrium stencil: the most simple and efficient d2Q5 weights, on the one side, and the most isotropic, hydrodynamic weights on the another, are not expected to be most stable in multi-dimensional constant-velocity field, [17,19].

In this section, we will reveal the apparent numerical dispersivity of the d2Q9 TRT scheme, created together by the third- and fourth-order truncation corrections in non-uniform channel flow. It should be said that in constant-velocity field, the first and second moments do not detect such terms as \( \xi^2 \mathcal{C} \) and \( \delta^2 \mathcal{C} \), only impacting the higher moments, [13]. The situation is quite different here because, although formally truncated, the numerical dispersion will produce correction \( D_0 \delta k r \delta^2 \mathcal{C} \) in Eq. (4) which is detected by the second moment of the averaged concentration distribution \( \bar{C}(x, t) \) in Eq. (4). The most accurate parameter sub-space will be identified by reducing or vanishing \( \delta k r \).

3.1. Exact mass-conservation equation

When the two relaxation functions are space–time independent, the post-collision non-equilibrium components \( \{g_q^\mp \} \) in Eq. (9) obey two equations referred to as the recurrence equations [50,19]:

\[
g_q^\mp (\bar{r}, t) = \Delta t e_q^\mp + \Delta q e_q^\mp - \Lambda^+ (\Delta^2 q^\mp - \Delta^2 q^\mp )
+ (\Lambda - \frac{1}{4}) (\Delta^2 q^\mp - \Delta^2 q^\mp ) e_q^\pm - \frac{1}{2} (\Delta_t q^\mp + (\Lambda^+ + \Lambda^\mp ) \Delta_t q^\mp ) q = 0, \ldots, Q_m .
\]  

(25)

These equations are exactly valid for any multi-dimensional TRT scheme with any equilibrium (we signalize a typo in Eq. (2.2) [19] for term of \( \Lambda = \frac{1}{4} ) \). They are expressed via the temporal and spatial central-difference operators. In time, \( \Delta_t \psi(\bar{r}, t) = \frac{1}{2} (\psi(\bar{r}, t + 1) - \psi(\bar{r}, t - 1)) \) and \( \Delta^2_t \psi (\bar{r}, t) = \psi(\bar{r}, t + 1) - 2\psi(\bar{r}, t) + \psi(\bar{r}, t - 1) \). In space, the central-differences apply link-wisely: \( \Delta q^\psi (\bar{r}, t) = \frac{1}{2} (\psi(\bar{r} + \bar{c}_q, t) - \psi(\bar{r} - \bar{c}_q, t)) \) and \( \Delta^2 q^\psi (\bar{r}, t) = \psi(\bar{r} + \bar{c}_q, t) - 2\psi(\bar{r}, t) + \psi(\bar{r} - \bar{c}_q, t) \), \( \forall \psi = \{e_q^\pm, g_q^\pm \} \). Exact mass conservation equation reads

\[
\sum_{q=0}^{Q_m} g_q^+(\bar{r}, t) = 0 .
\]  

(26)

Summing Eqs. (25), the time-operators applied to \( \sum_{q=0}^{Q_m} g_q^+(\bar{r}, t) \) vanish due to Eq. (26) and the exact mass conservation equation takes the form:

\[
\Delta t \sum_{q=0}^{Q_m} e_q^+ + \Delta q e_q^- = \Lambda^+ (\sum_{q=0}^{Q_m} \Delta q^2 e_q^+ - \sum_{q=0}^{Q_m} \Delta q^2 e_q^- ) - (\Lambda - \frac{1}{4}) (\sum_{q=0}^{Q_m} \Delta q^2 e_q^+ + \sum_{q=0}^{Q_m} e_q^- )^2 = C(\bar{r}, t) .
\]  

(27)

When \( \Lambda = \frac{1}{4} \), Eq. (27) takes the form of the central-difference scheme applied to the equilibrium components:

\[
\Lambda = \frac{1}{4} \quad \Delta t C + \sum_{q=1}^{Q_m} \Delta q e_q^- = \Lambda^+ (\sum_{q=1}^{Q_m} \Delta q^2 e_q^+ - \Delta^2 q^2 C) .
\]  

(28)
This distinguished discretization property conducts $\Lambda = \frac{1}{2}$ to advanced stability. \cite{17,19}. In Appendix A, we extend analysis \cite{19} of Eq. (27) for variable velocity field. As previously, we assume the linear equilibrium distribution with respect to mass variable $C$: $e^i_q(\vec{r}, t) = E^i_q(U)C(\vec{r}, t)$, $\nu q$. The fourth-order accurate approximation takes the form:

$$\partial_t C = [R_1 + R_2 + R_3 + R_4]C,$$

(29)

where the four operators $R_k$ are expressed via the two families of the differential operators, $[S_{2k}]C$ and $[S_{2k-1}]C$:

$$[S_{2k}]C = \sum_{q=1}^{Q_m} \partial_q^{2k} E^+_q C, \quad [S_{2k-1}]C = \sum_{q=1}^{Q_m} \partial_q^{2k-1} E^-_q C, \quad \partial_q = (\nabla, \vec{c}_q) = \sum_{\alpha=1}^{d} \partial_{\alpha} c_{q\alpha}, \quad k \geq 1.$$  

(30)

In considered case, $E^+_q = E^+_q(c_e, \vec{U})$ and $E^-_q = E^-_q(\vec{U})$. Hereby, $\partial_q^k C$ denotes $n$th-order directional derivative; $[S_n^q]C$ means that the operator $S_q$ applies $n$-times to $C(\vec{r}, t)$. All operators (30) are independent of the relaxation rates. It is important to say that all temporal derivatives are accounted in Eq. (29), by sequentially replacing $\partial_q^{2k-1}$ and $\partial_q^{2k}$ in Taylor’s expansion of $\Delta t$ and $\Delta t^2$ with the spatial operators, by employing the lower-order approximations of Eq. (29). The advantage of the recurrence equations is that any-order analysis develops systematically on the base of the Taylor expansion, independently of the dimension of the discrete-velocity set and specific equilibrium formulation.

3.2. Second-order equation and numerical diffusion

This analysis accounts that according to Eqs. (13), (16), $\sum_{q=1}^{Q_m} E^+_q = 1$ and $\sum_{q=1}^{Q_m} E^-_q \vec{c}_q = \vec{U}(\vec{r})$. Assume the simplest configuration where the equilibrium parameters as $c_e$ and weights, and the relaxation eigenvectors $\Lambda^\pm$, are set constant over the grid. At the first-order Eq. (29) reads

$$\partial_t C = [R_1]C, \quad [R_1]C = -[S_1]C, \quad [S_1]C = \sum_{q=1}^{Q_m} \partial_{\alpha} E^-_q(\vec{U})c_{q\alpha} = \nabla \cdot \vec{U}C.$$ 

(31)

At the second-order we replace in Eq. (27), $\Lambda^{-}([\sum_{q=1}^{Q_m} \alpha R^2_q] \vec{c}_q) = \Lambda^{-}[S_2]C$ and $\Lambda^{-}[\Delta t^2]C \approx \Lambda^{-}\alpha^2 C$ by $\Lambda^{-}[S_1^2]C$, with the help of Eq. (31). Summing the first- and second-order components, we separate $[S_2]C$ into a sum of the two components, $[S_2](cEtq^{(m)})C$ and $[S_2](E^{(u)})C$, and then the second-order approximation of the transport equation reads using Eq. (16):

$$\partial_t C + [S_2]C = [R_2]C, \quad [R_2]C = \Lambda^{-}[D_2]C, \quad [D_2]C = [S_2]C - [S_1^2]C,$$

where

$$[S_2](cEtq^{(m)})C = [S_2](Ec^{(m)})C + [S_2](E^{(u)})C,$$

$$[S_2](Ec^{(m)})C = \sum_{\alpha, \beta} \partial_{\alpha} E^{(m)}q_{\alpha}c_{q\beta} = \sum_{\alpha=1}^{d} \partial^2_{\alpha} C = c_e \Delta C,$$

$$[S_2](E^{(u)})C = \sum_{\alpha, \beta} \partial_{\alpha} E^{(u)}q_{\alpha}c_{q\beta} = \sum_{\alpha=1}^{d} \partial^2_{\alpha} U^2 + \sum_{\alpha \neq \beta} \partial_{\alpha} \partial_{\beta} U_{\alpha} U_{\beta},$$

$$[S_1^2]C = \sum_{q=1}^{Q_m} t^{(a)}_{q} \alpha \partial_{\alpha} U_{\alpha} c_{q\alpha} = \sum_{q=1}^{Q_m} t^{(a)}_{q} \alpha \partial_{\alpha} \partial_{\beta} U_{\alpha} U_{\beta}.$$ 

(32)

The component $-\Lambda^{-}[S_1^2]C$ of the diffusion part $\Lambda^{-}[D_2]C$ is referred to as the numerical diffusion of the scheme. In constant velocity field, its tensor has entries $D^{(num)}_{\alpha\beta} = -\Lambda^{-} U_{\alpha} U_{\beta}$. The diffusion term $\Lambda^{-}[S_2(E^{(u)})]C$ aims to create the anti-numerical-diffusion tensor. However, in the minimal models, its last term $\sum_{\alpha \neq \beta} \partial_{\alpha} \partial_{\beta} U_{\alpha} U_{\beta}$ vanishes, making them impossible to remove the cross-numerical-diffusion entries with the TRT scheme. In full models, the diagonal links do this, without further corrections in multi-dimensional constant velocity field at least. In what concern the present work, in channel flow $\vec{U} = U(x, y)$, the cross-diagonal entries $-\Lambda^{-} U_{x} U_{y}$ vanish and Eq. (32) reads with

$$[S_1]C = U_x(y) \partial_{y} \partial_{x} C, \quad [S_1^2]C = U_x^2 \partial_{x} C, \quad [S_2]C = c_e \Delta C + U_x^2 \partial_{x} C, \quad [D_2]C = c_e (\partial_{x}^2 C + \partial_{y}^2 C).$$ 

(33)

Thereby, for any weight-family obeying Eqs. (16), the modeled second-order equation (32) reads in channel flow:

$$\partial_t C + U_x(y) \partial_{y} \partial_{x} C = D_0(\partial_{x}^2 C + \partial_{y}^2 C), \quad D_0 = c_e \Lambda^{-}, \quad y \in [0, H].$$

(34)

This equation is equivalent to Eq. (1) for the same $Re$ (cf. Eq. (15)). The numerical scheme is then expected to produce Eq. (4) for the averaged concentration, which reads in lattice units:
\[ \partial_t \tilde{C} + U \partial_x \tilde{C} = D_0 (1 + k_T) \tilde{C}, \quad k_T = \frac{Pe^2}{210}, \quad Pe = \frac{U H}{c_e \Lambda}, \quad \text{with} \]

\[ U = \langle U_x(y) \rangle = \frac{1}{H} \int_0^H U_x(y) dy = \frac{U_0 H^2}{12}, \quad U_x(y) = \frac{U_0}{2} y (H - y). \quad (35) \]

In what follows, we examine \( \text{err}_D \), the relative error to modeled dispersion coefficient \( D \) in Eq. (35):

\[ \text{err}_D = \frac{D^{(\text{num})}}{D} - 1, \quad D = D_0 (1 + k_T). \quad (36) \]

where \( D^{(\text{num})} \) will be extracted from the measured variance of the averaged concentration field. Notice that the difference \( \text{err}_D (E_3^{(u)} = 0) \), between the value \( \text{err}_D \) obtained by dropping/including correction \( E_3^{(u)} \) in Eq. (17), is expected to read in parabolic profile (where \( \langle U_x^2 \rangle = \frac{6uy^2}{\Lambda^2} \)):

\[ \text{err}_D (E_3^{(u)} = 0) = -\frac{\langle U_x^2 \rangle}{c_e (1 + k_T)} = -\frac{6u^2}{5c_e (1 + k_T)}, \]

\[ \text{err}_D (E_3^{(u)} = 0) \mid_{k_T > 1} \approx -\frac{6 \times 210 u^2}{5c_e Pe^2} \mid_{Pe^2 > 210} = \frac{252 c_e (\Lambda^-)^2}{H^2} \mid_{\Lambda^2 \rightarrow 0} \rightarrow 0. \quad (37) \]

This tells us that in the presence of the Taylor dispersion, the relative contribution of the numerical diffusion becomes insignificant when \( c_e (\Lambda^-)^2 \) is small. Typically, we decrease \( c_e \) and, especially \( \Lambda^- \), to attain high \( Pe \) numbers, therefore \( c_e (\Lambda^-)^2 \) decreases faster than \( Pe \) increases. This explains the results [25] which only show the improving due to specific anti-numerical-diffusion matrix-entries over the MRT scheme with \( E_3^{(u)} \)-term, for relatively large diffusion values as \( c_e = \frac{1}{3} \), \( \Lambda^- = \{ 2, \frac{1}{2} \} \). Furthermore, no difference between the two schemes is found [25] as \( Pe > 16 \) for \( \Lambda^- = 1/20 \), when also dropping/including of the \( E_3^{(u)} \)-term does not play any role, in agreement with our estimate (37).

