

A Two-Field Numerical Model for Mass Transfer in Two-Phase Flows: Effect of the Jump Constant and Diffusivity Ratio on Model Accuracy

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Abstract: Accurate numerical modeling of interfacial mass transfer in two-phase flows requires enforcing a sharp concentration discontinuity at the interface, whose amplitude is set by the Henry constant He , across concentration boundary layers whose relative thickness is governed by the diffusivity ratio D_i/D_e . Classical 1-fluid methods embed this discontinuity into an additional interfacial term within a homogenized model relying on a smeared mixture scalar, which degrades accuracy as He departs from unity. The paper [1] introduced a two-field formulation on fixed Cartesian meshes that enforces Henry's law and flux continuity explicitly via a ghost-fluid mass-flux approximation in cut cells, at a computational cost comparable to the one-fluid approach. The present work extends that contribution through a systematic parametric study spanning $He \in [0.01, 100]$ and $D_i/D_e \in [0.01, 100]$, covering the three transfer regimes: internal, conjugate, and external, defined by the composite parameter $He\sqrt{D_i/D_e}$. Accuracy of the two-field scheme is quantified against the 1-fluid baseline through two-dimensional static diffusion and rotating-disk benchmarks. The results identify the regions of the $(He, D_i/D_e)$ plane where the two-field approach delivers the greatest accuracy gain, and characterise its systematic limitations in the conjugate regime where both phases offer comparable resistance to mass transfer.

Keywords: Interfacial mass transfer, Two-field formulation, Volume-of-Fluid, Henry constant, Diffusivity ratio.

1. Introduction

Interfacial mass transfer in two-phase flows involves the transport of a dissolved species across a fluid–fluid interface at which a sharp concentration discontinuity is imposed by thermodynamic equilibrium. This discontinuity is governed by Henry's law ($C_i = He C_e$ at the interface), and its numerical representation is the central difficulty: the concentration jump amplitude scales with He while the relative thickness of the concentration boundary layers on each side of the interface is governed by the diffusivity ratio D_i/D_e . Both parameters span several orders of magnitude in gas-liquid systems, so a method validated at one operating point can perform very differently elsewhere in parameter space.

Two main strategies have been developed to handle this discontinuity on fixed Cartesian meshes. *One-fluid* approaches [4, 5, 6] reformulate the two-phase mass transfer problem into a single mixture convection-diffusion equation by absorbing the Henry jump into an additional interfacial correction term and a smoothed effective diffusivity. This approach is simple and computationally efficient [7, 8, 9], but it inevitably smears the concentration discontinuity over the interface cells, and accuracy degrades when He departs significantly from unity. *Two-field* approaches maintain a separate concentration scalar in each phase and enforce Henry's law explicitly at the interface, thereby preserving the sharp discontinuity. On body-fitted meshes, this yields accurate predictions across all transfer regimes [16, 17]. On fixed Cartesian grids, the two-scalar VOF framework of [11] has been extended to reactive transfer [12, 28] and high-Péclet convection via sub-grid scale reconstructions [13, 14, 15, 27], but at increased implementation

complexity. The companion paper [1] proposes an efficient two-field alternative on a fixed Cartesian mesh: one majority-phase concentration per cell, one-dimensional interface geometry in cut cells, and a ghost-fluid mass-flux formula [23] that simultaneously satisfies Henry's law and flux continuity. Validated at $(\text{He} = 30, D_i/D_e = 100)$, the scheme reduces the concentration error by up to two orders of magnitude relative to the 1-fluid approach at comparable computational cost. However, no systematic assessment of its accuracy over the full $(\text{He}, D_i/D_e)$ parameter space has been reported, this is the central objective of the present work.

The Henry constant and the diffusivity ratio fundamentally alter the concentration field structure and the distribution of mass-transfer resistance between the two phases. Three regimes are identified by the composite parameter $\text{He}\sqrt{D_i/D_e}$, originally proposed by [26] (Fig. 1): the *internal* regime ($\text{He}\sqrt{D_i/D_e} \ll 1$), dominated by interior-phase resistance; the *external* regime ($\text{He}\sqrt{D_i/D_e} \gg 1$), dominated by exterior-phase resistance; and the *conjugate* regime ($\text{He}\sqrt{D_i/D_e} \sim 1$), where both phases offer comparable resistance [16, 17].

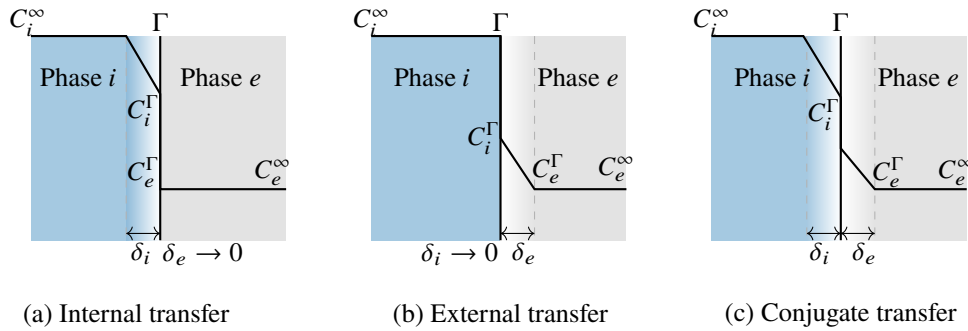


Figure 1: Concentration profiles across the three mass transfer regimes. Phase i : interior; phase e : exterior. $\text{He} = C_i/C_e|_\Gamma$.

The present work spans all three regimes by independently varying He and D_i/D_e , and identifies the regions where the two-field scheme outperforms the one-fluid baseline as well as its limitations. The mathematical model and numerical method are recalled in Sections 2–3 (full derivations are given in [1]); parametric results on two-dimensional static diffusion and rotating-disk benchmarks are presented in Section 4; conclusions are drawn in Section 5.

2. Problem Statement

The mathematical framework follows that of the companion paper [1]; the reader is referred there for complete derivations. The essential equations are recalled here for self-consistency.

2.1 Flow configuration

Two immiscible fluids are considered: an interior phase Ω_i and an exterior phase Ω_e , separated by a moving interface $\Gamma = \partial\Omega_e \cap \partial\Omega_i$. The exterior-phase volume fraction F ($F = 1$ in Ω_e , $F = 0$ in Ω_i) characterises the phase distribution and is advected by a conservative VOF scheme with Piecewise Linear Interface Calculation (PLIC) [24]:

$$\frac{\partial F}{\partial t} + \text{Re Sc} (\mathbf{u} \cdot \nabla) F = 0, \quad (1)$$

where $\text{Sc} = \mu_e/(\rho_e D_e)$ is the exterior-phase Schmidt number and $\text{Re} = \rho_e V L/\mu_e$ the Reynolds number based on reference velocity V and length L . In all configurations considered in this work, the Navier-Stokes equations are not solved: $\mathbf{u}$ is either zero (static diffusion benchmark) or prescribed as a rigid-body rotation. This decoupling allows the accuracy of the concentration solver to be assessed independently of

hydrodynamic complexity.

