

SPECIES TRANSPORT IMMERSED BOUNDARY SOLVER FOR QCM BIOSENSOR: INITIAL DEVELOPMENTS

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Abstract

Detection of life-threatening pathogens in water can be done by Quartz Crystal Microbalance (QCM) biosensors. The pathogenic species get trapped at the crystal surface leading to a measurable change in the crystal resonant frequency. As a microfluidic device, QCM operates under diffusion-limited conditions and in its current design, most of the analyte is trapped in regions with no or limited crystal sensitivity. Our long term goal is to improve the QCM sensor sensitivity through optimization of its geometry. The optimization will leverage the immersed boundary method to mitigate the need of creating a separate mesh for each tested design. The device performance will be evaluated by simulating the analyte transport in the sensor. In this contribution, we present the development and verification of a mass-preserving flux correction at the immersed boundary, which is the basis of the required transient solver for analyte transport in the presence of immersed boundaries.

Keywords: CFD, immersed boundary method, scalar transport, OpenFOAM, biosensor.

1 Introduction

Biosensors based on Quartz Crystal Microbalance (QCM) are often utilized [1] for detection or continuous monitoring of pathogens in water. These biosensors contain a piezoelectric quartz crystal, the resonant frequency of which changes when the pathogens are captured at the crystal surface [2]. However, with the standard QCM biosensor geometry, most of the pathogens are captured in regions with limited to zero crystal sensitivity, which hinders the detection efficiency of the QCM biosensor. Thus, there is a continuous effort to increase the biosensor efficiency [3].

One way to achieve higher efficiency is to alter the geometry of the biosensor flow cell [4]. To find a suitable alternation of the geometry, automatic geometry optimization approaches based on a computational model of the biosensor can be used. However, a computational model of a QCM biosensor has to be able to model the flow with transport of the pathogens, which can be costly.

Our long term goal is to prepare a computationally viable model usable for future QCM sensor geometry optimization. The model will take advantage of a computationally cheap approach to represent geometry alternations via an immersed boundary method (IBM) [5]. The IBM allows us to save a lot of computational time on re-meshing, since one single computational mesh can be used for all tested geometries. The geometry alternations are only projected onto the mesh via an indicator scalar field and adjustment of governing equations.

However, the IBM needs to be coupled with a computationally feasible option to model the transport of pathogens. In this work, we discuss how the IBM method can be coupled with species balance equations to model the transport. Our particular focus lies in the biosensor application where the concentrations of pathogens are usually low, and even an error in the overall species balance that is small in absolute values can cause significant relative discrepancies. In such a setting, the biggest problem showed itself to be the presence of spurious fluxes across the immersed boundary (IB).

Although the numeric diffusion is small in magnitude, it has a high effect on the species balance and is able to break the overall mass balance in the system. Interestingly, while the IBM has been developed since the 1970s [6] and numerous applications where it has been coupled with scalar transport are documented, see, e.g., [7, 8, 9, 10], we were not able to find a correction to the spurious fluxes across the IB usable for the studied application. Therefore, investigating the source of error and its correction is the main novelty of this contribution.

2 Mathematical model

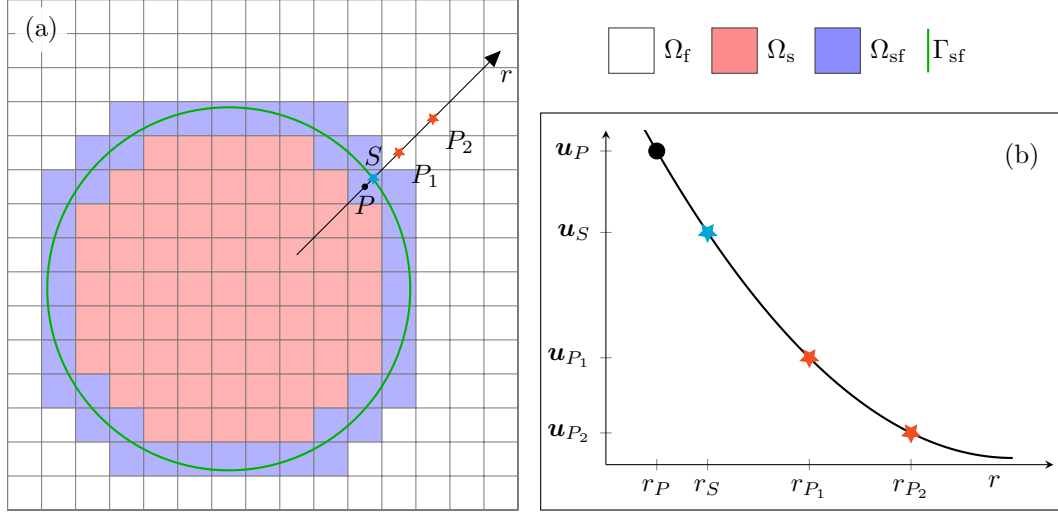


Figure 1: (a) Division of the computational mesh Ω into Ω_f , Ω_{sf} , and Ω_s required by the immersed boundary method. (b) Principle of reconstruction of the no-slip boundary condition for $\mathbf{u}$ on the solid-fluid interface Γ_{sf} . Inspired by [11].