3.3. Longitudinal numerical dispersion in channel flow

Our starting point is equation (29) where we examine the third- and fourth-order corrections, \( R_3 \) given by Eq. (A.17) and \( R_4 \) given by Eq. (A.21), respectively. The high-order corrections associated with the \( E_3^{(u)} \)-term are neglected by the present analysis, justified by Eq. (37) and confirmed by further numerical validation. Using idea of the Taylor analysis, \( C(x, y, t) \) is decomposed around its averaged value \( \bar{C}(x, t) \): \( C(x, y, t) = \bar{C}(x, t) + C'(x, y, t) \) in one-dimensional velocity field \( U_x(y) \). We then identify four following components in the right-hand side of Eq. (29):

\[ \begin{align*}
(1) \quad R^{(3,1)} &= c_{3,1} c_e U_x(y) \partial_x \partial_y^2 C', \\
(2) \quad R^{(3,2)} &= -4 \times 3t_d^{(a)} c_{3,2} U_x(y) \partial_y^2 \partial_x C' = -3(1 - 2t_d^{(a)}) c_{3,2} U_x(y) \partial_x \partial_y^2 C', \quad \text{with} \\
& \quad c_{3,1} (\Lambda^-, \Lambda) = 2(\Lambda^-)^2 + \Lambda - \frac{1}{4}, \quad c_{3,2} = (\Lambda - \frac{1}{12}),
\end{align*} \quad (38) \]

and

\[ \begin{align*}
(3) \quad R^{(4,1)} &= c_{4,1} c_e \partial_x^2 \partial_y^2 (\partial_x^2 C), \\
(4) \quad R^{(4,3)} &= c_{4,3} c_e \partial_y^2 (\partial_x^2 C), \quad \text{with} \\
& \quad c_{4,1} (\Lambda^-, \Lambda) = -L^- (\Lambda^-)^2 + \Lambda - \frac{1}{4}, \quad c_{4,3} (\Lambda^-, \Lambda) = \Lambda^- (\Lambda - \frac{1}{6}), \quad \Lambda^- = \frac{D_0}{c_e}.
\end{align*} \quad (39) \]

The two terms (38) originate, respectively, from two different components in \( [R_3] C \), namely \( c_{3,1} [S_1 S_2] C \) and \( -c_{3,2} [S_3] C \) in Eq. (A.15). In turn, the two terms (39) appear from \( c_{4,1} [S_2] C \) and \( c_{4,3} [S_4] C \), respectively, in \( [R_4] C \) (see Eq. (A.21)). If we plug the Taylor Ansatz (6): \( D_0 \partial_x^2 \approx U_y(y) \partial_x C \), the sum of two first terms becomes

\[ R^{(3,1)} + R^{(3,2)} \approx \frac{\gamma^{(1)}}{D_0} U_x(y) U_y(y) \partial_x \partial_y^2 C. \quad \gamma^{(1)} = c_{3,1} c_e - 3(1 - 2t_d^{(a)}) c_{3,2}. \quad (40) \]

This term produces correction \( D_0 \gamma^{(1)} k_T^{(1)} \) to dispersion coefficient \( D_0 (1 + k_T) \) in averaged equation (35):

\[ k_T^{(1)} = \frac{\langle U_x(y) U_y(y) \rangle}{D_0} = \frac{\langle U_y(y)^2 \rangle}{D_0}, \quad U_x(y) = \mathcal{U} + U'(y), \quad \mathcal{U} = \langle U_x(y) \rangle, \quad \langle U'(y) \rangle = 0. \quad (41) \]

In channel Poiseuille flow,
\( k_T^{(1)} = \frac{\int_0^H (U'(y))^2 \, dy}{D_0 H} = \frac{U^2}{5D_0} = \frac{Pe^2}{5H^2} \). 

(42)

In turn, if we plug the Taylor Ansatz (6) into the sum \( R^{(4,1)} + R^{(4,3)} \) (see Eq. (39)) it becomes

\[ R^{(4,1)} + R^{(4,3)} \approx \gamma^{(2)} \partial_x^2 U'(y) \partial_x \tilde{C} . \gamma^{(2)} = \frac{C_4 \partial_x^2 + C_4 \cdot 3 \cdot e}{D_0} . \]

(43)

This intrinsic modification of the advection term suggests the altering of the apparent Taylor Ansatz (6):

\[ D_0 \partial_x^2 C' = U'(y) \partial_x \tilde{C} - \gamma^{(2)} (\partial_x^2 U'(y)) \partial_x \tilde{C} . \]

(44)

Now, following the Taylor analysis, we solve equation (44) for \( C'(x, y, t) \) and present solution as

\[ C'(x, y, t) = \frac{\alpha(y) + \beta(y)}{D_0} \partial_x \tilde{C}(x, t) , \text{ with } \alpha(y) = \int_0^y \int_0^y U'(y') \, dy' , \beta(y) = -\gamma^{(2)} U'(y) + K , \]

(45)

(the integration constant \( K \) can be found from condition \( C'(y) = 0 \)). The first component \(-D_0^{-1} \partial_x (\alpha(y) U'(y)) \partial_x \tilde{C}(x, t)\) produces the Taylor coefficient \( k_T D_0 \) following Eq. (7). The additional (truncation) term in the RHS, \(-D_0^{-1} \partial_x (\beta(y) U'(y)) \partial_x \tilde{C}(x, t)\) produces correction \( \gamma^{(2)} k_T D_0 \) to \( k_T D_0 \). The sum of two contributions, \( \gamma^{(1)} k_T^{(1)} \) and \( \gamma^{(2)} k_T^{(1)} \), predicts correction \( \delta k_T = (\gamma^{(1)} + \gamma^{(2)}) k_T^{(1)} \) to Taylor’s coefficient \( k_T \), meaning that the apparent dispersion coefficient is given as \( D_0 (1 + k_T + \delta k_T) \):

\[ \delta k_T = \delta k_T (\tilde{t}_c^{(0)} = \frac{1}{2}) + \delta k_T (\tilde{t}_c^{(0)}) \, \text{, where} \]

\[ \delta k_T (\tilde{t}_c^{(0)} = \frac{1}{2}) = (c_e (\Lambda^2) + \Lambda - \frac{1}{6}) k_T^{(1)} , \]

(47)

\[ \delta k_T (\tilde{t}_c^{(0)}) = -3(1 - 2t_c^{(0)})(\Lambda - \frac{1}{12}) k_T^{(1)} , \quad \tilde{t}_c^{(0)} \in [0, \frac{1}{2}] . \]

(48)

In these relations, the entire correction \( \delta k_T \) is decomposed into two components. The first one, \( \delta k_T (\tilde{t}_c^{(0)} = \frac{1}{2}) \) presents its solution when \( \tilde{t}_c^{(0)} = \frac{1}{2} \), and, in particular, in d2Q5 scheme. The second component \( \delta k_T (\tilde{t}_c^{(0)}) \) is added when velocity-weight is different from \( \frac{1}{2} \). The \( \delta k_T \) behaves as the second-order correction to Taylor dispersion coefficient. It is proportional to \( Pe^2 \) but, in addition, it depends on four free-tunable model parameters, as: (i) equilibrium scale parameter \( c_e \), (ii) diffusion coefficient \( \Lambda^2 \), (iii) free eigenfunction product \( \Lambda^2 \), and (iv), equilibrium velocity-weight stencil \( \tilde{t}_c^{(0)} \). The dependency on \( \Lambda \) only vanishes for \( \tilde{t}_c^{(0)} = \frac{1}{2} \) in d2Q9 scheme. The dependency on the weights only vanishes for \( \Lambda = \frac{1}{4} \). Notice that \( \delta k_T \) does not depend on \( U \) directly but velocity stability limit restricts the product \( \Lambda \cdot c_e \) to interval \( [0, \frac{U_{max}}{H/Pe}] \). In Section 3.4 we reinterpret these results in terms of the dispersion error \( (36) \) and identify most accurate solutions in channel, by also accounting for the summation error.

3.4. “Optimal-dispersion” parameter-space in channel

The derived solution (46)-(48) is expected to be quite general for the longitudinal numerical dispersion with prefactor \( k_T^{(1)} \) depending on velocity-profile. This assumption is confirmed by our recent analysis of the Taylor dispersion in circular pipe (to be reported), that is, the dependency \( \delta k_T (\Lambda, \tilde{t}_c^{(0)}) \) upon free parameters remains valid, but its absolute value needs to be adjusted by some parameter-independent constant. We will relate this to summation/discretization errors in computation of the variance. Similar situation takes place in a channel.

Indeed, one should expect that the “optimal-dispersion” solution \( \Lambda = \frac{1}{6} \) also provides the “optimal-dispersion” choice for d2Q5 scheme at moderate and high Pe numbers, because \( \delta k_T \) vanishes for \( \Lambda = \frac{1}{6} \) in Eq. (47) as \( c_e (\Lambda^2) \rightarrow 0 \). However, all d2Q5 results will show that the dispersion error (36) almost vanishes for \( \Lambda = \frac{1}{4} \), rather than for \( \Lambda = \frac{1}{6} \). One possible explanation of that could be related to summation error peculiar to computation of the second-order moment via the analytical averaging. To illustrate similar effect, let us compute the Taylor coefficient in Eq. (49) via summation, by prescribing exact solution \( \alpha(y) \) in grid nodes \( y_i \):

\[ k_T^{sum} = -D_0^{-2} \frac{1}{H} \sum_{i=1}^{H} U'(y_i) \alpha(y_i) = \frac{Pe^2}{210} + \delta k_T^{sum} . \delta k_T^{sum} = \frac{Pe^2}{5H^2} \left( -\frac{5}{64} - \frac{7}{24H^2} + \frac{155}{448H^2} \right) . \]

(49)

Let us hypothesize now that the weight-independent and \( \Lambda \)-independent correction \( \delta k_T^{sum} \) appears in the apparent diffusion coefficient. By adding \( \delta k_T^{sum} \) to \( \delta k_T \) in Eq. (46), \( \delta k_T (\tilde{t}_c^{(0)} = \frac{1}{2}) \) increases by \(-\frac{5k_T^{(1)}(0)}{64} = (-\frac{1}{12} + \frac{1}{192})k_T^{(1)} \). To simplify expressions
let us first drop $k_T^{(4)}$ (we come back to this point at the end of this work). The numerical dispersion given by Eqs. (46)–(48) with Eq. (42) for $k_T^{(3)}$ then becomes in straight Poiseuille flow:

$$\delta k^T = \delta k^T(t_c^{(a)}) = \frac{1}{2} \delta k^T(t_c^{(a)}) , \quad \text{with} \quad \delta k^T(t_c^{(a)}) = \frac{1}{2} \left( c_T(\Lambda^2)^2 + \Lambda - \frac{1}{4} \frac{Pe^2}{5H^2} \right) ,$$

$$\delta k^T(t_c^{(a)}) = -3(1 - 2t_c^{(a)})(\Lambda - \frac{1}{12}) \frac{Pe^2}{5H^2} , \quad t_c^{(a)} \in [0, \frac{1}{2}] .$$

The relative dispersion error (36) due to the numerical dispersion estimated with Eqs. (50)–(52) reads:

$$d2Q9 : \text{err}^{th}_{D}(t_c^{(a)}) = \frac{\delta k^T(t_c^{(a)})}{D} = \frac{(c_T(\Lambda^2)^2 + 2\Lambda(3t_c^{(a)} - 1) - c_T^{(a)})Pe^2}{5H^2(1 + Pe^2/210)} ,$$

$$d2Q5 : \text{err}^{th}_{D}(t_c^{(a)}) = \frac{\delta k^T(t_c^{(a)})}{D} = \frac{(c_T(\Lambda^2)^2 + \Lambda - \frac{1}{4})Pe^2}{5H^2(1 + Pe^2/210)} ,$$

$$d2Q9 - d2Q5 : ||\text{err}^{th}_{D}|| = \text{err}_{D}(t_c^{(a)}) - \text{err}_{D}(t_c^{(a)}) = \frac{\delta k^T(t_c^{(a)})}{D} \frac{D_0(1 + k_T)}{D_0(1 + k_T)} = -3(1 - 2t_c^{(a)})(\Lambda - \frac{1}{12}) \frac{Pe^2}{5H^2(1 + Pe^2/210)} .$$

This last line shows the difference between the d2Q9 and d2Q5, it only vanishes for $\Lambda = \frac{1}{4}$ when err$^{th}_{D}(t_c^{(a)})$ becomes weight-independent. Therefore, it is expected that the d2Q9 will produce the same numerical dispersivity as the d2Q5 for $\Lambda = \frac{1}{12}$. Besides, err$^{th}_{D}$ reduces with the space resolution as the second-order correction at fixed Pe. This solution has the interesting limits when $Pe \to \infty$:

$$d2Q9 : \text{err}^{th}_{D}(t_c^{(a)}) = \frac{\delta k^T(t_c^{(a)})}{D} = \frac{21(4\Lambda(3t_c^{(a)} - 1) - c_T^{(a)})}{H^2} ,$$

$$d2Q9(t_c^{(a)} = \frac{1}{3}) : \text{err}^{th}_{D}(t_c^{(a)}) = -\frac{7}{H^2} , \forall \Lambda ,$$

$$d2Q9(\Lambda = \frac{1}{12}) : \text{err}^{th}_{D}(t_c^{(a)}) = \frac{7}{H^2} , \forall t_c^{(a)} ,$$

$$d2Q5 : \text{err}^{th}_{D}(t_c^{(a)}) = \frac{42(\Lambda - \frac{1}{4})}{H^2} , \forall t_c^{(a)} .$$

Remarkably that in the limit of high Pe, err$^{th}_{D}$ only depends on $\Lambda$ and $t_c^{(a)}$. That is, err$^{th}_{D}(t_c^{(a)})$ is predicted to be independent of the velocity amplitude and Pe when $c_T$ and/or $\Lambda^2$ are sufficiently small. Another singular property is that in d2Q5, err$^{th}_{D}(t_c^{(a)})$ vanishes when $\Lambda = \frac{1}{4}$. However, in two cases when either err$^{th}_{D}$ is $\Lambda$-independent for $t_c^{(a)} = \frac{1}{3}$, or weight-independent for $\Lambda = \frac{1}{12}$, it has the same but non-zero amplitude as Pe increases. In the opposite limit Pe $\to 0$, err$^{th}_{D}$ becomes weight-independent $\forall \Lambda$:

$$\text{err}^{th}_{D}(t_c^{(a)}) = \text{err}^{th}_{D}(t_c^{(a)}) = \frac{21(4\Lambda(3t_c^{(a)} - 1) - c_T^{(a)})}{H^2} .$$

This tells us that as $k_T \to 0$, err$^{th}_{D}(t_c^{(a)})$ behaves similar as the numerical-diffusion contribution err$^{th}_{D}(E^{(a)}_{L}) = -\frac{d^2 U}{\pi c_T}$ (cf. Eq. (37)). Therefore, at small Pe, Eq. (60) enforces the using of small values $\frac{d^2 U}{\pi c_T}$, below the necessary stability limit $\sqrt{U^2} = 2c_T$ (if $E^{(a)}_{L}$ is included) or $\sqrt{U^2} = c_T$ (if $E^{(a)}_{L}$ is omitted).