2.2 Species transport and interfacial conditions

A dilute chemical species is transported within each phase $p \in \{i, e\}$. Concentrations are non-dimensionalised by the initial interior-phase concentration $\tilde{C}_i(t=0)$, yielding initial conditions $C_i = 1$ in Ω_i and $C_e = 0$ in Ω_e . The governing convection–diffusion equation in each subdomain reads

$$\frac{\partial C_p}{\partial t} + \text{Re Sc} (\mathbf{u} \cdot \nabla) C_p = \nabla \cdot \left(\frac{D_p}{D_e} \nabla C_p \right), \quad \forall \mathbf{x} \in \Omega_p, \quad (2)$$

where D_i/D_e is the ratio of interior to exterior diffusion coefficients. Two conditions must be satisfied simultaneously at the interface:

$$\nabla C_e \cdot \mathbf{n}_{ie}|_{\Gamma} + \frac{D_i}{D_e} \nabla C_i \cdot \mathbf{n}_{ie}|_{\Gamma} = 0, \quad \text{mass-flux continuity,} \quad (3a)$$

$$C_i|_{\Gamma} = \text{He } C_e|_{\Gamma}, \quad \text{thermodynamic equilibrium,} \quad (3b)$$

where $\mathbf{n}_{ie}$ is the outward normal from the interior phase (i). These conditions are illustrated in Fig. 2.

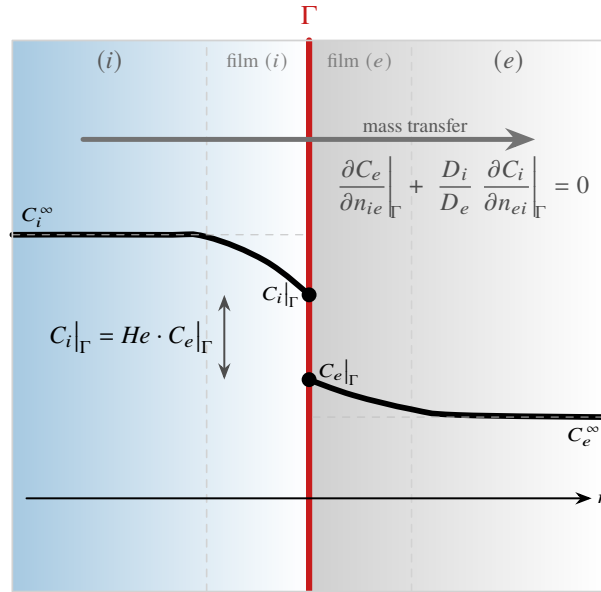


Figure 2: Diffusion boundary layers at interface Γ : concentration profiles C_i and C_e satisfy Henry's law $C_i|_{\Gamma} = \text{He} \cdot C_e|_{\Gamma}$ (eq. 3b) and flux continuity (eq. 3a) at Γ .

Equation (3b) states Henry's law, where $\text{He} > 1$ (resp. $\text{He} < 1$) implies a higher concentration in the interior phase (i) (resp. exterior phase (e)), both explicitly enforced at the discrete level through the two-field scheme.

2.3 Operator splitting

The equation (2) is advanced over each time interval $]t^{(n)}, t^{(n+1)}]$ by a two-step operator-splitting scheme [1, 6, 8] comprising a transport step followed by a diffusion step,

$$\frac{\partial C_p^*}{\partial t} + \text{Re Sc} (\mathbf{u} \cdot \nabla) C_p^* = 0, \quad C_p^*(\mathbf{x}, t^{(n)}) = C_p(\mathbf{x}, t^{(n)}), \quad (4a)$$

$$\frac{\partial C_p^{**}}{\partial t} = \nabla \cdot \left(\frac{D_p}{D_e} \nabla C_p^{**} \right), \quad C_p^{**}(\mathbf{x}, t^{(n)}) = C_p^*(\mathbf{x}, t^{(n+1)}), \quad (4b)$$

with $C_p(\mathbf{x}, t^{(n+1)}) = C_p^{**}(\mathbf{x}, t^{(n+1)})$. The transport step is synchronised with the VOF advection (1); the diffusion step is solved on the frozen interface with the two phasic fields coupled through conditions (3a)–(3b). Each step requires dedicated pre-processing of the concentration field: minority-phase reconstruction before transport; majority-phase selection before diffusion; the complete procedure is illustrated in Fig. 3 and fully described in [1].