Computational mesh First, let us assume a finite volume computational mesh Ω , which in our case represents the biosensor geometry. With the addition of obstacles, Ω is divided as $\Omega_f \cup \Omega_{sf} \cup \Omega_s$, where the subscripts f, s, sf denote parts fully immersed in the fluid phase, representing the solid phase, and the solid-fluid interface, respectively. This division is represented by the color function λ , which is defined for each cell $\Omega_P \in \Omega$ as

$$\lambda = \begin{cases} 0 & \text{if } \Omega_P \in \Omega_f \\ 1 & \text{if } \Omega_P \in \Omega_s \\ \tilde{\lambda} \in (0, 1) & \text{if } \Omega_P \in \Omega_{sf} \end{cases} \quad (1)$$

where $\tilde{\lambda}$ is defined as the volume fraction of the solid phase within the cell Ω_P . The division of the domain for a circular particle is shown in Figure 1a, with the true particle boundary Γ_{sf} colored green.

Immersed boundary method Using the approach described in the above paragraph, the solid phase is included virtually without the need for a conforming mesh. However, the presence of the solid has to be enforced in the system governing equations. In the following, we build on the approach of Municchi and Radl [12, 13] and Isoz et al. [5]. In particular, we firstly display basic principles for the case of the fluid governing equations and then focus on species transport.

For the problem at hand, we apply the standard variant of the laminar incompressible Navier-Stokes equations for a Newtonian fluid extended with by an additional IB forcing term $\mathbf{f}_{ib}$,

$$\begin{aligned} \mathcal{M}(\mathbf{u}) &= -\nabla \tilde{p} + \mathbf{f}_{ib}, & \mathcal{M}(\mathbf{u}) &= \frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot (\mathbf{u} \otimes \mathbf{u}) - \nabla \cdot (\nu \nabla \mathbf{u}), \\ \nabla \cdot \mathbf{u} &= 0, & \mathbf{f}_{ib} &= \text{ceil}(\lambda) (\mathcal{M}(\mathbf{u}_{ib}) + \nabla \tilde{p}) \end{aligned} \quad (2)$$

where $\tilde{p}$ is the kinematic pressure, ν kinematic viscosity and $\mathbf{u}$ is the fluid velocity. The forcing term $\mathbf{f}_{ib}$ is active only within the solid and in its vicinity, as given by the λ field.

Lastly, the prescribed velocity values $\mathbf{u}_{ib}$ are set for the internal cells and static Ω_s as $\mathbf{u}_{ib} = \mathbf{0}$. To ensure the correct no-slip boundary condition at the solid-fluid interface Γ_{sf} , the values in centroids of cells in Ω_{sf} are reconstructed based on the on the estimated position of the surface and fluid velocity in its vicinity, see Figure 1b.

In detail, a line r is constructed that passes through the points S and P and is orthogonal to Γ_{sf} . The length $\delta_P = \text{volume}(\Omega_P^h)^{1/3}$ is based on the characteristic cell size and is used to construct the points P_1 and P_2 . Then, the $\mathbf{u}$ values at these points are interpolated from the nearest neighbors using a suitable interpolation scheme. The value of $\mathbf{u}_{ib}$ in P is obtained by a polynomial approximation of degree $n \leq 2$. For the case of $n = 2$, the following equation is written,

$$\mathbf{u}_{ib}(P) = \frac{\mathbf{u}_{P_2} - 2\mathbf{u}_{P_1} + \mathbf{u}_S}{2\delta_P^2} d_{PS}^2 + \frac{4\mathbf{u}_{P_1} - \mathbf{u}_{P_2} - 3\mathbf{u}_S}{2\delta_P} d_{PS} + \mathbf{u}_S, \quad (3)$$

where d_{PS} is distance between the cell center P and the particle surface S . If the given cell is close to the system boundary or another solid obstacle, the points P_1 or P_2 may not belong to Ω_f . To be specific, when $P_1 \in \Omega_f$ and $P_2 \notin \Omega_f$ the first order approximation is then expressed as,

$$\mathbf{u}_{ib}(P) = \frac{\mathbf{u}_{P_1} - \mathbf{u}_S}{\delta_P} d_{PS} + \mathbf{u}_S. \quad (4)$$