The theoretical predictions (53)–(54) are illustrated in Fig. 3 when the advection velocity is set on the d2Q5 stability line $U = U_{max} = \frac{u}{2}$ with $U_{max}$ given by Eq. (22). The results for err$^{th}_{D}(c_T)$ in d2Q5 are depicted in three first diagrams for three values $\Lambda^2 \in \left(\frac{1}{2}, \frac{1}{4}, \frac{1}{4}\right)$. They correspond to $\text{Pe} = [2, 1, 0.55]$ in three Tables 3–5 from [25] and they will be compared in next section to numerical results. We set here $H = 12$ as in majority of our numerical solutions. When $\Lambda^2$ is large (the leftmost diagram), Pe is small, the dependency err$^{th}_{D}(c_T)$ is not monotonic on the stability line, and err$^{th}_{D}$ reduces to zero for $c_T = \frac{1}{2}$ where $U_s = 0$. When $\Lambda^2$ decreases, the dependency err$^{th}_{D}(c_T)$ becomes smoother (second diagram), and finally, err$^{th}_{D}$ becomes $c_T$-independent for small $\Lambda^2$ (third diagram). In this third diagram, the results are almost $\Lambda^2$-independent as $\Lambda^2$ decreases and err$^{th}_{D}$ scales as $\Lambda^2$ (if $\Lambda^2$ is included). The results in the last diagram are depicted for d2Q9($t_c^{(a)} = \frac{1}{3}$) where err$^{th}_{D}$ is $\Lambda$-independent and then three values $\Lambda^2$ are plotted together. This last diagram shows three similar situations for err$^{th}_{D}(c_T)$: the non-monotonomous behavior for relatively large $\Lambda^2$, followed by almost linear dependency err$^{th}_{D}(c_T)$ for intermediate $\Lambda^2$, and then $c_T$-independent result for small $\Lambda^2$. When $c_T \to 0$, err$^{th}_{D}$ takes the same, independent of $\Lambda^2$ and Pe, asymptotic value (57). Several typical solutions to vanish err$^{th}_{D}$ in d2Q9 scheme are:
The theoretical predictions (54) for relative diffusion error \( \text{err}_{D}^{(6)} \) due to numerical dispersion in d2Q5 scheme are depicted in three first diagrams when \( \Lambda^- \in \left[ \frac{1}{2}, \frac{1}{3} \right] \), from the left to the right, and \( \Lambda \in \left[ \frac{1}{2}, \frac{1}{4}, \frac{1}{3} \right] \) (dotted (blue), dashed (magenta), solid (red) and dash-dotted (black) lines). The fourth diagram plots d2Q9 result (53) for \( t_c^{(a)} = \frac{1}{3} \) where \( \text{err}_{D}^{(3)} \) is \( \Lambda \)-independent, with \( \Lambda^- \in \left[ \frac{1}{2}, \frac{1}{3}, \frac{1}{4} \right] \) (dashed (magenta), dotted (blue), solid (red)). The peak velocity is located on the stability line (22); \( H = 12 \) for all diagrams. (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

\[
d_{2Q9} : \quad c_e (\Lambda^-)^2 = \frac{1}{6} \text{ if } t_c^{(a)} = \frac{1}{3}, \\
\text{then } P_{\text{max}}^{\text{diff}} = \frac{2}{3} \sqrt{c_e \Lambda^{-}} = \frac{4}{3} \sqrt{2c_e}, \quad c_e \in [0, \frac{1}{4}],
\]

\[
d_{2Q9} : \quad \Lambda (t_c^{(a)} = \frac{1}{3} \frac{t_c^{(a)}}{4(3t_c^{(a)}) - 1}, t_c^{(a)} \in [\frac{1}{2}, \frac{1}{3}], \text{ if } c_e (\Lambda^-)^2 \approx 0 (Pe \rightarrow \infty).
\]

Equation (61) tells us that by vanishing \( \delta k_{\text{T}} \) on the advection stability line (22) for \( c_e \in [0, \frac{1}{4}] \), the scheme is limited to \( P_{\text{max}}^{\text{diff}} = \frac{2}{3} \sqrt{c_e H} \) for \( t_c^{(a)} = \frac{1}{3} \). On the other side, as has been already mentioned, the velocity constraint (22) is expected to relax for \( t_c^{(a)} = \frac{1}{3} \). When \( Pe \) is sufficiently large, \( \text{err}_{D}^{(6)} \) vanishes due to relationship (62) where \( \Lambda \) specifically depends on \( t_c^{(a)} \). This solution only exists in the interval \( t_c^{(a)} \in [\frac{1}{2}, \frac{1}{3}] \) and it reduces to \( \Lambda = \frac{1}{4} \) for \( t_c^{(a)} = \frac{1}{3} \) in d2Q5 scheme. The d2Q5 scheme vanishes \( \text{err}_{D}^{(6)} \) for

\[
d_{2Q5} : \quad c_e (\Lambda^-)^2 = \frac{1}{4} - \Lambda, \quad \Lambda \in [0, \frac{1}{4}] \text{ then} \]

\[
\Lambda^- = \frac{Pe}{H} \left( \frac{1}{4} - \Lambda \right), \quad \text{or}
\]

\[
c_e = \frac{3 - \Lambda}{(\Lambda^-)^2}, \quad \text{e.g., } c_e = \frac{1}{3}, \quad \Lambda^- = \frac{1}{2}, \quad \Lambda = \frac{1}{6},
\]

\[
d_{2Q5} : \quad \Lambda = \frac{1}{4} \text{ if } c_e (\Lambda^-)^2 \approx 0 (Pe \rightarrow \infty).
\]

The TRT choice (65) is curious because it vanishes the dispersion error for popular parameter choice, by adopting hydrodynamic choice \( c_e^2 = \frac{1}{4} \) for \( c_e \) and specific BGK choice \( \tau = 1 \) for \( \Lambda^+ \), together with advanced diffusion choice \( \Lambda = \frac{1}{6} \). Nevertheless, solution (66) is of particular interest, because it is expected to behave most stably and accurately. The numerical results in Section 4 will examine all these predictions for d2Q5 and d2Q9 models with zero-normal-flux boundary condition.

4. Numerical results and truncation predictions

4.1. Numerical set-up

The initial concentration condition is set as

\[
C(x_0, t = 0) = 1, \quad C(x \neq x_0, t = 0) = 0.
\]

The first raw spatial moments of the averaged concentration, \( \mu_n(t) = \int_{-\infty}^{\infty} x^n \hat{C}(x, t) dx \) and the central moments \( \mu_n^*(t) = \int_{-\infty}^{\infty} (x - \mu(t))^n \hat{C}(x, t) dx \), \( n = 0, 1, 2, \) are expected to obey

\[
\mu_0 = 1, \quad \mu_1 = \mu(t), \quad \mu_2 = 2Dt + \mu_1^2, \quad \mu_2^* = 2Dt, \quad D = D_0(1 + k_f).
\]

In all simulations, the periodic boundary conditions are applied at inlet/outlet, the measurements are performed when the concentration front is far from these ends. The average concentration \( \hat{C}(x) \) and its raw moments are computed as the arithmetical mean values. The zero moment is fulfilled exactly due to mass-conserving specular reflection rule applied for horizontal walls. We report time-independent values \( L^{(num)} \) and \( D^{(num)} \), \( L^{(num)} = (\mu_1(t + \delta t) - \mu_1(t))/\delta t \) and \( D^{(num)} = (\mu_2^*(t + \delta t) - \mu_2^*(t))/(2\delta t) \), located zero velocity midway the grid nodes in parabolic velocity field, \( L^{(num)} \) is expected as
Table 1

Exp. 1. The d2Q9 MRT-A model [25] (Tables 3–5 there) and the d2Q5-BB are compared for $\alpha_{r0}$% when $H = 32$. The three series of results are presented for $\Lambda^- = \{\frac{1}{2}, \frac{1}{3}, \frac{1}{6}\}$, increasing $Pe$ with $U$ in each series. The d2Q5 is applied with parameter choice (65) in case (a) and (b), as following: (a) $\Lambda^- = \frac{1}{2}$, $c_r = \frac{1}{2}$, $\Lambda = \frac{1}{2}$, (b) $\Lambda^- = \frac{1}{3}$, $c_r = \frac{1}{3}$, $\Lambda = \frac{1}{3}$. In case (c), $\Lambda^- = \frac{1}{6}$, $c_r = \frac{1}{2}$ and $\Lambda = \frac{1}{6}$ following Eq. (66).

<table>
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<th>d2Q5</th>
<th>Pe</th>
<th>MRT-A</th>
<th>d2Q5</th>
<th>Pe</th>
<th>MRT-A</th>
<th>d2Q5</th>
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</tr>
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<tr>
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<td>73.9</td>
<td>$-1.927 \times 10^{-3}$</td>
<td>739</td>
<td>$-1.09 \times 10^{-3}$</td>
<td></td>
</tr>
</tbody>
</table>

$$U^{(\text{num})} = \frac{1}{H} \sum_{i=1}^{H} U_x(y_i) = U(1 + \frac{1}{2H^2}).$$

(69)

In d2Q5, the specular reflection reduces to bounce-back rule (BB hereafter). The d2Q5 has the same solutions for $U^{(\text{num})}$ and $D^{(\text{num})}$ either using the bounce-back or periodic conditions at the horizontal walls, and $U^{(\text{num})}$ obeys Eq. (69) exactly. The d2Q5 shares these properties for any equilibrium weights applying specular reflection. Since these two schemes, hereafter abbreviated as d2Q5-BB and d2Q9-SNL, guarantee zero-normal-flux boundary conditions without any restriction of the tangential advection–diffusion flux, we employ them to validate the bulk truncation analysis of the numerical dispersion.

4.2. Taylor dispersion with the d2Q5 model

We recall that the molecular diffusion coefficient $D_0$ is modeled via product of the equilibrium parameter $c_r$ from Eq. (13) and the positive eigenfunction $\Lambda^-$ of the anti-symmetric collision mode (see Eq. (11)). When channel width $H$ is fixed, the d2Q5 allows to select (i) $c_r \in [0, \frac{1}{2}]$, (ii) $\Lambda^- > 0$ and (iii) $U \in [0, U^{\text{max}}]$, with $U^{\text{max}} = \frac{1}{2} |U^{\text{max}}(c_r)|$, $|U^{\text{max}}(c_r)|$ is set by Eq. (22) and illustrated in Fig. 2: the largest two-dimensional velocity amplitude: $\max_{c_r} (|U^{\text{max}}|) = \sqrt{2}/2$ takes place for $c_r = \frac{1}{3}$. These three parameters are inter-connected via $Pe = UH/c_r$. The MRT operator allows, in addition, to freely prescribe eigenfunction $\Lambda^+$ of the symmetric mode which is defined from free-tunable choice of $\Lambda$: $\Lambda^+ = \Lambda/\Lambda^-$. The numerical results and theoretical predictions of the numerical dispersions are compared for all computations.

It is expected that the d2Q9 and d2Q5 TRT schemes with $E^{(u)}_q$-term in Eqs. (17), (19), on the one side, and the matrix-based MRT-A model [25] without it, on the other side, remove their numerical diffusion and produce the same second-order ADE in channel flow. However, the MRT-A model [25] has been found more accurate than the $E^{(u)}_q$-based MRT model for small $Pe$. We guess that the reported improving is mostly related to different amounts of the numerical dispersion; this situation can be reversed for another or optimized parameter choice, as will be first demonstrated for d2Q5 scheme.

4.2.1. Experiment 1

The MRT-A collision operator employed [25] differs from the TRT because, first, it introduces non-zero cross-entries in standard MRT collision basis for removing of the numerical diffusion; and secondly, because it sets two slightly different symmetric eigenfunctions: $\Lambda^+_c = (1/1.2 - \frac{1}{2}) = \frac{1}{2}$ for two shear-stress vectors and $\Lambda^+_v = (1/1.1 - \frac{1}{2}) = \frac{1}{2}$ for two energy vectors. The numerical dispersion has not been predicted for MRT-A but in principle, it may depend on all products of the symmetric/anti-symmetric eigenfunctions. Namely, MRT-A produces $\Lambda_v = \Lambda^+_v \Lambda^- = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$ in series of three measurements with $\Lambda^- = (\frac{1}{2}, \frac{1}{2}, \frac{1}{2}, \frac{1}{2})$. In this section, we will provide the results for $\Lambda$ from this list, even if it is expected from the previous analysis [19] that $\Lambda = \frac{1}{2}$ and $\Lambda = \frac{1}{6}$ will have poor accuracy and stability, respectively. We also add $\Lambda = \frac{1}{4}$ for its distinguished stability properties and $\Lambda = \frac{1}{12}$ for its advection accuracy.

We first adopt the parameter choice [25] from their Tables 3–5 for $H = 32$. The computations [25] are all run with $c_r = \frac{1}{2}$ where MRT-A applies $t^{(m)}_c = t^{(u)}_c = \frac{1}{2}$, $t^{(o)}_c = \frac{1}{2}$ (this can be readily obtained equating their equilibrium (37) to Eq. (13)). The results of simulations with the MRT-A from Tables 3–5 in [25] and d2Q5-BB TRT scheme (19) are compared in Table 1. The d2Q5-BB vanishes predicted numerical dispersion with the help of Eq. (65) in two first series of computations, with (a) $\Lambda^- = \frac{1}{2}$, $c_r = \frac{1}{2}$ and (b) $\Lambda^- = \frac{1}{3}$, $c_r = \frac{1}{3}$, in both cases we set $\Lambda = \frac{1}{3}$. In the third series with $\Lambda^- = \frac{1}{6}$, we apply $c_r = \frac{1}{2}$ and $\Lambda = \frac{1}{6}$ following Eq. (66). In each of the three series of simulations, $Pe$ increases together with mean velocity $U$ which takes the same values for MRT-A and d2Q5 in cases (b) and (c), but in case (a), $c_r$ and $U$ are decreased together by a factor of nine with the d2Q5. The results in Table 1 show that in all considered cases, by vanishing numerical dispersion, the d2Q5-BB outperforms the MRT-A by several orders of magnitude for dispersion error $\alpha_{r0}$, in the entire range $Pe \in [2, 128]$ examined [25], on the same grid and with the same values $\Lambda^-$. This confirms that the reported gain in accuracy with the MRT-A for Taylor dispersion in channel is most likely caused by a smaller amount of the numerical dispersion, rather than by the advanced anti-numerical-diffusion mechanism.
Table 2
Exp. 1, \( H = 12 \). The theoretical predictions (54) for err_D^\text{th} and numerical results err_D are compared for d2Q5-BB when \( U = U^{\text{max}}(c_e) \) for different \( \Lambda \). This data is presented in Fig. 4 for \( P_{\text{e}}^{\text{max}} \), the results can be compared with d2Q5-SNL\( (\epsilon_0 = 1/3) \) in Table 13. Unstable results are absent.