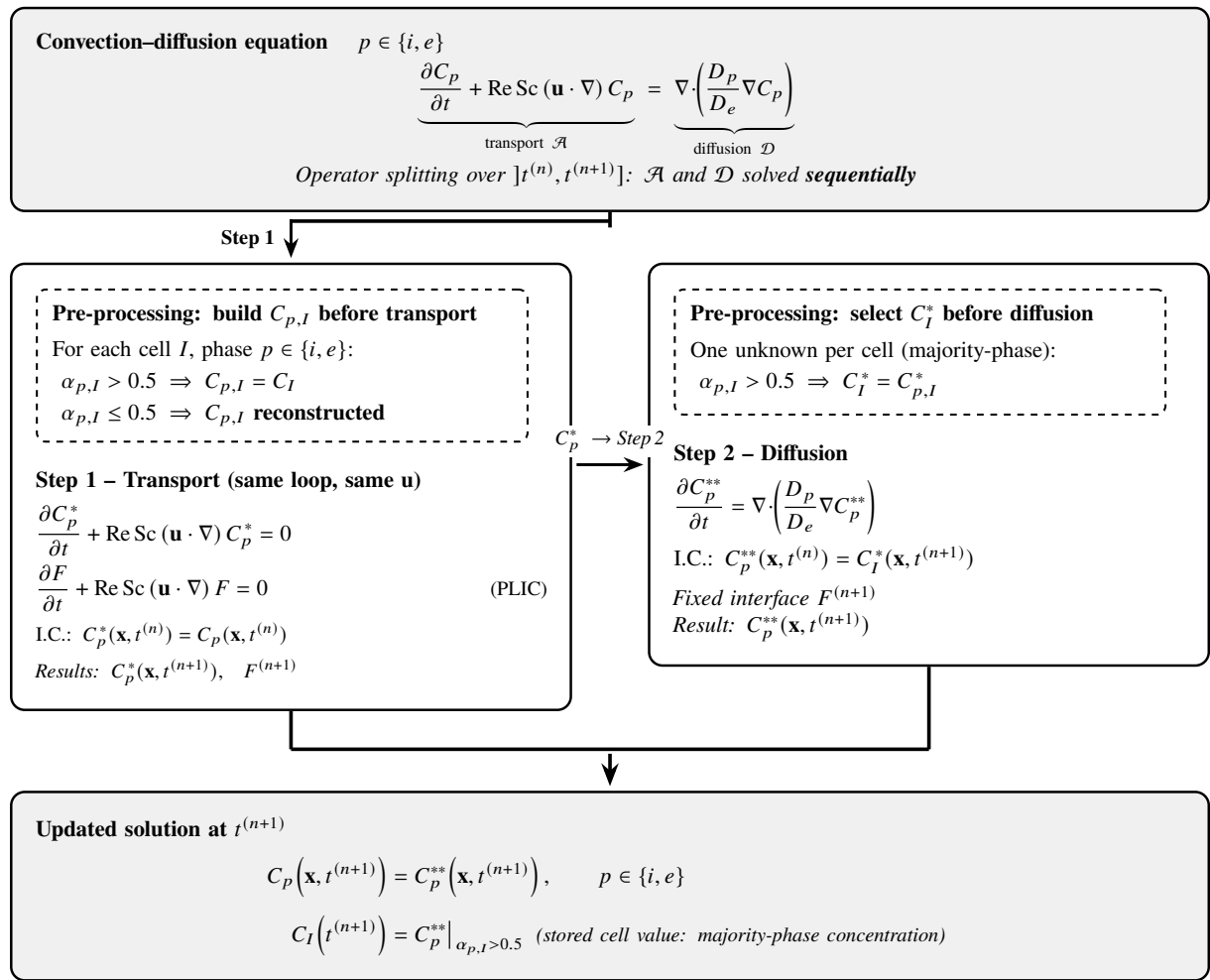


Figure 3: Operator-splitting procedure for the concentration equation (2) over one time step $]t^{(n)}, t^{(n+1)}]$. *advection step*: phasic concentrations $C_{p,I}$ are reconstructed from the stored majority-phase value (minority-phase cells use a 1-D ghost-fluid estimate), then C_p^* and the VOF field F are advanced together with velocity $\mathbf{u}$. *diffusion step*: C_I^* serves as initial condition; the phasic diffusion equations for C_e^{**} and C_i^{**} are solved on the frozen interface $F^{(n+1)}$, with Henry’s law and flux continuity enforced at Γ .

3. Proposed Numerical Method

The complete derivation and validation of the numerical scheme are reported in [1]; only the key ingredients and notations relevant to the parametric study are recalled here.

3.1 Cell notations and majority-phase convention

A cell Ω_I indexed by $I = (i, j, k)$ is called a *cut cell* whenever it contains both phases, i.e., $0 < f_I < 1$, where f_I is the discrete exterior-phase volume fraction at node I . The *majority phase* of cell I is defined as the exterior phase if $f_I \geq 0.5$ and as the interior phase otherwise. A single concentration unknown c_I , representing the majority-phase concentration, is stored at each cell centre. $\mathcal{N}_I^M$ denotes the set of neighbours of I that share the same majority phase, and $\mathcal{N}_I^m$ the set of neighbours whose majority phase is opposite to that of I (i.e. cells that lie across the interface).

3.2 Step 1 – Synchronized species and interface advection

As stated in Section 2.1, the velocity field is either zero or prescribed. The interface position is tracked on a structured Cartesian mesh using a conservative VOF scheme with Piecewise Linear Interface Calculation (PLIC) [24], which guarantees exact mass conservation. The concentration C_p^* (4a) and the VOF fraction F (1) are then transported simultaneously in the same loop, by means of three sequential directional sweeps. This synchronisation guarantees consistency between the phase-fraction and concentration fields [6, 8]. In cut cells, the minority-phase value required by the advection update is provided by the R_{2F-int} reconstruction (Section 3.4). The complete update formulas are given in [1].

3.3 Step 2 – Coupled diffusion and ghost-fluid interface treatment

Between two cells I and $J \in \mathcal{N}_I^m$ with opposite majority phases, the interface is located at the normalised distance $\theta_{\Gamma_{IJ}} = (0.5 - f_I)/(f_J - f_I)$ from node I , where $x_{IJ} = \|\mathbf{x}_I - \mathbf{x}_J\|$. For each such interface-crossing face, the discrete mass flux is approximated by a ghost-fluid formula [23] that simultaneously enforces Henry's law (3b) and flux continuity (3a) (full derivation in [1]). The resulting two-phase mass flux, for all $J \in \mathcal{N}_I^m$, reads:

$$\Phi_{IJ}^{2F} = \frac{m(\sigma_{IJ})}{x_{IJ}} D_{p_I^M, IJ} \left[c_J (\delta_{p_I^M, e} + \text{He} \delta_{p_I^M, i}) - c_I (\delta_{p_I^M, i} + \text{He} \delta_{p_I^M, e}) \right], \quad (5)$$

where the effective diffusion coefficient at the interface is the weighted harmonic mean:

$$\frac{1}{D_{p_I^M, IJ}} = \frac{(1 - \theta_{\Gamma_{IJ}}) (\text{He} \delta_{p_I^M, i} + \delta_{p_I^M, e})}{D_{p_I^M}} + \frac{\theta_{\Gamma_{IJ}} (1 + \delta_{p_I^M, e} (\text{He} - 1))}{D_{p_I^M}}. \quad (6)$$

Equations (5)–(6) show that the two-phase flux depends explicitly on both He and D_i/D_e ; this is why the accuracy of the scheme is expected to vary systematically with these two parameters. For same-phase neighbours $J \in \mathcal{N}_I^M$, the standard single-phase flux $\Phi_{IJ}^{1F} = m(\sigma_{IJ}) D_{p_I^M} (c_J - c_I)/x_{IJ}$ is used.

3.4 Minority-phase reconstruction in cut cells

The ghost-fluid interfacial concentrations also serve the advection step (4a): a minority-phase estimate $c_{p_I^m, I}$ is required in each cut cell I , and is reconstructed from them through a weighted average over all interface-crossing neighbours (R_{2F-int}):

$$c_{p_I^m, I} = \frac{\sum_{J \in \mathcal{N}_I^m} \alpha_J c_{p_I^m, \Gamma_{IJ}}}{\sum_{J \in \mathcal{N}_I^m} \alpha_J}. \quad (7)$$

This strategy was identified as the most accurate minority-phase reconstruction in [1].

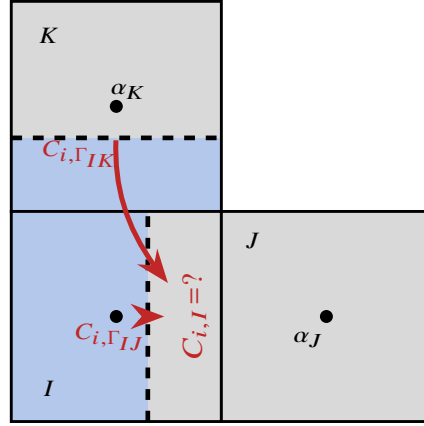


Figure 4: The R_{2F-int} scheme (Eq. (7)): the minority-phase concentration in cut cell I is estimated from ghost-fluid interfacial values $C_{p^m,\Gamma_{IK}}$ and $C_{p^m,\Gamma_{IJ}}$ evaluated at the SLIC interface segments of neighbours K and J , weighted by α_K and α_J .