At last, when the given cell is at the domain boundary or very close to another solid obstacle, that is, $P_1, P_2 \notin \Omega_f$, the zero-order approximation $\mathbf{u}_{ib}$ is used and computed based on the value of λ as

$$\mathbf{u}_{ib}(P) = \lambda \mathbf{u}_S + (1 - \lambda) \mathbf{u}_P. \quad (5)$$

The discretized form of the flow equations (2) is solved via a standard PIMPLE-like loop. For further details and verification of this approach, the readers are referred to Isoz et al. [5].

Scalar transport For species, i.e., scalar transport, we apply a similar principle as shown above with minor modifications. The transport equation for the i -th specie is given as

$$\frac{\partial(c_T x_i)}{\partial t} + \nabla \cdot ((c_T x_i) \mathbf{u}) = \nabla \cdot (D_i \nabla (c_T x_i)) + s_{ib}, \quad i = 1, \dots, n-1, \quad x_n = 1 - \sum_{i=1}^{n-1} x_i \quad (6)$$

where x_i , D_i and c_T are the molar fraction, the diffusion coefficient for the i -th component, and the total concentration, respectively. The last term s_{ib} is an IB-related source term designed to keep the species outside the solid phase.

For the cases where there is a surface reaction at Γ_{sf} , the term s_{ib} can be defined similarly to $\mathbf{f}_{ib}$ in (2) with the values in Ω_{sf} defined similarly to $\mathbf{u}_{in}$ in (3)-(5). However, in the case studied, our goal is merely to prevent the species x_i , $i = 1, \dots, n$ from crossing Γ_{sf} , which should already be ensured by the computed velocity field. Thus, in our case $s_{ib} = 0$.

However, since the position of Γ_{sf} in Ω_{sf} is reconstructed only approximately, there are always spurious fluxes across the IB present. In specific cases, these fluxes can lead to the breakdown of the overall mass balance for the species in the system. Furthermore, in case of $s_{ib} \neq 0$ in (6), the approximate resolution of Γ_{sf} leads to an inaccuracy of the solution close to IB. More so for the transport of species, which tends to be sensitive to the spurious fluxes. This issue is also described in the review by Xiao et al. [10]. Usually, as in [12], the inaccuracy close to IB is resolved via modification of s_{ib} . However, such an approach further deteriorates the problem of mass balance in the system.

3 Scalar transport correction

The IB-induced error in species transfer is studied in an ad hoc designed test. The test comprises a two-dimensional laminar flow around a circular obstacle. The obstacle is assumed nonporous. The test geometry has dimensions of $50 \times 50 \times 1$ FV cells, which corresponds to $L \times L = 0.5 \times 0.5$ m. The obstacle has the diameter of 20 cells and is placed in the center of the geometry. The geometry and dimensions of the test are shown in Figure 2a and b.

Outlet, inlet and wall boundaries are prescribed with boundary conditions $\mathbf{n}_{outlet} \cdot (\nabla \mathbf{u}_{outlet}) = 0$, $\mathbf{u}_{inlet}^T = (0, -5, 0)$ mm/s, $\mathbf{u}_{wall} = 0$ for fluid velocity and $p_{outlet} = 0$, $\mathbf{n}_{inlet} \cdot \nabla p_{inlet} = 0$, $\mathbf{n}_{wall} \cdot \nabla p_{wall} = 0$ for fluid pressure, respectively. For the species, the tracer molar fraction is prescribed uniform at the inlet, $x_{i,inlet} = 1$ and $\mathbf{n}_{outlet,wall} \cdot \nabla x_{i,outlet,wall} = 0$ elsewhere. The test parameters comprise the fluid kinematic viscosity $\nu = 10^{-5} \text{ m}^2 \text{ s}^{-1}$ and diffusivity $D = 0 \text{ m s}^{-2}$. The test Reynolds