<table>
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<th>( P_{\text{e}}^{\text{max}} \approx 9.24 )</th>
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Table 3
This table gives asymptotic prediction (59) for err_D^\text{th} for \( P_{\text{e}} \to \infty \) versus \( \Lambda \) in d2Q5 scheme when \( c_e(\Lambda^-)^2 \approx 0 \) for \( H = 12 \). This estimate agrees with the numerical results for \( P_{\text{e}} > \approx 3 \times 10^2 \) in Tables 2, 4–7.

| \( \epsilon_0 \times 100 \) | 7.29167 | 0 | -2.43056 | -4.86111 | -6.80556 |

Fig. 4. Exp. 1. The diffusion error err_D is plotted versus \( P_{\text{e}} \) when \( \Lambda^- \) decreases: \( \Lambda^- \in \{1/3, 1/4, 1/6\} \) from the left to the right diagram. Numerical results (“symbols”) and theoretical predictions (54) (lines) are depicted for \( H = 12 \) in the top row and \( H = 32 \) in the bottom row; at each diagram, \( \Lambda \) takes four values: \( 1/3 \) (“circles”, blue), \( 1/4 \) (“squares”, magenta), \( 1/6 \) (“lozenges”, red) and \( 1/12 \) (“triangles”, black). The Pe grows with \( U \) up to \( P_{\text{e}}^{\text{max}} \) for \( L^\text{max}(c_e = 1/3) = \sqrt{3}/9 \). The data in Table 2 corresponds to \( P_{\text{e}}^{\text{max}} \). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Now, mean-velocity amplitude \( U \) is increased up to \( U^{\text{max}}(c_e = 1/3) \) in d2Q5 (last line in Table 1), by growing \( P_{\text{e}} \) to \( \approx 740 \) for \( \Lambda^- = 1/20 \), but err_D remains very small, about 10^-3%. Therefore, all results in Table 1 confirm the validity of the optimized parameters (65)–(66) in d2Q5 model. This analysis is extended to d2Q9 model in Section 4.3. Fig. 4 illustrates these three series of measurements for four values \( \Lambda \in \{1/30, 1/4, 1/6, 1/12\} \), with \( H = 12 \) (top row) and \( H = 32 \) (bottom row); the numerical and truncation results for \( H = 12 \) are further reported in Table 2 for \( P_{\text{e}}^{\text{max}}(c_e = 1/3) \) corresponding to \( L^\text{max} = \frac{\sqrt{3}}{9} \) on the advection stability line \( L^\text{max}(c_e) = \frac{2\sqrt{3}}{3}c_e/3 \). The analytical estimate (54) is plotted together with the numerical results in Fig. 4 and for all other results below. An excellent agreement between the numerical and theoretical results is achieved for all computations, a very small discrepancy is only observable for a few points with \( H = 12 \) but it disappears for \( H = 32 \). In principle, we should expect that the larger \( \Lambda \) values, as \( \Lambda = 1/30 \), here, will produce
larger deviations from the theoretical predictions because the amplitudes of the coefficients in (neglected) truncation errors increase with $\Lambda$.

The averaged concentration profiles in Fig. 5 confirm the difference in $\text{err}_D$ for four $\Lambda$ values from Table 2 when $Pe = Pe^{\text{max}}$: the positive-valued $\text{err}_D(\Lambda)$ means larger numerical dispersion and hence, a larger spreading of the profile (see $\Lambda^{-} = 0.5$ where all $\Lambda$ have $\text{err}_D > 0$); this is inversely with the negative-valued $\text{err}_D(\Lambda)$ (see $\Lambda^{-} = 1.20$, $\text{err}_D(\Lambda) < 0$ for $\Lambda < 0.5$). Furthermore, the concentration profiles confirm that $\Lambda = 0.4$ (third diagram) produces quasi-exact solution due to vanishing of the numerical dispersion.

Finally, we increase $Pe^{\text{max}}$ up to $\approx 3400$ in Table 2 by decreasing $(\Lambda^{-})^2$ to $1/6 \times 10^{-4}$. Table 3 shows predicted values $\text{err}_D^{\text{th}}$ of $Pe \rightarrow \infty$ versus $\Lambda$ for this series of measurements. The theoretical predictions for $\text{err}_D^{\text{th}}$ from Table 2 tell us that the asymptotic values are reached for $Pe$ about $3 \times 10^2$ when $H = 12$. Since $c_e(\Lambda^{-})^2 \approx 0$, $\Lambda = 0.4$ has the advanced accuracy in agreement with Eq. (66), with $\text{err}_D \approx -0.1$. We will observe exactly the same accuracy with $\Lambda = 0.4$ in all next computations, when either $c_e$ or $(\Lambda^{-})^2$ is small enough.

Altogether, the results show that (i) $|\text{err}_D|$ increases with $Pe$ when $Pe \ll 300$ for $H = 12$ and $Pe \ll 100$ for $H = 32$; (ii) $\text{err}_D$ becomes $Pe$-independent with higher $Pe$; (iii) for all $Pe$, $\text{err}_D$ depends on $\Lambda$: (iv) when $c_e(\Lambda^{-})^2$ is small (three last columns in Table 2), $\Lambda = 0.4$ annihilates $\text{err}_D$ even in small and intermediate range, $Pe \approx 6-16$. When all model parameters and $U$ are fixed, $\text{err}_D$ reduces in proportion to $H^2$, unless when $\delta k_T$ is eliminated and then the convergence is faster (cf. for $\Lambda = 0.4$: $\text{err}_D \approx 0.1$% in Table 2 for $H = 12$ and $\text{err}_D \approx 10^{-3}$% in Table 1 for $H = 32$). Finally, the reported interval $Pe \in [1.7, 740]$ was stable with $c_e = 1/4$ when $\Lambda \in [0.4, 0.4]$. However, with the reduction of $(\Lambda^{-})^2$ to $1/6 \times 10^{-4}$, $\Lambda = 1/2$ loses stability, and this happens with $\Lambda = 1/60$ already for $(\Lambda^{-})^2 = 10^{-3}$, in qualitative agreement with the predictions of stability analysis. In the next experiments, we further increase $Pe$ by reducing both $c_e$ and $\Lambda^{-}$.

4.2.2. Experiments 2–5

In these series of measurements $Pe$ enlarges in two different ways. First, in Exp. 2, $(\Lambda^{-})^2$ decreases as shown in Table 4. Second, in Exp. 3, $c_e$ decreases as shown in Table 5. Third, in Exp. 4, $(\Lambda^{-})^2$ is reduced by factor 10 with respect to Exp. 3 and $Pe$ increases to $Pe \approx 10^4$, as shown in Table 6. The results are plotted together for these three experiments in Fig. 6. The averaged velocity $U$ is set equal to $U^{\text{max}}(c_e)$ and the four values $\Lambda = \{0.4, 0.4, 0.6, 1.2\}$ are examined in all cases. The asymptotic predictions (59) for $\text{err}_D^{\text{th}}(\Lambda)_{Pe \rightarrow \infty}$ from Table 3 remain valid here and they are depicted by lines in Fig. 6: $\text{err}_D^{\text{th}}$ decreases from about $-7\%$ for $\Lambda = 0.4$ to $7\%$ for $\Lambda = 0.4$.

Additionally, Exp. 5 in Table 7 examines very small values of $c_e$. These results confirm that $\text{err}_D(\Lambda)$ keeps nearly the same asymptotic values as in Exp. 2–Exp. 4. Unstable points are marked with $\times$ and they are lacking on the graphs, the stability is discussed in Section 4.2.4.

The results clearly show that $\text{err}_D$ becomes independent of $U$, $\Lambda^{-}$ and $c_e$, meaning that $\text{err}_D$ is $Pe$-independent on given grid as $Pe$ increases. At the same time, the $\text{err}_D$ varies in proportion to $(\Lambda^{-})^2$, in excellent agreement with the prediction in Eq. (59). Thereby, all these results display that $\text{err}_D$ is set by $\Lambda$ alone when, typically, $Pe > 3 \times 10^2$ for $H = 12$. Altogether, these and previous results confirm the validity of Eqs. (54) and (59) in a wide range of parameters: $c_e \in [0.2 \times 10^{-4}, 0.4]$ and $(\Lambda^{-})^2 \in [0.1 \times 10^{-4}, 9/4]$, when $\Lambda \in [(0.4, 0.4)]$.

4.2.3. Experiment 6: convergence rates with $\Lambda = 0.4$ and $\Lambda = 0.6$

All the results above have shown that when $c_e(\Lambda^{-})^2$ is negligible, the choice (66): $\Lambda = 0.4$ behaves most accurately. It may still exist a very small unaccounted by our analysis discrepancy, e.g., because of summation, truncation correction
because of the variation of \( E[0] \)-term and/or high-order truncation terms. In Exp. 6, we examine the convergence rate for \( \Lambda = \frac{64}{3} \) and \( \Lambda = \frac{1}{2} \). Here, \( U \) is fixed to 1/300, \( c_e \) to \( \frac{1}{2} \) and \( \text{Pe} \approx 48 \), when \( H \) reduces from 6 to 138 with the simultaneous increase of \( \Lambda \) from 1/80 to 23/80. The results are reported in Table 8 and illustrated in the left diagram in Fig. 7. On the finest grid, these series of computations approximately reach the “optimal-diffusion” choice [15,19,39]: \( (\Lambda^-)^2 = \frac{1}{12}, \Lambda = \frac{1}{6} \). The theoretical prediction (54) becomes for fixed velocity \( U, c_e \) and \( \text{Pe} \):
Table 7
Exp. 5, the d2Q5-BB, \( H = 12 \). The table shows error of \( \text{c}_{\text{e}} \) (in percents) when \( (\Lambda^{-})^2 = \frac{1}{4} \) and \( \text{c}_{\text{e}} \) takes very small values. The data with asterisk fluctuates around the steady state. The results agree with the asymptotic prediction \((59)\) shown in Table 3.

<table>
<thead>
<tr>
<th>Pe</th>
<th>( c_{\text{e}} )</th>
<th>( \Lambda )</th>
<th>( \text{err} )</th>
<th>( \text{err} )</th>
<th>( \text{err} )</th>
</tr>
</thead>
<tbody>
<tr>
<td>2771.28</td>
<td>( \frac{1}{2} \times 10^{-2} )</td>
<td>( \frac{1}{2} \times 10^{-2} )</td>
<td>6.9321</td>
<td>-0.08863</td>
<td>-2.4289</td>
</tr>
<tr>
<td>1385.64</td>
<td>( 1 \times 10^{-4} )</td>
<td>( 1 \times 10^{-3} )</td>
<td>6.9378*</td>
<td>-1 \times 10^{-1}</td>
<td>-2.4467</td>
</tr>
<tr>
<td>2771.28</td>
<td>( \frac{1}{2} \times 10^{-4} )</td>
<td>( \frac{1}{2} \times 10^{-3} )</td>
<td>6.93*</td>
<td>-1 \times 10^{-1}</td>
<td>-2.4488*</td>
</tr>
</tbody>
</table>

Fig. 7. Exp. 6, the d2Q5 model. Left diagram: the numerical results from Table 8 for \( \text{c}_{\text{e}} \) with \( (\Lambda^{-})^2 = \frac{1}{4} \) (“squares”, red) and \( (\Lambda^{-})^2 = \frac{1}{2} \) (“circles”, blue), are compared to prediction \((70)\) by increasing \( H \) at fixed \( \text{Pe} = 48 \), \( c_{\text{e}} = \frac{1}{4} \) and \( \Lambda = \frac{1}{4} \), when \( (\Lambda^{-}) \) linearly increases with \( H \) as shown in the middle diagram. Right diagram: the numerical results are compared for \( \text{Pe} = H, \text{Pe} = \frac{2}{3} H \), and \( \text{Pe} = 2H \), \( \text{Pe} = \frac{2}{3} H \), \( c_{\text{e}} = \frac{1}{4} \) and \( (\Lambda^{-}) = \frac{1}{4} \times 10^{-1} \) in both cases. The results are plotted for \( (\Lambda^{-}) = \frac{1}{4} \), \( \text{Pe} = H \) with “circles” (blue) and \( \text{Pe} = 2H \) with “squares” (magenta), and \( (\Lambda^{-}) = \frac{1}{4} \) with “lozenges” (red) and “triangles” (black). (For interpretation of the references to color in this figure legend, the reader is referred to the web version of this article.)

Table 8
Exp. 6, the d2Q5-BB, \( H \in [6, 138] \). This table shows the convergence behavior for \( \text{err}_{\Lambda} \) with channel resolution \( H \) for fixed \( \text{Pe} = 48 \), when \( c_{\text{e}} = \frac{1}{4} \), \( \text{Pe} = \frac{2}{3} H \), and \( (\Lambda^{-}) \) increases from 1/80 \((H = 6)\) to 23/80 \((H = 138)\). The \( \text{err}_{\Lambda} \) is given in percents. The theoretical prediction \((70)\) for \( \text{err}_{\Lambda}^{\text{th}} \) is given for \( (\Lambda^{-}) = \frac{1}{4} \) in the last column; \( \text{err}_{\Lambda}^{\text{th}} (\Lambda = \frac{1}{4}) \approx 5.57 \times 10^{-3} \% \) for all data. The last line shows the exponent \( \alpha \) of pow fit.

<table>
<thead>
<tr>
<th>( H )</th>
<th>( \text{err}_{\Lambda} (\Lambda = \frac{1}{4}) )</th>
<th>( \text{err}_{\Lambda} (\Lambda = \frac{1}{2}) )</th>
<th>( \text{err}_{\Lambda} (\Lambda = \frac{1}{4}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>6</td>
<td>-1.441</td>
<td>-9.141</td>
<td>-8.905</td>
</tr>
<tr>
<td>12</td>
<td>-8.682 \times 10^{-2}</td>
<td>-2.237</td>
<td>-2.222</td>
</tr>
<tr>
<td>18</td>
<td>-1.280 \times 10^{-2}</td>
<td>-9.876 \times 10^{-1}</td>
<td>-9.844 \times 10^{-1}</td>
</tr>
<tr>
<td>24</td>
<td>-2.707 \times 10^{-4}</td>
<td>-5.523 \times 10^{-1}</td>
<td>-5.513 \times 10^{-1}</td>
</tr>
<tr>
<td>30</td>
<td>3.164 \times 10^{-3}</td>
<td>-3.513 \times 10^{-1}</td>
<td>-3.508 \times 10^{-1}</td>
</tr>
<tr>
<td>36</td>
<td>4.396 \times 10^{-3}</td>
<td>-2.422 \times 10^{-1}</td>
<td>-2.419 \times 10^{-1}</td>
</tr>
<tr>
<td>42</td>
<td>4.920 \times 10^{-3}</td>
<td>-1.764 \times 10^{-1}</td>
<td>-1.763 \times 10^{-1}</td>
</tr>
<tr>
<td>48</td>
<td>5.194 \times 10^{-3}</td>
<td>-1.337 \times 10^{-1}</td>
<td>-1.337 \times 10^{-1}</td>
</tr>
<tr>
<td>54</td>
<td>5.334 \times 10^{-3}</td>
<td>-1.045 \times 10^{-1}</td>
<td>-1.044 \times 10^{-1}</td>
</tr>
<tr>
<td>60</td>
<td>5.413 \times 10^{-3}</td>
<td>-8.356 \times 10^{-2}</td>
<td>-8.353 \times 10^{-2}</td>
</tr>
<tr>
<td>138</td>
<td>5.604 \times 10^{-3}</td>
<td>-1.122 \times 10^{-2}</td>
<td>-1.127 \times 10^{-2}</td>
</tr>
<tr>
<td>( \alpha )</td>
<td>-0.0899</td>
<td>-2.0282</td>
<td>-2.0056</td>
</tr>
</tbody>
</table>

\[
\text{err}_{\Lambda}^{\text{th}} = \frac{42(\text{H}^2 \text{Pe}^2 + (\Lambda - \frac{1}{4})c_{\text{e}} \text{Pe}^2)}{c_{\text{e}} \text{H}^2 (210 + \text{Pe}^2)}, \quad (\Lambda^{-}) = \frac{\text{H} \text{Pe}}{c_{\text{e}}}, \quad \text{then } \text{err}_{\Lambda}^{\text{th}} = \frac{42\text{H}^2}{c_{\text{e}}(210 + \text{Pe}^2)} \text{ if } (\Lambda^{-}) = \frac{1}{4} \text{, } \forall \text{H} .
\]

This estimate gives the same value for all values of \( H \) in Table 8 when \( (\Lambda^{-}) = \frac{1}{4} \), \( \text{err}_{\Lambda}^{\text{th}} (\Lambda = \frac{1}{4}) \approx 5.57 \times 10^{-3} \% \). The numerical results agree well when \( H \in [48, 138] \), with \( \text{err}_{\Lambda} \in [5.2, 5.6] \times 10^{-3} \% \). Furthermore, the numerical results confirm the fourth-order convergence for fixed \( \text{Pe} \) and \( \text{Pe}^2 \). At the same time, \( \text{err}_{\Lambda} (\Lambda = \frac{1}{4}) \) is found in almost exact agreement with the result \((70)\) for \( H \geq 12 \) and this choice only shows the second-order convergence. In resume, this example demonstrates the advanced fourth-order convergence of \( (\Lambda^{-}) = \frac{1}{4} \) even in intermediate range \( \text{Pe} = 48 \), because of its vanishing of the numerical dispersion. The rightmost diagram in Fig. 7 displays the effect of the velocity amplitude, by reducing \( \text{Pe} \) alone with \( \text{Pe} \) by a factor of 2. In agreement with the prediction \((70)\), \( \text{err}_{\Lambda} \) is insensitive to velocity magnitude for \( (\Lambda^{-}) = \frac{1}{4} \), as long as \( \text{Pe} \) is sufficiently large and \( \text{Pe}^2/\text{Pe}^2 \) is kept constant, unlike with \( (\Lambda^{-}) = \frac{1}{6} \) on the coarser grids \( H \leq 18 \).