3.5 Temporal discretisation in cut cells

The discrete time derivative in cut cells accounts for the simultaneous coexistence of both phases by weighting their concentrations with the respective volume fractions:

$$\sum_{p \in \{i,e\}} f_{p,I} \frac{c_{p,I}^{(n+1)} - c_{p,I}^{(n)}}{\Delta t^{(n)}}. \quad (8)$$

Only one concentration scalar $c_I := c_{p_I^M,I}$ is stored per cell (the majority-phase value); the minority-phase concentration $c_{p_I^m,I}$, required by Eq. (8), is not a direct unknown and must therefore be reconstructed. Since a neighbour $J \in \mathcal{N}_I^{p_I^m}$ has its majority phase equal to the minority phase of I , its stored concentration c_J carries direct information about that phase. The $T_{2F-neigh}$ scheme estimates $c_{p_I^m,I}$ as a volume-fraction-weighted average of those neighbours, evaluated explicitly at time $t^{(n)}$:

$$c_{p_I^m,I}^{(n)} = \frac{\sum_{J \in \mathcal{N}_I^{p_I^m}} f_{p_J^M,J} c_J^{(n)}}{\sum_{J \in \mathcal{N}_I^{p_I^m}} f_{p_J^M,J}}, \quad (9)$$

where $\mathcal{N}_I^{p_I^m}$ denotes the set of cut-cell neighbours whose majority phase coincides with the minority phase of cell I , and the weight $f_{p_J^M,J}$ is the volume fraction of that phase in neighbour J . Weighting by $f_{p_J^M,J}$ gives more influence to neighbours predominantly filled with the minority phase, where the majority-phase concentration is most representative.

If no such neighbour exists ($\mathcal{N}_I^{p_I^m} = \emptyset$), the minority-phase variable is reconstructed through alternative strategies described in [1].

The explicit evaluation of $c_{p_I^m,I}^{(n)}$ decouples the minority-phase reconstruction from the implicit solve on $c^{(n+1)}$, keeping the overall system linear without additional coupling.

All results in the present parametric study are obtained with R_{2F-int} for the transport reconstruction and $T_{2F-neigh}$ for the temporal term.

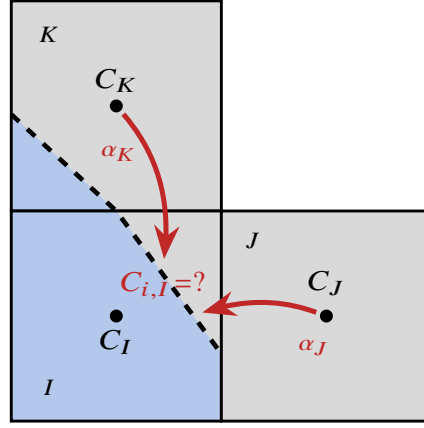


Figure 5: The $T_{2F-neigh}$ scheme (Eq. (9)): the minority-phase concentration in cut cell I is reconstructed as a weighted mean of the concentrations stored at neighbours K and J whose majority phase matches the minority phase of I ; weights α_K, α_J are the local volume-fractions.

3.6 One-fluid baseline

The 1-fluid formulation [4, 5, 6] is used as the accuracy reference throughout the parametric study. Applying a spatial filter to the two-field model (2) yields a single mixture concentration $\tilde{C} = F C_e + (1 - F) C_i$, governed by [4, 6, 8]:

$$\frac{\partial \tilde{C}}{\partial t} + \text{Re Sc} (\mathbf{u} \cdot \nabla) \tilde{C} = \nabla \cdot \left(\tilde{D} \left(\nabla \tilde{C} - \frac{1 - \text{He}}{F + (1 - F)\text{He}} \tilde{C} \nabla F \right) \right), \quad (10)$$

with $\tilde{D} = D_e D_i / (F D_i + (1 - F) D_e)$. The term proportional to ∇F smears the concentration discontinuity over interface cells when $\text{He} \neq 1$, which is the primary source of error in the one-fluid approach. Equation (10) is solved with the same operator-splitting strategy as the two-field scheme (Section 2.3), ensuring consistency between the interface and concentration fields [6, 8, 1]. In cut cells, the time derivative is discretised with the fixed-control-volume scheme $T_{1F/FCV}$, weighting the temporal term by the full cell volume $m(\Omega_I)$ [1].

4. Results

The implementation of the one-fluid formulation used as accuracy baseline throughout this section, was validated in [1] by comparison with the numerical results of [8] and against the analytical solution at ($\text{He} = 30, D_i/D_e = 100$).

4.1 Two-dimensional static diffusion benchmark

A circular disk of radius R_0 is placed at the centre of a square domain $[-L, L]^2$, where L is determined by requiring that the diffusive flux at radius $r = L$ be at most 10^{-8} times the flux at the circular interface ($r = R_0$), thereby ensuring compatibility with the zero-flux boundary conditions imposed on all domain boundaries. The velocity field is identically zero ($\mathbf{u} = \mathbf{0}$), reducing the problem to pure coupled diffusion in each phase, subject to the interfacial jump conditions. The disk centre is slightly offset from the origin at $\mathbf{x}_0 = (0.125/\pi, 0.125\sqrt{2}/2) R_0$ to avoid spurious symmetry effects. Initial conditions are $C_i = 1$ in the inner phase and $C_e = 0$ in the external. An analytical solution for this configuration, derived in [1], serves as the reference for all accuracy assessments.

All configurations are advanced to the dimensionless final time $t^* = t D_e / R_0^2 = 1$. Three temporal

resolutions are compared, labelled Δt_1 , Δt_2 , and Δt_3 , with respective time-step sizes

$$\Delta t_1 = \frac{h}{10}, \quad \Delta t_2 = \frac{h}{40}, \quad \Delta t_3 = \frac{h}{160}, \quad (11)$$

where h is the cell spacing non-dimensionalized by R_0 . For each $(\text{He}, D_i/D_e)$ configuration, the error ratio $\varepsilon_{2F}/\varepsilon_{1F}$ is reported, where ε denotes the relative L^2 error between the numerical and analytical concentration fields [1]. A ratio below 1 indicates that the two-field scheme outperforms the 1-fluid baseline; a ratio above 1 indicates degraded accuracy. The parameter space covers $\text{He} \in [0.01, 100]$ and $D_i/D_e \in [0.01, 100]$, spanning the internal, conjugate, and external transfer regimes defined in Section 1.

Among the schemes evaluated in [1], the combination of the R_{2F-int} transport reconstruction with the $T_{2F-neigh}$ temporal reconstruction consistently achieved the best accuracy across the parameter space. The following subsections present the mesh and time-step convergence of this scheme on the static benchmark (Section 4.2), followed by its assessment under transport conditions using a rotating-disk configuration (Section 4.3).

4.2 Mesh and time-step convergence of $T_{2F-neigh}$

4.2.1 Mesh refinement study (Δt_2)

Figure 6 shows the error ratio $\varepsilon_N/\varepsilon_{1F}$ as a function of He for the three mesh resolutions ($n_x/d = 4, 16, 64$) at the intermediate time step Δt_2 . Each curve corresponds to one value of D_i/D_e . The horizontal dashed line marks the one-fluid baseline ($\varepsilon_N = \varepsilon_{1F}$). Blue and red shaded regions indicate accuracy gain and loss with respect to the 1-fluid reference, respectively. The accuracy of $T_{2F-neigh}$ improves consistently with mesh refinement across the entire $(\text{He}, D_i/D_e)$ parameter space.

In the external regime ($\text{He}\sqrt{D_i/D_e} \gg 1$), $T_{2F-neigh}$ remains in the gain region (blue shading) at all three mesh resolutions, and the accuracy advantage grows with refinement. Error ratios decrease monotonically with mesh refinement, reaching 3% at the fine mesh. The accuracy gap between the two schemes thus widens progressively with refinement, always in favour of $T_{2F-neigh}$: at the fine mesh, the two-field scheme is one to two orders of magnitude more accurate than the 1-fluid approach in this regime.

In the internal regime ($\text{He}\sqrt{D_i/D_e} \ll 1$), the behaviour depends critically on D_i/D_e . For all curves except $D_i/D_e = 1$, the two-field scheme lies in the gain region at all three mesh resolutions. The most pronounced gain is observed for $D_i/D_e = 0.1$, which lies below all other curves. The $D_i/D_e = 0.01$ blue curve lies above it, showing that very small diffusivity ratios yield less gain than $D_i/D_e = 0.1$. The $D_i/D_e = 1$ red curve constitutes the main exception: at the coarse mesh ($n_x/d = 4$), it lies entirely in the loss region throughout the internal regime. Mesh refinement progressively brings this curve back into the gain region: at $n_x/d = 16$ it already falls below parity in the internal regime, and the improvement continues at $n_x/d = 64$.

In the conjugate regime ($\text{He}\sqrt{D_i/D_e} \sim 1$), the behaviour splits into two groups. All curves with $D_i/D_e \neq 1$ remain in the gain region throughout the conjugate regime at all three mesh resolutions, and their error ratios decrease monotonically with mesh refinement, confirming that the two-field scheme systematically outperforms the 1-fluid baseline for these configurations even near the conjugate point. The $D_i/D_e = 1$ red curve constitutes the exception: it enters the loss region near $\text{He} \approx 0.5$ – 2 at all three mesh levels. However, mesh refinement progressively reduces both the peak value of the ratio and the number of He points above parity, the loss region shrinks with refinement, though it does not fully disappear at the Δt_2 level.

Table 1 reports the absolute one-fluid error ε_{1F} at the coarsest mesh ($n_x/d = 4$) as a reference, together

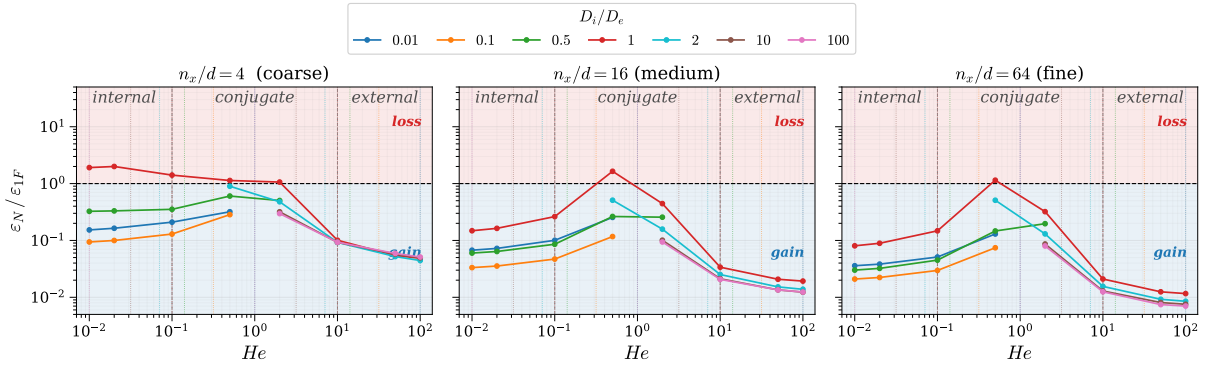


Figure 6: Relative accuracy of $T_{2F-neigh}$ compared with the 1-fluid model ($\varepsilon_N/\varepsilon_{1F}$) as a function of He , at three mesh resolutions. Each curve corresponds to one value of D_i/D_e . The dashed horizontal line marks parity ($\varepsilon_N = \varepsilon_{1F}$); blue and red shading indicate gain and loss regions. Vertical lines mark the regime boundaries $He\sqrt{D_i/D_e} = 0.1$ and 10 for $D_i/D_e = 1$ (grey dashes) and for each D_i/D_e curve.

with the spatial convergence rate p computed for the two finer meshes as

$$p = \frac{\log(\varepsilon_{1F}^{n_4}/\varepsilon_{1F}^{n_f})}{\log(n_f/4)},$$

where $n_f \in \{16, 64\}$. A value $p \approx 1$ indicates first-order spatial convergence, while $p \approx 2$ indicates second-order.

Table 1: 1-fluid reference errors and spatial convergence rates at Δt_1 . Cell colour indicates the transfer regime based on $He\sqrt{D_i/D_e}$: internal ($\ll 1$), conjugate (~ 1), external ($\gg 1$). (a) Absolute error ε_{1F} at $n_x/d = 4$; (b)–(c) spatial convergence order $p = \log(\varepsilon_{1F}^{n_4}/\varepsilon_{1F}^{n_f})/\log(n_f/4)$ between grids $n_x/d = 4 \rightarrow 16$ and $4 \rightarrow 64$.

(a) Absolute error ε_{1F} , $n_x/d = 4$

$He \backslash D_i/D_e$	0.01	0.1	0.5	1	2	10	100
0.01	5.6×10^{-1}	5.8×10^{-1}	1.3×10^{-1}	1.8×10^{-2}	–	–	–
0.02	5.3×10^{-1}	5.5×10^{-1}	1.3×10^{-1}	1.7×10^{-2}	–	–	–
0.1	4.1×10^{-1}	4.2×10^{-1}	1.1×10^{-1}	2.1×10^{-2}	–	–	–
0.5	2.6×10^{-1}	1.8×10^{-1}	4.4×10^{-2}	2.1×10^{-2}	2.1×10^{-2}	–	–
2	–	–	2.5×10^{-2}	1.4×10^{-2}	3.2×10^{-2}	4.8×10^{-2}	5.1×10^{-2}
10	–	–	–	4.4×10^{-2}	5.6×10^{-2}	6.6×10^{-2}	6.9×10^{-2}
50	–	–	–	1.8×10^{-2}	2.1×10^{-2}	2.3×10^{-2}	2.4×10^{-2}
100	–	–	–	1.0×10^{-2}	1.2×10^{-2}	1.3×10^{-2}	1.3×10^{-2}