4.2.4. Effective stability
We examine if the stable solutions have been obtained by locating the peak velocity on the two-dimensional stability line \((22)\). Stability predictions give clear preference to \( (\Lambda^{-})^2 = \frac{1}{4} \) and, if \( (\Lambda^{-})^2 > \frac{1}{6} \), to \( (\Lambda^{-}) \in \left[ \frac{5}{6}, \frac{1}{4} \right] \) \((\text{see } 17,37,19)\). The necessary stability conditions \((22)\) are expected to be stable with this parameter choice. The exact dependency \( U^2(c_{\text{e}}, (\Lambda^{-})^2) \) has
Table 9
This table shows the numerical results for $\text{err}_D(E_q^{(u)} = 0)$ in constant velocity field, when equilibrium term $E_q^{(u)}$ is omitted. They coincide with Eq. (71) (in percent). This solution is the same for d2Q5-BB and d2Q9-SNL if $E_q^{(u)}$ is included, then $\text{err}_D = 0$.

<table>
<thead>
<tr>
<th>$U/L = 1/60$</th>
<th>$\text{err}_D[%]$</th>
<th>$U/L = 1/f$</th>
<th>$\text{err}_D[%]$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c_e = 1/4$</td>
<td>$-8.333 \times 10^{-2}$</td>
<td>$1/60$</td>
<td>$-8.333 \cdot 10^{-2}$</td>
</tr>
<tr>
<td>$1/3$</td>
<td></td>
<td></td>
<td></td>
</tr>
<tr>
<td>$1/4$</td>
<td>$-1.111 \cdot 10^{-1}$</td>
<td>$1/30$</td>
<td>$-3.333 \cdot 10^{-2}$</td>
</tr>
<tr>
<td>$1/8$</td>
<td>$-2.222 \times 10^{-1}$</td>
<td>$1/15$</td>
<td>$-1.333$</td>
</tr>
<tr>
<td>$1/200$</td>
<td>$-5.556$</td>
<td></td>
<td>$-100$</td>
</tr>
</tbody>
</table>

been only constructed for d1Q3 model [37], this solution is very complicated and its further approximations were constructed [18]. It has also been recognized that the d1Q3 curves govern the effective stability of the minimal models in advection-dominated zone (see [37]), while the non-negativity condition of the immobile weight bounds the stable domain on the right, as in Eq. (22). The stability in upper subdomain $\Lambda > \frac{1}{4}$ has not been examined in detail because the accuracy typically deteriorates there. At the same time, the choice $\Lambda = \frac{1}{4}$ has been studied carefully, [37,19], and its stable velocity amplitude is drop far below stability line (22) when $c_e$ and/or $\Lambda^-$ decrease towards zero.

First, Table 4 shows that when $c_e = \frac{1}{4}$, $\Lambda = \frac{1}{12}$, the scheme remains stable reducing $(\Lambda^-)^2$ to $\frac{1}{4} \times 10^{-4}$, at least. At the same time, $\Lambda = \frac{1}{10}$ becomes unstable for $(\Lambda^-)^2 = 10^{-3}$. Second, Table 5 shows that by decreasing $c_e$ for fixed value $(\Lambda^-)^2 = \frac{1}{4} \times 10^{-3}$, only $\Lambda = \frac{1}{4}$ and $\Lambda = \frac{1}{2}$ allow to reduce $c_e$ below $\frac{1}{12}$. Third, by further decrease of $(\Lambda^-)^2$ to $\frac{1}{4} \times 10^{-3}$ in Table 6, $\Lambda = \frac{1}{12}$ leaves stability line even for $c_e = \frac{1}{4}$. Fourth, by increasing $(\Lambda^-)^2$ to $\frac{1}{4} \times 10^{-4}$ in Table 7, $\Lambda = \frac{1}{12}$ and $\Lambda = \frac{1}{4}$ remain stable even for very small values $c_e$, up to $c_e = \frac{1}{4} \times 10^{-4}$. Notice however that for reaching of the quasi-steady regime, $U$ was reduced in the two last rows in Table 7 below the stability line $U^{\text{max}} = 2/\sqrt{2c_e}$, but still exceeding the non-negativity line $U = (1 - \sqrt{1 - 4c_e})/3$. With further decrease of $\Lambda^-$, e.g., to $\Lambda^- = 10^{-1}$, the small values of $c_e$ from Table 7 do not reach steady-state regime even with $\Lambda = \frac{1}{4}$. So far, the highest reached value of $Pe$ for maximum velocity amplitude $U^{\text{max}}$ and $H = 12$ is about $Pe = 9915$ in Table 6. This result is obtained with $c_e = 1/192$ and $(\Lambda^-)^2 = \frac{1}{4} \times 10^{-3}$, for $\Lambda = \frac{1}{4}$ and $\Lambda = \frac{1}{2}$. Notice that $|\text{err}_D|$ decreases by a factor of 70 between these two $\Lambda$ values. The $\Lambda^-$ was not further reduced because of the increasing computational time to reach steady values of $D^{\text{num}}$.

On the whole, $\Lambda = \frac{1}{4}$ is clearly recommended both for accuracy and stability in straight Poiseuille flow, because one may increase velocity up to stability line (22) (except for very small values $c_e < 0, \approx 10^{-1}$) for almost zero numerical dispersion. We emphasize that although $c_e$ is commonly fixed (e.g. $c_e = \frac{1}{4}$ in [25], $c_e = \frac{1}{3}$ in [24]), our results show that the highest values of $Pe$ are stable for much smaller values of $c_e$ when $\Lambda \approx \frac{1}{4}$. As one more example, small thermal diffusivity values in high Rayleigh numbers simulations were achieved [42] with d2Q5 scheme by reducing $c_e$ (see Eq. (47) there with $c_e = (4 + a)/10$).

4.2.5. Numerical diffusion and numerical dispersion

Applying the d2Q5-BB/d2Q9-SNL schemes with constant velocity, the first moment yields $U^{\text{num}} = U$, and the second moment produces exact diffusion coefficient $D^{\text{num}} = D_0$, providing that $E_q^{(u)}$ is included into Eqs. (13)–(20). If $E_q^{(u)}$ is omitted (excluding $U\nu_\text{eff}$-terms from Eq. (19)), the numerical diffusion of the scheme is expected to be added to molecular diffusion: $D^{\text{num}} = D_0 + D^{\text{num}}$, with $D^{\text{num}} = -\Lambda^- U^2 = D_0 U^2$. In this case, the necessary stability condition (22):

$$U^2 \leq 2c_e$$

reduces to $U^2 \leq c_e$, for all velocity sets [see (17)]. Furthermore, approaching this stability line, $\text{err}_D(E_q^{(u)} = 0) = -1$, that is, the apparent diffusion coefficient reduces from $D_0$ to 0:

$$U, \text{err}_D(E_q^{(u)} = 0) = -U^2/c_e ,$$

$$\text{err}_D(E_q^{(u)} = 0) = -1 \text{ if } U^2 = c_e .$$

The numerical results in Table 9 confirm these predictions exactly. Therefore, in constant velocity field, $E_q^{(u)}$ should not be omitted unless $U^2 < c_e$.

In Poiseuille profile, all above d2Q5 computations included $E_q^{(u)}$ via $U^2$-terms in Eq. (19). The expected difference in $\text{err}_D$ for case without $E_q^{(u)}$ and with $E_q^{(u)}$ is given by Eq. (37). This estimate is $\Lambda$-independent. Fig. 8 perfectly confirms Eq. (37) for data from Exp. 1, when $\Lambda^- = (\frac{1}{2}, \frac{1}{4}, \frac{1}{2})$, with $\Lambda = \frac{1}{4}$ and $\Lambda = \frac{1}{2}$. This figure clearly shows that the difference in $\text{err}_D$ between the two distributions, without $E_q^{(u)}$ and with $E_q^{(u)}$, reduces with $\Lambda^-$, from about $-40\%$ for $\Lambda^- = \frac{1}{2}$, $\Lambda^\approx 10$ to about $-0.15\%$ for $\Lambda^- = \frac{1}{4}$, $\Lambda^\approx 3 \times 10^2$. In accord with our predictions, numerical diffusion becomes irrelevant when $\Lambda^-$ increases in the presence of mechanical dispersion.

Experiment 7. Now we compare the independent results [24] for Taylor dispersion with our predictions. In this isotropic two-dimensional problem, the d3Q7 MRT collision [24] with two relaxation rates, $\tau_D$ for diffusion coefficient $D = \mathcal{E}(\tau_D - \frac{1}{2})\frac{L^2}{\Delta t}$ (in physical units) and a free value $\tau_p$ for symmetric modes, is expected to produce the same solutions as the d2Q5
Fig. 8. Exp. 1, d2Q5, the same physical parameters as in Fig. 4, \( c_{\xi} = \frac{1}{4} \), \( H = 12 \). This figure illustrates the decreasing role of the non-removed numerical diffusion when \( Pe \) increases with the velocity from the left to the right where \( \Lambda = \{ \frac{1}{3}, \frac{1}{4}, \frac{1}{8} \} \), respectively. The symbols depict the difference in relative diffusion error for the computations without \( E^{(u)}_q \)-term and with it, with \( \Lambda = \frac{1}{4} \) ("squares") and \( \Lambda = \frac{1}{8} \) ("lozenges"). The lines plot \( \Lambda \)-independent theoretical prediction (37): \( \text{err}_D(E^{(u)}_q) = -\frac{\langle U \rangle}{\text{err}_D} \).

Table 10
The four first (TRT) and the four last (BGK) columns show: (i) numerical diffusion given by Eq. (37), \( \text{err}_D(E^{(u)}_q) = 0 \) \(-\frac{\text{err}^2_U}{\text{err}_D^2} \); (ii) numerical dispersion given by Eq. (54), \( \text{err}_D^0 = \frac{\langle (\Lambda^{-2} - 1) \rangle^2}{\text{err}_D} \); (iii) their sum, which is prediction for \( \text{err}_D \) and (iv), numerical value \( \text{err}_D \). The data is in percents. The parameters correspond to Fig. 6 from [24], with \( c_{\xi} = 1/4, Pe = 50, U = Pe c_{\xi} / H \).

<table>
<thead>
<tr>
<th>( \text{err}_D(E^{(u)}_q) = 0 )</th>
<th>( \text{err}_D )</th>
<th>sum</th>
<th>( \text{err}_D(E^{(u)}_q) = 0 )</th>
<th>( \text{err}_D )</th>
<th>sum</th>
<th>( \text{err}_D(E^{(u)}_q) = 0 )</th>
<th>( \text{err}_D )</th>
<th>sum</th>
<th>( \text{err}_D(E^{(u)}_q) = 0 )</th>
<th>( \text{err}_D )</th>
<th>sum</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Lambda^{-} = 0.1 ), ( \Lambda^{+} = 0.5 ), ( \Lambda = 0.05 )</td>
<td>( H = 32 )</td>
<td>( -5.68 \times 10^{-2} )</td>
<td>( -7.47 \times 10^{-1} )</td>
<td>( -8.04 \times 10^{-1} )</td>
<td>( -8.06 \times 10^{-1} )</td>
<td>( -8.99 \times 10^{-1} )</td>
<td>( -9.55 \times 10^{-1} )</td>
<td>( -9.53 \times 10^{-1} )</td>
<td>( H = 64 )</td>
<td>( -1.42 \times 10^{-2} )</td>
<td>( -2.01 \times 10^{-2} )</td>
</tr>
</tbody>
</table>

TRT scheme. The notation convention applies as follows: \( \Lambda^{-} = \tau_p - \frac{1}{4}, \Lambda^{+} = \tau_p - \frac{1}{2}, c_{\xi} = \mathcal{E} \). Since the \( E^{(u)}_q \)-term was omitted (see Eqs. (10) and (25) in [24]), the reported results are expected to contain numerical diffusion. Our prediction then sums the contribution because of the numerical-diffusion, \( \text{err}_D(E^{(u)}_q) = 0 \) given by Eq. (37), with the truncation dispersion \( \text{err}_D^0 \) given by Eq. (54).

The following parameters apply in Table 1 [24]: \( c_{\xi} = \frac{1}{4}, \Lambda^{-} = 0.1, D_0 = 2.5 \times 10^{-2} \), \( \Lambda^{+} = 0.5 \), \( H = 64 \). In first example, \( Pe = 10, U = 3.90625 \times 10^{-3} \) and \( \text{err}_D = -0.068\% \). Our predictions given: \( \text{err}_D(E^{(u)}_q) = 0 \approx -4.96 \times 10^{-3}\% \), \( \text{err}_D^0 \approx -6.53 \times 10^{-2}\% \), \( \text{err}_D = \text{err}_D(E^{(u)}_q) = 0 + \text{err}_D^0 \approx -0.07\% \). The highest investigated value [24] is \( Pe = 160 \), modeled with \( U = 0.0625 \). This gives \( \text{err}_D = -0.216997\% \) (according to private communication, the difference between this value and one reported in Table 1 is due to unaccounted there end-effect). The predictions give: \( \text{err}_D(E^{(u)}_q) = 0 \approx -1.53557 \times 10^{-2}\% \), \( \text{err}_D^0 \approx -2.00867 \times 10^{-1}\% \), \( \text{err}_D = \text{err}_D(E^{(u)}_q) = 0 + \text{err}_D^0 \approx -0.216123\% \). The two results are found in perfect agreement with computations [24]. Next, in accord with our predictions, \( Pe = 50 \) and \( Pe = 160 \) display nearly the same accuracy, with \( \text{err}_D|_{Pe=50} = -0.201\% \) in Table 1 [24]. We further explore results for \( Pe = 50 \) from Fig. 6 in [24] for different resolutions (the numerical data is available due to private communication). Table 10 displays the two separate contributions given by Eqs. (37) and (54) in the two first columns, their sum gives the prediction for \( \text{err}_D \) displayed in the third column, the numerical result [24] is shown last. The velocity diminishes in proportion to \( H \) on the three grids, \( H = \{32, 64, 128\} \). The agreement is very good between the computations and theory for all four examined TRT/BGK combinations of the relaxation rates.