(b) Conv. order p : $n_x/d = 4 \rightarrow 16$

$He \backslash D_i/D_e$	0.01	0.1	0.5	1	2	10	100
0.01	0.7	0.8	0.5	0.0	–	–	–
0.02	0.7	0.8	0.5	0.0	–	–	–
0.1	0.8	0.9	0.6	0.5	–	–	–
0.5	1.2	1.0	0.9	1.9	1.3	–	–
2	–	–	1.0	1.1	1.0	1.0	1.0
10	–	–	–	0.9	0.9	0.9	0.9
50	–	–	–	0.9	0.9	1.0	1.0
100	–	–	–	0.9	0.9	1.0	1.0

(c) Conv. order p : $n_x/d = 4 \rightarrow 64$

$He \backslash D_i/D_e$	0.01	0.1	0.5	1	2	10	100
0.01	0.8	0.9	0.7	0.4	–	–	–
0.02	0.8	0.9	0.7	0.4	–	–	–
0.1	0.8	0.9	0.8	0.7	–	–	–
0.5	1.0	1.0	0.9	1.4	1.2	–	–
2	–	–	1.0	1.0	1.0	1.0	1.0
10	–	–	–	0.9	0.9	0.9	1.0
50	–	–	–	0.9	1.0	1.0	1.0
100	–	–	–	0.9	1.0	1.0	1.0

4.2.2 Time-step refinement study

Table 2 presents, for each of the three time-step levels (Δt_1 , Δt_2 , Δt_3), the error ratio $\varepsilon_N/\varepsilon_{1F}$ ($\times 100$) at the fine mesh ($n_x/d = 64$), alongside the absolute one-fluid error ε_{1F} as a reference. Values below 100 indicate improvement over the 1-fluid baseline.

The sensitivity to time-step size is strongly regime-dependent. In the external regime, $T_{2F-neigh}$ lies

Table 2: Effect of time-step refinement on $T_{2F-neigh}$ accuracy at the fine mesh ($n_x/d = 64$). Left sub-table: error ratio $\varepsilon_N/\varepsilon_{1F}$ ($\times 100$); right sub-table: 1-fluid reference error ε_{1F} . Three time-step levels are compared: Δt_1 , Δt_2 , Δt_3 . Cell colour: transfer regime based on $\text{He}\sqrt{D_i/D_e}$: internal ($\ll 1$), conjugate (~ 1), external ($\gg 1$).

(a) Ratio ($\times 100$), Δt_1									
$\text{He}\sqrt{D_i/D_e}$	0.01	0.1	0.5	1	2	10	100		
0.01	4	2	13	39	—	—	—		
0.02	4	2	14	45	—	—	—		
0.1	5	3	20	88	—	—	—		
0.5	13	9	87	160	80	—	—		
2	—	—	47	264	68	39	35		
10	—	—	—	6	4	4	4		
50	—	—	—	2	2	2	2		
100	—	—	—	2	2	2	2		

(b) ε_{1F} , Δt_1									
$\text{He}\sqrt{D_i/D_e}$	0.01	0.1	0.5	1	2	10	100		
0.01	6.0×10^{-2}	4.9×10^{-2}	1.8×10^{-2}	4.6×10^{-3}	—	—	—		
0.02	5.6×10^{-2}	4.6×10^{-2}	1.7×10^{-2}	4.0×10^{-3}	—	—	—		
0.1	4.2×10^{-2}	3.3×10^{-2}	1.1×10^{-2}	2.0×10^{-3}	—	—	—		
0.5	1.6×10^{-2}	1.1×10^{-2}	2.3×10^{-3}	1.1×10^{-3}	1.8×10^{-3}	—	—		
2	—	—	2.2×10^{-3}	3.9×10^{-4}	1.5×10^{-3}	2.4×10^{-3}	2.7×10^{-3}		
10	—	—	—	3.2×10^{-3}	4.0×10^{-3}	4.7×10^{-3}	4.8×10^{-3}		
50	—	—	—	1.3×10^{-3}	1.5×10^{-3}	1.6×10^{-3}	1.6×10^{-3}		
100	—	—	—	7.6×10^{-4}	8.2×10^{-4}	8.6×10^{-4}	8.7×10^{-4}		

(c) Ratio ($\times 100$), Δt_2									
$\text{He}\sqrt{D_i/D_e}$	0.01	0.1	0.5	1	2	10	100		
0.01	4	2	3	8	—	—	—		
0.02	4	2	3	9	—	—	—		
0.1	5	3	5	15	—	—	—		
0.5	13	7	15	115	51	—	—		
2	—	—	20	32	13	9	8		
10	—	—	—	2	2	1	1		
50	—	—	—	1	1	1	1		
100	—	—	—	1	1	1	1		

(d) ε_{1F} , Δt_2									
$\text{He}\sqrt{D_i/D_e}$	0.01	0.1	0.5	1	2	10	100		
0.01	6.0×10^{-2}	4.9×10^{-2}	2.0×10^{-2}	5.8×10^{-3}	—	—	—		
0.02	5.6×10^{-2}	4.6×10^{-2}	1.8×10^{-2}	5.2×10^{-3}	—	—	—		
0.1	4.2×10^{-2}	3.3×10^{-2}	1.3×10^{-2}	3.1×10^{-3}	—	—	—		
0.5	1.6×10^{-2}	1.1×10^{-2}	3.6×10^{-3}	3.9×10^{-4}	7.5×10^{-4}	—	—		
2	—	—	1.4×10^{-3}	8.9×10^{-4}	2.1×10^{-3}	3.1×10^{-3}	3.3×10^{-3}		
10	—	—	—	3.3×10^{-3}	4.1×10^{-3}	4.8×10^{-3}	4.9×10^{-3}		
50	—	—	—	1.3×10^{-3}	1.5×10^{-3}	1.6×10^{-3}	1.6×10^{-3}		
100	—	—	—	7.7×10^{-4}	8.2×10^{-4}	8.7×10^{-4}	8.8×10^{-4}		

(e) Ratio ($\times 100$), Δt_3									
$\text{He}\sqrt{D_i/D_e}$	0.01	0.1	0.5	1	2	10	100		
0.01	4	2	1	3	—	—	—		
0.02	4	2	2	3	—	—	—		
0.1	5	3	2	5	—	—	—		
0.5	13	7	6	24	23	—	—		
2	—	—	8	11	5	4	4		
10	—	—	—	2	1	1	1		
50	—	—	—	1	1	1	1		
100	—	—	—	1	1	1	1		

(f) ε_{1F} , Δt_3									
$\text{He}\sqrt{D_i/D_e}$	0.01	0.1	0.5	1	2	10	100		
0.01	6.0×10^{-2}	4.9×10^{-2}	2.0×10^{-2}	6.1×10^{-3}	—	—	—		
0.02	5.6×10^{-2}	4.6×10^{-2}	1.9×10^{-2}	5.5×10^{-3}	—	—	—		
0.1	4.2×10^{-2}	3.3×10^{-2}	1.3×10^{-2}	3.4×10^{-3}	—	—	—		
0.5	1.6×10^{-2}	1.1×10^{-2}	4.0×10^{-3}	6.3×10^{-4}	4.8×10^{-4}	—	—		
2	—	—	1.3×10^{-3}	1.1×10^{-3}	2.3×10^{-3}	3.2×10^{-3}	3.4×10^{-3}		
10	—	—	—	3.4×10^{-3}	4.1×10^{-3}	4.8×10^{-3}	5.0×10^{-3}		
50	—	—	—	1.4×10^{-3}	1.5×10^{-3}	1.6×10^{-3}	1.6×10^{-3}		
100	—	—	—	7.7×10^{-4}	8.2×10^{-4}	8.7×10^{-4}	8.8×10^{-4}		

firmly in the gain region at all three time-step levels, with an accuracy advantage of one to two orders of magnitude over the 1-fluid baseline regardless of Δt . The absolute change between Δt_1 and Δt_3 is at most a few percentage points, confirming that the correction delivered by $T_{2F-neigh}$ is insensitive to Δt when the mass-transfer resistance is concentrated in the exterior phase.

In the internal regime, all $(\text{He}, D_i/D_e)$ configurations remain in the gain region across the three time-step levels, but the degree of sensitivity varies with D_i/D_e . For $D_i/D_e \leq 0.1$, ratios are 2–5% at Δt_1 and essentially unchanged at Δt_3 , confirming that time-step refinement brings no additional benefit once spatial resolution dominates. For $D_i/D_e = 1$, the sensitivity is more pronounced: ratios reach about 40% at Δt_1 , which still in the gain zone, but approaches parity, and decrease systematically to about 3% at Δt_3 .

By contrast, the conjugate regime exhibits a pronounced time-step dependence, with two distinct behaviours depending on D_i/D_e . For $D_i/D_e \neq 1$, most configurations already lie in the gain region at Δt_1 , but with ratios approaching parity near the conjugate point (about 80% at $\text{He} = 0.5$, $D_i/D_e = 0.5$ and at $\text{He} = 0.5$, $D_i/D_e = 2$). Time-step refinement brings these values firmly below parity: at Δt_3 , all $D_i/D_e \neq 1$ configurations reach ratios of 4%–23%, representing gains of one order of magnitude or more over the 1-fluid baseline. For $D_i/D_e = 1$, the loss region observed at coarse Δt is progressively eliminated by time refinement. At $(\text{He} = 0.5, D_i/D_e = 1)$, the ratio drops from 160% (Δt_1) to 24% (Δt_3), a reduction by a factor of 6.7. At $(\text{He} = 2, D_i/D_e = 1)$, the progression is 264 to 11%, a factor of 24. This sensitivity is a direct consequence of the minority-phase reconstruction: when both phases carry comparable resistance, the cut-cell concentration changes significantly between successive time steps, and a coarse Δt forces the reconstruction to extrapolate over a large temporal increment, generating errors that grow with Δt . Time-step refinement therefore acts as an effective remedy for conjugate-regime inaccuracy.

A practical implication follows: configurations in the external or deep-internal regimes ($\text{He}\sqrt{D_i/D_e} \gtrsim 5$ or $\text{He}\sqrt{D_i/D_e} \lesssim 0.3$) may use the coarsest admissible time step with negligible accuracy penalty, whereas configurations near the conjugate point ($\text{He}\sqrt{D_i/D_e} \sim 1$) require a finer Δt .

4.3 Parametric study on rotating-bubble simulations

The dynamic benchmark uses the same two-dimensional geometry as the static case: circular disk of radius R_0 in a square domain with Neumann boundaries, advanced to $t^* = 1$, with the same three time-step levels $\Delta t_1, \Delta t_2, \Delta t_3$ defined in Eq. (11)), but subjects the bubble to a prescribed rigid-body rotation around a fixed axis $\mathbf{x}_c = (-0.5R_0, 0)$:

$$\mathbf{u}(x, y) = A[(y - y_c)\mathbf{e}_x - (x - x_c)\mathbf{e}_y], \quad (12)$$

where A is chosen so that the mass-transfer Péclet number equals $\text{Pe} = \text{Re} \text{Sc} = 5.74$. Because the velocity field is a rigid-body rotation, the interface remains circular and does not deform; the analytical concentration solution of the static case therefore remains valid in the rotating frame. This property is the key advantage of the rotating-bubble benchmark: it provides an exact reference solution while genuinely exercising the numerical advection of both the VOF interface and the concentration field.

Unlike the static case, the concentration field is now coupled to the interface motion: advection at each time step introduces additional numerical diffusion and reconstruction errors that superimpose on the purely diffusive error. The scheme $T_{2F-neigh}$, which delivered the most consistent accuracy gains in the static benchmark, is retained here; its results are compared directly against the static reference to isolate the contribution of transport.

Figure 7 shows the error ratio $\varepsilon_N/\varepsilon_{1F}$ as a function of He for the three mesh resolutions at time-step level Δt_1 . Solid curves with markers correspond to the dynamic case; dashed curves reproduce the static results for direct comparison. The table 3 reports the corresponding numerical values at the fine mesh ($n_x/d = 64$).

Several conclusions can be drawn from the comparison. In the external regime, $T_{2F-neigh}$ retains its

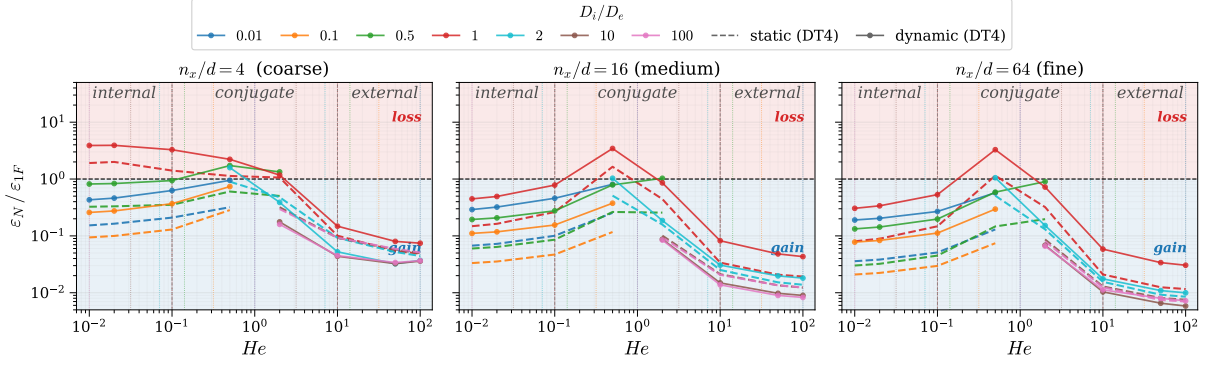


Figure 7: Effect of convection on the relative accuracy of $T_{2F-neigh}$ ($\varepsilon_N/\varepsilon_{1F}$) as a function of He , for three mesh resolutions at Δt_1 . Solid curves with markers: rotating-bubble results; dashed curves: static diffusion benchmark (from Fig. 6) shown for comparison. Colour encodes D_i/D_e ; blue and red shading indicate gain and loss regions.