It should be said that, while the numerical diffusion is independent of free relaxation rate and it is always negative, it is not so for the numerical dispersion which is positive when \( \Lambda > \frac{1}{3} - c_{\xi}(\Lambda^{-})^2 \) in d2Q5. The two effects can balance one another, in principle. For example, in simulations with \( \Lambda^{-} = 0.1, U \) is smaller than with \( \Lambda^{-} = 0.6 \) by a factor of 6. In this first case, the numerical dispersion dominates. This situation is reversed in the second case where the numerical diffusion increases as the velocity in square, by a factor of 6\(^2\) and it dominates numerical dispersion.
In conclusion, our predictions for numerical diffusion and dispersion in TRT scheme are confirmed via independent computations [24] and their sum explains the observed there dependency on the free relaxation rate \( \tau_p \). When \( E_q^{(u)} \)-term is dropped, the negative numerical diffusion plays a predominant role if \( U^2 \approx c_e \) and \( k_T \) is small. In the limit \( k_T (P_e^2) \rightarrow 0 \), the amplitude of \( \text{err}_D (E_q^{(u)}) = 0 \) is larger by a factor of 6 than the predicted value of the numerical dispersion \( \text{err}_D (P_e - \text{err}_D) \) in Eq. (60), and these two numerical corrections have the opposite signs: \( \text{err}_D (E_q^{(u)}) = 0 |_{k_T = 0} = -\frac{a}{D_p c_e} \) and \( \text{err}_D (P_e - \text{err}_D) = \frac{a}{D_p} \). Therefore, in the limit \( P_e \rightarrow 0 \), their sum gives the same, \( \Lambda \)-independent relative correction \( \text{err}_D \) as for constant velocity (71): \( \text{err}_D (E_q^{(u)}) = 0 |_{k_T = 0} = -\frac{a}{D_p} \). This result could be expected, because when \( P_e^2 \) is small, the dispersion is small, and numerical dispersion is small, the difference in \( \text{err}_D \) reduces for constant and parabolic profiles. The opposite happens in the limit \( P_e \rightarrow \infty \), when \( \text{err}_D (E_q^{(u)}) = 0 \) asymptotically vanishes while the contribution from the numerical dispersion dominates. Finally, we recall that several possibilities to remove numerical diffusion from the anisotropic diagonal, and anisotropic full matrix, d2Q5/d3Q7 models have been outlined at the end of Section 2.2.2.

4.3. The d2Q9-SNL model

We now consider the d2Q9-SNL scheme applying the standard specular-forward non-local reflection (SNL). In constant and parabolic channel profiles this scheme produces the same solutions as applying the periodic boundary conditions on the horizontal ends. We recall that the truncation analysis predicts correction \( b_k \) to Taylor coefficient \( k_T \) by Eqs. (50)–(52); its relative contribution to \( \text{err}_D \) is specified by Eqs. (53)–(55). In addition to free parameters of the d2Q5, the d2Q9 may independently vary the three families of its equilibrium weights (Fig. 1). Our computations confirm that, in agreement with the predictions, \( \text{err}_D \) is independent of the mass-weigh family \( t_q^{(m)} \) and \( D_p^{(u)} \)-weight family \( t_q^{(u)} \), but it is noticeably affected by the velocity-weight \( t_q^{(v)} \). We first illustrate this dependency on the velocity-weight. The computations involve the same parameters as with the d2Q5 scheme in Fig. 4 for \( U = U^{(\text{max})} (c_e) \), \( P_e = P_e^{(\text{max})} \) but applying the d2Q9-SNL in two configurations: (i) the “hydrodynamic” (standard) weights \( t_q^{(u)} = t_q^{(m)} = \frac{1}{2}, t_q^{(v)} = \frac{1}{2} \), and (ii) the “rotated” d2Q5 model [20]. The corresponding concentration profiles are shown in Figs. 9 and 10. They can be compared with the d2Q5 profiles from Fig. 5. The averaged profiles are very different for three weight-families. They are almost \( \Lambda \)-independent with the standard weights, in entire agreement with Eq. (53). We notice that the “rotated” d2Q5 is much less accurate than the d2Q5, especially for small values \( \Lambda^{-} \) (last two diagrams in the two figures). These results are further quantified in Tables 11 and 12 which show the difference \( |\text{err}_D| = |\text{err}_D (E_q^{(u)})| - |\text{err}_D (E_q^{(v)})| = \frac{1}{2} \) between the d2Q9-SNL and the d2Q5 from Fig. 4. The numerical results are compared to prediction (55) for \( |\text{err}_D^{th}| \).

On the whole, the numerical results are found in a very good agreement with the predictions, especially for \( \Lambda = \frac{1}{4} \) and \( \Lambda = \frac{1}{2} \); the amplitude of \( |\text{err}_D| \) is slightly smaller than the predicted value for \( \Lambda = \frac{1}{2} \), indicating the increasing role of the neglected truncation corrections. The “rotated” d2Q5 model underestimates the dispersive coefficient by a large extent with respect to d2Q5, e.g., \( |\text{err}_D (\Lambda = \frac{1}{2})| \) lies in the interval \( 0.06.33.0\% \) (see Table 12), what explains the noticeable deterioration of its profiles in Fig. 10. Next, in agreement with Eq. (55) where \( |\text{err}_D^{th}| = 0 \) for \( \Lambda = \frac{1}{12} \), Vs, Vqs and VPe, the difference between the standard weights and d2Q5 in Table 11 is very small when \( \Lambda = \frac{1}{12} \). At the same time, the results in Tables 11 and 12 further confirm that \( \Lambda = \frac{1}{12} \) is unstable on the velocity stability line when \( \Lambda^{-} \rightarrow 0 \). It is interesting

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**Table 11**

Exp. 1. This table shows the difference between d2Q9 (\( t_q^{(v)} = \frac{1}{2} \)) and d2Q5: \( |\text{err}_D| = |\text{err}_D (E_q^{(u)})| - |\text{err}_D (E_q^{(v)})| = \frac{1}{2} \) (in percents). The theoretical predictions are given by Eq. (55). Velocity is set on the stability line (22) for \( c_e = \frac{3}{4} \). The \( \text{err}_D (t_q^{(v)}) = \frac{1}{2} \) and \( \text{err}_D (t_q^{(v)}) = \frac{1}{2} \) are shown in Tables 2 and 13, respectively.

<table>
<thead>
<tr>
<th>( \Lambda )</th>
<th>( \text{Pe}^{(\text{max})} \approx 9.24 )</th>
<th>( \text{Pe}^{(\text{max})} \approx 27.71 )</th>
<th>( \text{Pe}^{(\text{max})} \approx 27.73 )</th>
<th>( \text{Pe}^{(\text{max})} \approx 438.18 )</th>
<th>( \text{Pe}^{(\text{max})} \approx 3394.11 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Lambda \cdot \Lambda^{-} )</td>
<td>( \frac{9}{2} )</td>
<td>( \frac{1}{2} )</td>
<td>( \frac{1}{2} \times 10^{-1} )</td>
<td>( \frac{1}{2} \times 10^{-3} )</td>
<td>( \frac{1}{2} \times 10^{-4} )</td>
</tr>
<tr>
<td>(</td>
<td>\text{err}_D^{(u)}</td>
<td>)</td>
<td>(</td>
<td>\text{err}_D^{(v)}</td>
<td>)</td>
</tr>
<tr>
<td>1/2</td>
<td>-3.51</td>
<td>-3.19</td>
<td>-5.94</td>
<td>-8.67</td>
<td>-12.1</td>
</tr>
<tr>
<td>1/4</td>
<td>-1.4</td>
<td>-1.36</td>
<td>-3.82</td>
<td>-3.83</td>
<td>-4.85</td>
</tr>
<tr>
<td>1/6</td>
<td>-0.702</td>
<td>-0.704</td>
<td>-1.91</td>
<td>-1.91</td>
<td>-2.42</td>
</tr>
<tr>
<td>1/12</td>
<td>0</td>
<td>-0.0278</td>
<td>0</td>
<td>-0.0756</td>
<td>0</td>
</tr>
</tbody>
</table>

**Table 12**

Exp. 1. Similar as in Table 11 but for “rotated” d2Q5 scheme [20]. Table shows \( |\text{err}_D| = |\text{err}_D (E_q^{(u)})| - |\text{err}_D (E_q^{(v)})| = \frac{1}{2} \) (in percents), together with the theoretical prediction (55).

<table>
<thead>
<tr>
<th>( \Lambda )</th>
<th>( \text{Pe}^{(\text{max})} \approx 9.24 )</th>
<th>( \text{Pe}^{(\text{max})} \approx 27.71 )</th>
<th>( \text{Pe}^{(\text{max})} \approx 27.73 )</th>
<th>( \text{Pe}^{(\text{max})} \approx 438.18 )</th>
<th>( \text{Pe}^{(\text{max})} \approx 3394.11 )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \Lambda \cdot \Lambda^{-} )</td>
<td>( \frac{9}{2} )</td>
<td>( \frac{1}{2} )</td>
<td>( \frac{1}{2} \times 10^{-1} )</td>
<td>( \frac{1}{2} \times 10^{-3} )</td>
<td>( \frac{1}{2} \times 10^{-4} )</td>
</tr>
<tr>
<td>(</td>
<td>\text{err}_D^{(u)}</td>
<td>)</td>
<td>(</td>
<td>\text{err}_D^{(v)}</td>
<td>)</td>
</tr>
<tr>
<td>1/2</td>
<td>-1.05 \times 10^{1}</td>
<td>-9.57</td>
<td>-28.6</td>
<td>-26</td>
<td>-36.4</td>
</tr>
<tr>
<td>1/4</td>
<td>-4.21</td>
<td>-4.07</td>
<td>-11.5</td>
<td>-11.2</td>
<td>-14.5</td>
</tr>
<tr>
<td>1/6</td>
<td>-2.11</td>
<td>-2.11</td>
<td>-5.73</td>
<td>-5.74</td>
<td>-7.27</td>
</tr>
<tr>
<td>1/12</td>
<td>0</td>
<td>-0.084</td>
<td>0</td>
<td>x</td>
<td>0</td>
</tr>
</tbody>
</table>
Table 13
Exp. 1, dQ9-SNL, \(H = 12\), \(\mathcal{U} = \mathcal{U}^{\text{max}}(c_t = \frac{1}{4})\). This table compares predicted dispersion error \((53)\) and numerical error for dQ9(\(c_t^{(0)} = \frac{1}{4}\)). These results can be compared with dQ5 in Table 2.

<table>
<thead>
<tr>
<th>(\Lambda)</th>
<th>Truncation prediction ((53)) for (\text{err}_D(c_t^{(0)} = \frac{1}{4})), (\forall \Lambda), in percents</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/2</td>
<td>-1.91</td>
</tr>
<tr>
<td>1/4</td>
<td>-1.38</td>
</tr>
<tr>
<td>1/6</td>
<td>-1.922</td>
</tr>
<tr>
<td>1/12</td>
<td>-1.993</td>
</tr>
</tbody>
</table>

Numerical results, \(\text{err}_D(c_t^{(0)} = \frac{1}{4})\), in percents

<table>
<thead>
<tr>
<th>(\Lambda)</th>
<th>Results</th>
</tr>
</thead>
<tbody>
<tr>
<td>1/2</td>
<td>-4.09</td>
</tr>
<tr>
<td>1/4</td>
<td>-4.78</td>
</tr>
<tr>
<td>1/6</td>
<td>-4.87</td>
</tr>
<tr>
<td>1/12</td>
<td>×</td>
</tr>
</tbody>
</table>

Fig. 9. Averaged concentration profiles are computed by the dQ9-SNL model with the “hydrodynamic” weights \(c_t^{(0)} = c_t^{(1)} = c_t^{(2)} = 0\). The parameters are the same as in Fig. 4: \(H = 12\), \(c_t = \frac{1}{4}\), \(\mathcal{U} = \mathcal{U}^{\text{max}}\), \(t = 7 \times 10^{-1}\). The diffusion eigenfunction \(\Lambda \in \{0.2, 0.4, 0.5\}\) decreases from the left to the right diagram. The results are displayed for four \(\Lambda\) values: \(\Lambda = \{\frac{1}{12} (\text{dashed}), \frac{1}{6} (\text{dotted}), \frac{1}{3} (\text{solid}), \frac{1}{4} (\text{dash-dotted})\}\). The analytical solution is plotted with solid (red) line. (Color online.)

Fig. 10. Averaged concentration profiles corresponding to the “rotated” dQ5 model with \(c_t^{(0)} = c_t^{(1)} = c_t^{(2)} = 0\). Other model parameters are the same as in Figs. 4 and 9. The diffusion eigenfunction \(\Lambda \in \{0.2, 0.4, 0.5\}\) decreases from the left to the right diagram. The \(\Lambda\) takes four values: \(\Lambda = \{\frac{1}{12} (\text{dashed}), \frac{1}{6} (\text{dotted}), \frac{1}{3} (\text{solid}), \frac{1}{4} (\text{dash-dotted})\}\). The analytical solution is plotted with solid (red) line. (Color online.)

that if this deficiency occurs for \(Pemax \approx 3394\) with dQ5 in Table 2, \(\Lambda = \frac{1}{12}\) loses stability already for \(Pemax \approx 438\) with dQ9(\(c_t^{(0)} = \frac{1}{4}\)) in Table 11, and even for \(Pemax \approx 27.7\) with “rotated” weights, dQ9(\(c_t^{(0)} = 0\)) in Table 12. Besides, we find that \(\Lambda = \frac{1}{4}\) loses stability for \(Pemax \approx 3394\) with the both, hydrodynamic and rotated weights, while it was stable with the dQ5. The same parameters, except the equilibrium weights, were applied in all these simulations.