Table 3: Error ratio $\varepsilon_N/\varepsilon_{1F}$ (%) for $T_{2F-neigh}$ at the fine mesh ($n_x/d = 64$, Δt_1): static diffusion (left) and rotating-bubble (right) benchmarks compared side by side. Cell colour indicates the transfer regime based on $He\sqrt{D_i/D_e}$: internal, conjugate, external.

(a) Static										(b) Dynamic									
He\ D _i /D _e		0.01	0.1	0.5	1	2	10	100		He\ D _i /D _e		0.01	0.1	0.5	1	2	10	100	
0.01	4	2	3	8	—	—	—	—		0.01	19	8	13	31	—	—	—	—	
0.02	4	2	3	9	—	—	—	—		0.02	20	8	14	34	—	—	—	—	
0.1	5	3	5	15	—	—	—	—		0.1	27	11	20	53	—	—	—	—	
0.5	13	7	15	115	51	—	—	—		0.5	57	30	59	328	105	—	—	—	
2	—	—	20	32	13	9	8	8		2	—	—	90	72	15	7	7	7	
10	—	—	—	2	2	1	1	1		10	—	—	—	6	2	1	1	1	
50	—	—	—	1	1	1	1	1		50	—	—	—	3	1	1	1	1	
100	—	—	—	1	1	1	1	1		100	—	—	—	3	1	1	1	1	

advantage over the one-fluid baseline at all three mesh resolutions. For $D_i/D_e \neq 1$, the dynamic and static error ratios are virtually identical, confirming that transport has no measurable effect when the mass-transfer resistance is entirely concentrated in the exterior phase and the diffusivity contrast is non-unity. The $D_i/D_e = 1$ red curve constitutes a minor exception: the ratio rises from 1% (static) to 3% (dynamic) at $He \geq 50$, a visible but modest degradation that leaves $T_{2F-neigh}$ firmly in the gain region.

In the internal regime, the dynamic error ratios are higher than their static counterparts by a factor of approximately 5 across all D_i/D_e values. The relative ordering of the curves is largely preserved between the static and dynamic cases: $D_i/D_e = 0.1$ orange curve remains the most accurate configuration in the internal regime, lying below $D_i/D_e = 0.5$ and $D_i/D_e = 0.01$ in absolute error ratio. The amplification is largest for $D_i/D_e = 0.01$ (factor ≈ 5), which exhibits the steepest internal concentration gradient. Despite this amplification, the two-field model outperforms the one-fluid baseline in all accessible internal-regime configurations. As the mesh is refined, the static curves descend rapidly towards 1–5% while the dynamic curves descend more slowly, so the gap between them progressively widens.

The conjugate regime remains the primary limitation. In the static benchmark, the error ratio reaches 115% at ($He = 0.5$, $D_i/D_e = 1$). Under transport, this peak rises to 328% at the same point, and the degradation extends to ($He = 0.5$, $D_i/D_e = 2$) (105%), demonstrating that advection widens the problematic region within the conjugate regime. The time-step study (Section 4.2.2) shows that refining Δt substantially mitigates this degradation in the static case.

Overall, $T_{2F-neigh}$ proves robust under transport conditions across most of the (He , D_i/D_e) parameter space. Its accuracy advantage over the 1-fluid baseline is preserved in both the external and internal regimes regardless of mesh resolution or time step. The conjugate regime at $D_i/D_e \approx 1$ and $He \sim 0.5$ –2 constitutes the only systematic limitation; its severity decreases substantially with time-step refinement.

5. Conclusion and Future Work

The accuracy of the two-field scheme $T_{2F-neigh}$ for interfacial mass transfer on Cartesian meshes has been investigated through a systematic parametric study spanning $He \in [0.01, 100]$ and $D_i/D_e \in [0.01, 100]$, covering the internal, conjugate, and external transfer regimes defined by the composite parameter $He\sqrt{D_i/D_e}$. Two two-dimensional benchmarks were considered: a static circular bubble in a purely diffusive field, and the same bubble subjected to a rigid-body rotation at moderate Péclet number.

External regime. This constitutes the most favourable operating domain for $T_{2F-neigh}$. In the static case, the error ratio remains low (about 3%) and insensitive to both mesh resolution beyond moderate grid densities and time-step level. Under advective transport, configurations with $D_i/D_e \neq 1$ are virtually unaffected; the $D_i/D_e = 1$ case exhibits a minor degradation that nonetheless leaves the scheme firmly in the gain region.

Internal regime. In the static case, low error ratios are obtained at fine mesh resolution across all diffusivity ratios considered. The exception arises at coarse mesh resolution for $D_i/D_e = 1$, which temporarily enters the loss region before recovering with spatial refinement. Under rotation, error ratios increase across all D_i/D_e values (by a factor of about 4–5), with the amplification being most pronounced for low diffusivity ratios. Despite this behaviour, $T_{2F-neigh}$ outperforms the one-fluid baseline in all accessible internal-regime configurations at all mesh levels considered.

Conjugate regime. This constitutes the primary limitation of $T_{2F-neigh}$. For $D_i/D_e \neq 1$, all configurations remain in the gain region at all mesh levels, and both spatial and temporal refinement consistently improve accuracy. For $D_i/D_e = 1$, error ratios exceed parity near the conjugate point in the static case, with the loss region shrinking but persisting under mesh refinement alone. Under advective transport, the loss region broadens and the peak error ratio increases substantially. Temporal refinement proves to be an effective remedy: the error ratio decreases by nearly an order of magnitude upon successive time-step

reductions, recovering the gain region without any modification to the spatial scheme.

The present study provides practical accuracy guidelines for a two-fields scheme $T_{2F-neigh}$. In the static case, reliable accuracy is achieved in the external regime for sufficiently large values of $He\sqrt{D_i/D_e}$, and in the internal regime for sufficiently fine spatial and temporal resolutions. Under advective transport, error ratios in the internal regime increase moderately at fine mesh resolution, while the external regime remains largely unaffected for $D_i/D_e \neq 1$. Configurations in the vicinity of the conjugate point are found to be sensitive to the time step, and temporal refinement is recommended in this parameter range to maintain accuracy.

Future work will focus on deformable interfaces at higher Schmidt numbers ($Sc \gg 1$), which require a dedicated treatment of the thin diffusive boundary layers, either by coupling the present approach with subgrid-scale models, or by introducing a dual-grid strategy in which the concentration field is resolved on a finer grid than the flow dynamics.

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