Table 13 shows numerical values \(\text{err}_D\) for “standard” weights. In agreement with prediction \((53)\) and the profiles, \(\text{err}_D\) is almost \(\Lambda\)-independent for \(c_t^{(0)} = \frac{1}{4}\), but, for example, \(\text{err}_D(\Lambda = \frac{1}{4})\) increases its amplitude by two orders of magnitude for \(Pemax \approx 277.13\), from \(\approx -7.7 \times 10^{-2}\) in dQ5 to \(\approx -4.76\%\) in “standard” dQ9-SNL. Next, we apply the particular solution \((62)\) for \(\Lambda(c_t^{(0)})\), the results are reported in Table 14. Notice that this solution has been derived in the limit \(c_t (\Lambda^{-2}) \to 0\), in particular, it yields \(\Lambda = \frac{5}{12}\) for \(c_t^{(0)} = \frac{5}{12}\). The results confirm that this choice has the advanced accuracy when \(Pemax\) is sufficiently high (see three last columns), where, similar to choice \(\Lambda = \frac{1}{4}\) in dQ5, \(|\text{err}_D|\) reduces to \(\approx 0.1\%\) with \(H = 12\). Much
more accurate solutions are obtained for smaller $Pe$ applying Eq. (61) (where $c_r(\Lambda^-)^2$ has been not neglected) rather than Eq. (62). For example, when $Pe \approx 9.24$ and $t_c^{(O)} = \frac{1}{2}$, it yields $\Lambda^- = \sqrt{1/(6c_r)}$, then, if $\Upsilon = 2/3t_c^{\text{max}} = 2/3\sqrt{1-2c_r}$, this solution imposes: $\Upsilon \approx 0.21$, $\Lambda^- \approx 0.61$, $c_r = 0.45$ and results in $err_D = -5.517 \times 10^{-2}$. This improves by a factor $10^2$ the reported in Table 14 value $err_D = 6.1311$. Thereby, the numerical results confirm that an efficient reducing of the numerical dispersive in d2Q9-SNL can be achieved with the help of parameter choice offered by Eqs. (61) and (62).

Next, Fig. 11 displays the entire dependency of $err_D$ on the velocity-weight when the velocity amplitude is halved with respect to its maximum value, in order to obtain stable results for all weights and $\Lambda$. The numerical results and theoretical predictions are plotted together. In accord with Eq. (50), the dependency of $err_D$ on the diagonal weight-value $t_d^{(O)} = 1/4 - t_c^{(O)}/2$ is linear and its amplitude increases in small and intermediate $Pe$ range presented here, $Pe \in [4.6, 138.6]$. These numerical results again confirm the weight-independence of the dispersion error when $\Lambda = \frac{1}{2}$. This choice, also justified for its advanced accuracy in advection due to removing of the third-order spatial coefficient of the truncation errors (see in Appendix A), can therefore be recommended when velocity is far below stability line. As predicted, at relatively high $Pe$, the d2Q5 with $\Lambda = \frac{1}{3}$ gains in accuracy (see last diagram in top row). All curves $err_D(t_c^{(O)})$ have a common, $\Lambda$-independent point for $t_c^{(O)} = \frac{1}{2}$ but this hydrodynamic velocity-weight has non-zero numerical dispersion as $Pe$ increases.

Finally, during revision of this work, an exact or quasi-exact solution for numerical dispersivity of the scheme was obtained due to finer accounting for the summation errors. Namely, replacing $U'(y) = U_h(y) - \Upsilon$ by its numerical counterpart $U'^{\text{num}}(y) = U_h(y) - \Upsilon^{\text{num}}$, with $\Upsilon^{\text{num}}$ given by Eq. (69), one replaces Eq. (49) with
Taylor–Aris

(iii) the truncation based flow links on parameters also coordinate on Fig. 12.

(b) the d2Q9, with the coordinate velocity-weight stencil \( t_c^{(a)} = \frac{1}{2} \), \( \forall \Lambda \) and (3) the d2Q9 with \( \Lambda = \frac{1}{2} \), \( \forall t_c^{(a)} \in [0, \frac{1}{2}] \). It follows that this result is also exact for any finite-difference scheme \( [28] \) which is equivalent to the TRT subclass \( \Lambda = \frac{1}{2} \). We confirm this observation by numerical computations for the forward-time central finite-difference schemes corresponding to \( \Lambda^- = \Lambda^+ = \frac{1}{2} \), on the different 5–9-points discretization stencils. Besides, the \( H^{-4} \) and \( H^{-6} \) corrections from Eqs. (74)–(76) reduce for all parameters the small discrepancy between the numerical and predicted result further, as demonstrated in Fig. 12.

All in all, the results from this section have demonstrated the combined role of the equilibrium velocity-weight and \( \Lambda \) on the accuracy and stability in d2Q9-SNL scheme, in the presence of the high mechanical dispersion and in the absence of the boundary effect. The truncation and spurious boundary effects of the bounce-back rule in the presence of the diagonal links are examined in parallel study \([46]\) and summarized in Section 5.

5. Summary and perspectives

In this work we have analytically predicted the apparent dispersion coefficient \( D_0 (1 + k_T + \delta k_T) \) in straight Poiseuille flow modeled with the two-relaxation-times advection–diffusion d2Q9 scheme. The correction \( \delta k_T \) over the predicted dimensionless dispersivity coefficient \( k_T = Pe^2 / 210 \) encompasses the numerical dispersivity of the scheme. This new result is based on the extension of the third- and fourth-order transient truncation analysis for space-variable velocity. Starting from the underlying recurrence equations, our methodology is especially interesting for link-wise collisions, as the TRT, where the truncation analysis develops independently of the dimension, velocity set and equilibrium weight–stencils, making its results available for differently-discretized convection and isotropic/anisotropic diffusion forms. The present analysis develops along the following three steps: (i) the Taylor Ansatz \( D_0 \delta^2 C \approx (U_c(y) - \bar{U}) \delta \bar{C} \) is applied to truncation corrections; (ii) the contributions which modify \( k_T \) are identified and the numerical dispersivity \( \delta k_T \) is derived summing all relevant components; (iii) the summation error in computation of the averaged equation is accounted for. Although numerical corrections to Taylor–Aris predictions can be created by other advection–diffusion numerical schemes, such as the finite-difference/finite-
element schemes, we are not aware of this type analysis in them. Nevertheless, we believe that the proposed combination of the truncation and Taylor–Aris dispersion analysis is also applicable in other numerical methods.

The derived apparent transport coefficient \( k_1 + \delta k_T \) was found in very good agreement with the numerical measurements of the variance in a very broad equilibrium and relaxation parameter range. Unlike in previous studies \([15,19,26,39,52]\), where either the third- or fourth-order truncation correction vanished for particular value assigned for product \( \Lambda \) of two eigenfunctions, here the entire contribution from all terms vanishes in the “optimal-dispersion” parameter sub-space where \( \delta k_T \approx 0 \). Following these rules, the simplest d2Q5 TRT model with the bounce-back rule demonstrated accuracy within \( 10^{-5} \)–\( 10^{-3} \% \) with Taylor predictions for \( H = 32 \) and outperformed the improved d2Q9 full-matrix model \([25]\) by several orders of magnitude (Table 1). On the whole, the optimized relative dispersion error was about \( 10^{-1} \% \) of magnitude over a Péclet number ranging four decades in a small channel of \( H = 12 \), with the d2Q5 bounce-back and d2Q9 specular-reflection schemes. The closed-form \( H^{-2} \)-order expression for \( \delta k_T \) in Eqns. (50)–(52). Its prefactor before \( Pe^2/H^2 \) depends on almost all parameters of the model, such as

1. \( c_e(\Lambda^-)^2 \), which is the product of the equilibrium scale parameter \( c_e \in [0,1] \) and the eigenfunction (in square) of molecular-diffusion coefficient \( D_0 = c_e \Lambda^- \);
2. velocity-weight equilibrium stencil \( \{t_{(o)}^{(0)}, t_d^{(0)}\} = 1/4 - t_{(o)}^{(0)}/2 \) \( \in [0,1] \);
3. free-tunable positive TRT-number \( \Lambda = \Lambda^- \Lambda^- \).

While \( D_0 = c_e \Lambda^- \) is linked to average velocity \( Ut \) and \( H \) via \( Pe \) formally, the weight-family and \( \Lambda \) are free parameters. The explicit dependency of \( \delta k_T \) on \( c_e(\Lambda^-)^2 = D_0 \Lambda^- \) means that, unlike the physical equation, the second-order modeled equation is not fully controlled by \( Pe \). In other words, selecting two different pairs of \( c_e \) and \( \Lambda^- \) with the same product \( D_0 \), their numerical solutions will differ for same velocity and grid resolution even when the weights and \( \Lambda \) are fixed.

However, as \( Pe \) increases and \( D_0 \) decreases, the term \( c_e(\Lambda^-)^2 \) becomes insignificant rapidly, the \( \delta k_T \) then scales as \( Pe^2 \) and its asymptotic relative dispersion error \( \|k_T/(1+k_T)\| \) becomes Péclet- and velocity-independent. We emphasize that in this limit, the modeled concentration distribution is practically set by \( Pe \) provided that \( \Lambda \) is fixed, similar to general result \([50]\) on the steady-state solutions of advection–diffusion schemes. Furthermore, \( \delta k_T \) becomes \( \Lambda \)-independent with the hydrodynamic velocity weight \( t_{(o)}^{(0)} = 1 \), while the “optimal-advection” choice \( \Lambda = \frac{1}{2} \) makes it weight-independent. Yet, these two options have the opposite in sign relative errors \( \|k_T/k_T\| = \frac{1}{2} \) in intermediate and high \( Pe \)-range (Eqs. (57) and (58)) while the “optimal-dispersion” choice \( \delta k_T \approx 0 \) is set by specific function \( \Lambda(t_{(o)}^{(0)}) \), only available when \( t_{(o)}^{(0)} \in \left\{ \frac{1}{2}, \frac{1}{4} \right\} \).

It is remarkable that when the coordinate velocity-weight is equal to \( \frac{1}{2} \), the “optimal-dispersion” solution is \( \Lambda \approx \frac{1}{4} \). In particular, the d2Q5 model is most accurate on the “optimal-stability” TRT subclass \( \Lambda = \frac{1}{4} \).

In agreement with the predictions \([17]\), the choice \( \Lambda = \frac{1}{4} \) effectively retains the necessary stability diagram of the d2Q5 model (Fig. 2) for maximum velocity amplitude in Poiseuille profile, except for very small values \( c_e \leq 10^{-4} \) –\( 10^{-3} \). For example, \( Pe_{H=12} \approx 10^4 \) was reached for \( c_e \approx 5 \times 10^{-5} \) on the velocity stability line, with \( (\Lambda^-)^2 = \frac{1}{4} \approx 10^{-3} \). Further increase of \( Pe \) is possible by decreasing \( \Lambda^- \), but at the price of slowing down the convergence rate to steady solutions of moments. Stable solutions were also obtained on the peak of 2D stability diagram of the d2Q5 scheme: \( \frac{|U|^{max}}{\delta c_e} = \frac{1}{\sqrt{2}} \), \( \frac{\Lambda^-}{U_f} \), for higher velocity amplitude than commonly applied. It should be said again that increasing of the efficiency with the velocity amplitude does not deteriorate the relative accuracy of the scheme in intermediate and high Péclet range. In small \( Pe \)-range, if the numerical diffusion, such as \( -\Lambda^-/(U_f^2) \), has been not eliminated, it will sum with the numerical dispersion (Fig. 8). The sum of these two contributions precisely explains the results \([24]\) (Table 10). Since the mechanical and truncation dispersion dominate the numerical diffusion as \( Pe \) increases, we expect our results to be valuable for different ADE schemes \([25,28]\), only distinguished for their anti-numerical-diffusion mechanism in isotropic problems.

Altogether, truncation and stability predictions have suggested the preference for the coordinate stencil with the simple bounce-back rule and \( \Lambda = \frac{1}{4} \) in modeling of the Taylor–Aris dispersion with straight impermeable boundaries. The present analysis is applicable for other channel flows, as Brinkman profile in porous channel, because, except the summation correction, the \( Pe^2/H^2 \)-prefactor in derived expression for numerical dispersivity is flow-independent. Moreover, our recent extension for Taylor dispersion in circular pipe has shown that, surprisingly, the d3Q7 model with the bounce-back rule produces velocity and diffusion/dispersion results free from the spurious boundary effect on discretized circular wall. It follows that the minimal models are appealing not only because of their advanced efficiency but especially that they have no diagonal links. At the same time, it is found that the dependency \( \delta k_T(\Lambda, t_{(o)}^{(0)}) \) keeps its form in three-dimensions only for isotropic fourth-order truncation correction, achieved for isotropic “hydrodynamic” mass-weight stencil \( \{t_{(o)}^{(m)}, t_d^{(m)}\} \), with

\[
\sum_{Q,R \neq \emptyset} \frac{1}{Q \cdot R} t_R^{(m)} t_Q^{(m)} = 1.
\]

However, any non-zero diagonal weights, as the hydrodynamic weights, create the artificial Knudsen-type boundary layers \([46]\), as the system response on the boundary restriction of the tangential advection–diffusion flux by the bounce-back rule \([45]\). Furthermore, the transverse velocity gradients in those induced boundary-layers produce the longitudinal numerical dispersion, in agreement with the Taylor mechanism and the three types of dispersions, namely, physical, truncation and boundary, are superposed. A simple remedy \([46]\) consists in using of the specific (typically very small) \( \Lambda \) values at the boundary nodes only. The rational behind is that the boundary \( \Lambda \)-values control the amplitude of the Knudsen layers, in agreement with the prediction \([50]\). This local reduction of spurious boundary layers allows to apply the simplest bounce-
Appendix A. Fourth-order analysis in variable velocity field

We extend the truncation analysis [19] to case when the equilibrium weights \( E_q^\pm \) may vary in space together with the velocity vector \( \vec{U} \). The eigenvalue functions \( \Lambda^\pm \) are set time- and space-independent. The equilibrium is applied in the linear form \( e_q(t, t) = E_q^\pm(U(t))C(t, t) \), where \( E_q^\pm \) is restricted to mass conservation condition: \( \sum_{q=0}^{M} E_q^\pm = 1 \). The analysis develops in general form suitable for any velocity set and isotropic/anisotropic weights (the anisotropic weights \( E_q^\pm \) allow to model isotropic diffusion form [19,28]). The present analysis does not employ any symbolic tools. Because of the linearity of the system with respect to \( C(t, t) \), we write the non-equilibrium components as \( g_q^\pm(t, t) = [G_q^\pm]C \) and then present the recurrence equations (25) in the form:

\[
\begin{align*}
G_q^\pm C &= [S^\pm_q + R^\pm_q + T^\pm_q + Z^\pm_q]C ,
q = 0, \ldots , M .
\end{align*}
\]  
(A.1)

A.1.}

In this equation, \([S^\pm_q]C\) and \([R^\pm_q]C\) describe the spatial variation of the equilibrium and, respectively, non-equilibrium components; \([T^\pm_q]C\) and \([Z^\pm_q]C\) define, accordingly, their variation in time:

\[
\begin{align*}
[S^\pm_q]C &= [\Lambda q E^\mp_q]C - \Lambda^\mp [\Lambda^\pm q E^\pm_q]C , \ [S^\pm_0]C = 0 ,
A.2.
\end{align*}
\]

\[
\begin{align*}
[R^\pm_q]C &= (\Lambda - \frac{1}{4}[\Lambda^\pm_q q^2]C , \ [R^\pm_0]C = 0 ,
A.3.
\end{align*}
\]

\[
\begin{align*}
[T^\pm_q]C &= [\Lambda q E^\mp_q]C + \Lambda^\mp [\Lambda^\pm_q q^2]C ,
A.4.
\end{align*}
\]

\[
\begin{align*}
[Z^\pm_q]C &= - (\Lambda - \frac{1}{4}[\Lambda^\pm_q q^2]C - \frac{1}{2}[\Lambda^\pm_q q^2]C - (\Lambda^\pm + \Lambda^\mp) [\Lambda q E^\pm_q]C .
A.5.
\end{align*}
\]

The temporal and spatial central-difference operators are expanded into the fourth-order Taylor series and expressed in terms of the two families of the differential operators, \([S_{2k}]C\) and \([S_{2k-1}]C\), also specified in Eq. (30):

\[
\begin{align*}
[S_{2k}]C = \sum_{q=1}^{M} \delta_{q}^{2k} E_{q}^{-1} C , \ [S_{2k-1}]C = \sum_{q=1}^{M} \delta_{q}^{2k-1} E_{q}^{-1} C , \ \delta_{q} = (\nabla \vec{z}_{q}) = \sum_{\alpha=1}^{d} \delta_{\alpha} c_{q q} , \ k \geq 1 .
A.6.
\end{align*}
\]

With their help, the fourth-order Taylor approximations applied to Eqs. (A.2) and (A.4) read, respectively:

\[
\begin{align*}
\sum_{q=1}^{M} [S^\pm_q]C \approx [S_{1}]C - \Lambda^{-}[S_{2}]C + \frac{1}{6}[S_{3}]C - \frac{\Lambda}{12}[S_{4}]C ,
A.7.
\end{align*}
\]

In this, we will sequentially replace all temporal derivatives via the spatial ones employing the previous order approximation of the mass conservation equation (26):

\[
\begin{align*}
\sum_{q=0}^{M} G_q^\pm(t, t)C = 0 , \text{ with } \sum_{q=0}^{M} E_q^\pm = 1 , \ \sum_{q=0}^{M} Z_q^\pm(t, t)C = 0 .
A.8.
\end{align*}
\]

We construct its fourth-order approximation in the form (29): \( \partial_t C = [R_{1} + R_{2} + R_{3} + R_{4}]C \). When \( n \geq 2 \), the nth-order term \([R_n]C\) is defined as:

\[
\begin{align*}
[R_n]C = - \sum_{q=0}^{M} [S_q^{\pm(n)} + T_q^{\pm(n)} + R_q^{\pm(n)}]C(t, t) , \ \sum_{q=0}^{M} Z_q^{\pm(n)}[C(t, t) , \ \sum_{q=0}^{M} Z_q^{\pm(n)}]C = 0 .
A.9.
\end{align*}
\]
At the first-order, $[R_1]C$ is defined from
\[
\sum_{q=0}^{Q_m}[T^+_q]C = \partial_t C , \quad \sum_{q=1}^{Q_m}[S^+_q]C = [S_1]C , \quad [R^+_q]C = [Z^+_q]C = 0 . \tag{A.10}
\]
\[
\partial_t C = [R_1]C , \quad [R_1]C = −[S_1]C .
\tag{A.11}
\]
At the second-order, with the help of Eq. (A.7), one gets
\[
\sum_{q=0}^{Q_m}[S^+_q]C = −\Lambda^{−}[S_2]C , \quad \sum_{q=0}^{Q_m}[T^+_q]C = \Lambda^{−}\partial_t [\partial_t C] = \Lambda^{−}[S^+_1]C , \quad [R^+_q]C = 0 . \tag{A.12}
\]
Then, by summing Eq. (A.11) and Eq. (A.12), the second-order mass conservation equation takes the form of Eq. (32):
\[
\partial_t C = [R_1 + R_2]C , \quad [R_2]C = \Lambda^{−}[D_2]C , \quad [D_2]C = [S_2 − S^+_2]C . \tag{A.13}
\]
At the third-order we obtain
\[
\sum_{q=1}^{Q_m}[S^+_q]C = \frac{1}{6}[S_3]C , \tag{A.14}
\]
\[
\sum_{q=1}^{Q_m}[R^+_q]C = (\Lambda − \frac{1}{4})\sum_{q=1}^{Q_m}[\Lambda^2_q\partial_q^{+}]C = (\Lambda − \frac{1}{4})\sum_{q=1}^{Q_m}[\partial_q^{+}(\partial_q E^− + \partial_q E^+)] = (\Lambda − \frac{1}{4})[S_3 − S_1 S_2]C
\]
\[
= −(\Lambda − \frac{1}{4})[S_1 D_2]C + (\Lambda − \frac{1}{4})[S_3 − S^+_1]C ,
\]
\[
\sum_{q=0}^{Q_m}[T^+_q]C = \Lambda^{−}[\partial_t^2 C^{(3)}] + \frac{1}{6}[\partial_t^3 C]^{(3)} = −2(\Lambda^{−})^2[S_1 D_2]C − \frac{1}{6}[S^+_1]C . \tag{A.15}
\]
In this last relation, we took use of: $[\partial_t^2 C]^{(3)} = [(R_1 + R_2)^2C]^{(3)} = 2R_1 R_2 C = −2\Lambda^{−}[S_1 D_2]C$, $[\partial_t^3 C]^{(3)} = −[S^+_1]C$. Summing $[R_3]C$ with Eq. (A.13), the third-order-accurate mass-conservation equation reads
\[
\partial_t C = [R_1 + R_2 + R_3]C ,
\]
\[
[R_3]C = −\frac{1}{6}\sum_{q=1}^{Q_m}[(S^+_q) + T^+_{q, 3} + R^+_{q, 3}]C
\]
\[
= 2(\Lambda^{−})^2[S_1 D_2]C + (\Lambda − \frac{1}{4})[S_1 D_2]C + (\Lambda − \frac{1}{12})[S^+_3 − S_3]C . \tag{A.16}
\]
Therefore, Eq. (A.15) takes the same form [19] as in constant velocity field:
\[
\partial_t C = [R_1 + R_2 + R_3]C ,
\tag{A.17}
\]
\[
[R_3]C = c_3,1[S_1 D_2]C + c_3,2[S^+_1 − S_3]C , \quad c_3,1(\Lambda^{−}, \Lambda) = 2(\Lambda^{−})^2 + \Lambda − \frac{1}{4} , \quad c_3,2(\Lambda) = \Lambda − \frac{1}{12} ,
\]
then
\[
c_3,1 = 0 , \quad c_3,2 = 0 \text{ if } (\Lambda^{−})^2 = \Lambda = \frac{1}{12} \text{ or } \Lambda^{−} = \Lambda^{+} = \sqrt{1/12} . \tag{A.18}
\]
This last choice was called the optimal-advection choice [15,19] because it vanishes the advection correction in modeled equation. This choice is extremely accurate for advection-dominant problems [17,19,47]. Moreover, in combination with $c_e = \frac{1}{2}$, $U = \frac{1}{2}$ the BGK scheme (A.18) vanishes both the third- and fourth-order corrections in one-dimensional constant flow (see (A.9)–(A.11) in work [13]).

Finally, at the fourth-order, using Eqs. (A.11), (A.13) and (A.16) in Eq. (A.7) we apply: $[\partial_t^2 C]^{(4)} = [R_2^2 + 2R_1 R_3]C$, $[\partial_t^3 C]^{(4)} = [3R_2^2 R_2]C$, $[\partial_t^4 C]^{(4)} = [S^+_1]C$, $[\partial_t^5 C]^{(4)} = [R_2 C] = \Lambda^{−}[D_2]C$,
\[
\sum_{q=1}^{Q_m}[S^+_{q, 4}]C = −\frac{1}{12}\Lambda^{−}[S_4]C ,
\]
\[
\sum_{q=0}^{Q_m}[T^+_{q, 4}]C = \Lambda^{−}[R_2^2 + 2R_1 R_3]C + \frac{1}{6}[3R^2_2 R_2]C + \frac{\Lambda^{−}}{12}[S^+_4]C
\]
\[
\begin{align*}
[L^{-2}(\Lambda^{-2})^2D_2^2]C + \frac{1}{2}S_2^4 [L^{-2}D_2]C - 2[S_1R_3]C + \frac{\Lambda^{-2}}{12} [S_4^1]C \\
= \frac{1}{12} [L^{-2}(12\Lambda^{-2})^2D_2^2]C + 6[S_2^2D_2]C - 24[S_1R_3]C + [S_4^1]C
\end{align*}
\]

and

\[
\sum_{q=1}^{Q_m} [R_q^{(4)}]C = (\Lambda - \frac{1}{4}) \sum_{q=1}^{Q_m} \partial^2_q (S_q^{(2)} + T_q^{(2)} + Z_q^{(2)})]C,
\]

where

\[
[S_q^{(2)}]C = -L^{-2}\partial^2_q E_q^+, \quad \sum_{q=1}^{Q_m} \partial^2_q S_q^{(2)}]C = -L^{-2}[S_4]C,
\]

\[
\sum_{q=1}^{Q_m} \partial^2_q T_q^{(2)}]C = \sum_{q=1}^{Q_m} \partial^2_q (\partial_t E_q^+) + 2\Lambda^{-2}[\partial_q^2 E_q^+]C,
\]

\[
= \sum_{q=1}^{Q_m} \partial^2_q E_q^+ ([\partial_t C]^{(2)} + \Lambda^{-2}[\partial_q^2 E_q^+]) = S_2[L^{-2}D_2 + 2\Lambda^{-2}S_1^1]C = \Lambda^{-2}[S_2^1]C,
\]

\[
[Z_q^{(2)}]C = -(\Lambda^{-1} + \Lambda^+) [\partial_t G_q^{(1)}]C = -(\Lambda^{-1} + \Lambda^+) [\partial_t (\partial_q E_q^+ + \partial_q E_q^-)]C,
\]

\[
\sum_{q=1}^{Q_m} \partial^2_q Z_q^{(2)}]C = -(\Lambda^{-1} + \Lambda^+) [(S_2^1S_2 - S_1S_3)]C \approx -[(\Lambda^{-1} + \Lambda^+) [(S_1S_2 - S_3)]C.
\]

Replacing \([R_2]C\) and \([R_3]C\) by their respective solutions \((A.13)\) and \((A.16)-(A.17)\), the fourth-order truncation term \([R_4]C\) reads

\[
[R_4]C = -\sum_{q=1}^{Q_m} (S_q^{(4)} + T_q^{(4)} + R_q^{(4)})]C
\]

\[
= -\frac{1}{12} \Lambda^{-2}[12(L^{-2})^2D_2^2 + 6D_2S_1^2 - 24S_1R_3 + S_1^4 - S_4]C
\]

\[
+ (\Lambda - \frac{1}{4})[\Lambda^{-2}(S_4 - S_2^1)]C + (\Lambda - \frac{1}{4})(\Lambda^{-2} + \Lambda^+) [(S_1S_2 - S_3)]C
\]

\[
= c_{4.1}[D_2^2]C + c_{4.2}[S_2^2D_2]C + c_{4.3}[S_4 - S_1S_3]C + c_{4.4}[S_4^1 - S_1S_3]C,
\]

\[
c_{4.1}(\Lambda, \Lambda) = -\Lambda^{-2}((\Lambda^{-2}) + \Lambda - \frac{1}{4},
\]

\[
c_{4.2}(\Lambda, \Lambda) = \Lambda^{-2}(4\Lambda^{-2} + \Lambda - \frac{3}{4} + \frac{4(4\Lambda - 1)}{4(\Lambda^{-2})^2},
\]

\[
c_{4.3}(\Lambda, \Lambda) = \Lambda^{-2}(\Lambda - \frac{1}{6}),
\]

\[
c_{4.4}(\Lambda, \Lambda) = \frac{\Lambda^{-2}(8\Lambda - 1 + \frac{4(4\Lambda - 1)}{(\Lambda^{-2})^2})}{\Lambda}.
\]

We note typos in Eq. (2.10) of work \([19]\) for coefficient \(c_{4.4}(\Lambda^{-2}, \Lambda)\). Thus, we obtain the same form \([19]\) of the truncation corrections as in constant velocity field but now in terms of the operators \((A.6)\), bearing in mind that \(E_q^\pm\) may become space-dependent.

It has been shown \([19]\) that the coefficient \(c_{4.4}(\Lambda^{-2}, \Lambda)\) determines the effective stability of the full schemes when their second-order numerical diffusion is eliminated. This coefficient vanishes on the so-called “extended optimal-stability subclass” \([37]\) for specific dependency \(\Lambda((\Lambda^{-2})^2). This parameter choice may retain the advanced stability properties of \(\Lambda = \frac{1}{4}\) in 1D or for proper equilibrium weights in multidimensional, \([37,19]\).

In pure diffusion case \(\tilde{U} = 0\), Eq. \((A.21)\) reduces to

\[
[R_4]C = [c_{4.1}S_2^2 + c_{4.3}S_4]C, \quad c_{4.1} = 0, \quad c_{4.3} = 0 \text{ if } (\Lambda^{-2}) = \frac{1}{12} \text{ and } \Lambda = \frac{1}{6}.
\]
The TRT choice \((A.22)\) was called the optimal-diffusion \((15,19)\) or “quartic” \([39]\). The fourth-order diffusion form \((R_4)\)C has been examined \([19]\) for isotropy, especially in d2Q9 scheme. The hydrodynamic mass-weight stencil \(\{t_c^{(m)}, t_d^{(m)}\}\), with

\[
3 \sum_{q,a=\pm 1} t_q^{(a)} t_q^{(a)\ast} = 1
\]

maintains the isotropy of the fourth-order form, giving \((\frac{1}{12}, \frac{1}{8})\) in d2Q9 scheme. In isotropic case, specific solution for equilibrium parameter \(c_0((\Lambda^{-1})^2, \Lambda) = -c_{4.3}/c_{4.1}\) vanishes the fourth-order correction for any relaxation rates (see Eq. (B.7) \([15]\), Eq. (5.9) in \([19]\)).

Finally, we emphasize that the “optimal-advection” choice \(\Lambda = \frac{1}{t_c}\) and “optimal-diffusion” choice \(\Lambda = \frac{1}{t_d}\) vanish, respectively, the third- and fourth-order spatial corrections in bulk for any equilibrium, advection–diffusion or hydrodynamic, because of specific organization of the coefficients in steady-state Chapman–Enskog series, \([50,53]\).

References