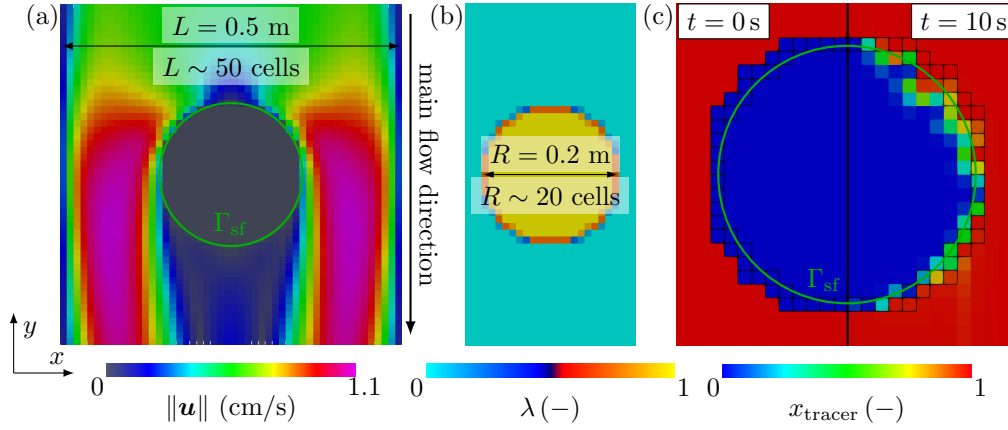


Figure 2: Test to illustrate the required correction for spurious fluxes across IB. (a) Test geometry and velocity field, (b) definition of the solid obstacle via λ field, (c) initial and final tracer concentration inside the particle.

number is 100. Note that given the initial state of the tracer concentration and the switched-off diffusion, any nonzero concentration inside the particle is nonphysical. The test is evaluated for 10 s of the simulation time, which corresponds only to 0.1 of the tracer residence time. The nonphysical concentration field inside Ω_s is shown in Figure 2c.

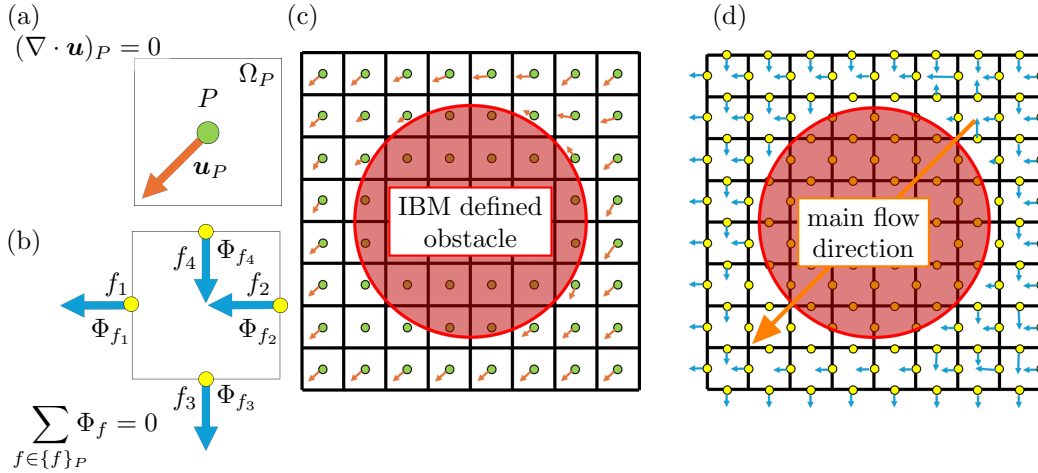


Figure 3: Finite volume method treatment of advection. (a) Velocity $\mathbf{u}_P$ stored in the centroid P of the cell Ω_P and the local mass balance, (b) flux-based discretization of the local mass balance in Ω_P . The expected immersed boundary method influence on a circular obstacle and in its proximity (c) velocity and (d) fluxes.

In Figure 2c, the error in tracer transport is evident in the penetration of the boundaries, not only affecting the interface cells (Ω_{sf}), but also propagating into the internal cells (Ω_s). This is similar to observations reported in the literature [10]. The spurious fluxes across the IB are caused by the convective term in (6). Due to the convective term discretization in FVM, see [14], for a cell $\Omega_P \in \Omega_{\text{sf}}$, the correction has to be implemented at the level of fluxes across the faces $\{f\}_P$ comprising the boundary of Ω_P . The relation between $\mathbf{u}_P$, the mass balance in Ω_P and the fluxes Φ_f , $f \in \{f\}_P$ is depicted in Figures 3a and b. The velocity and flux fields for the flow around a circular immersed boundary are shown in Figures 3c and d.

However, since FVM is a numerical method, the available solution always has some residual error below the set tolerance. For the case presented in Figure 2, the relative tolerance with respect to pressure and fluid velocity is set as 10^{-7} . Consequently, with the test results displayed in the range below tolerance, the residual non-zero field circulating within the obstacle is revealed; see

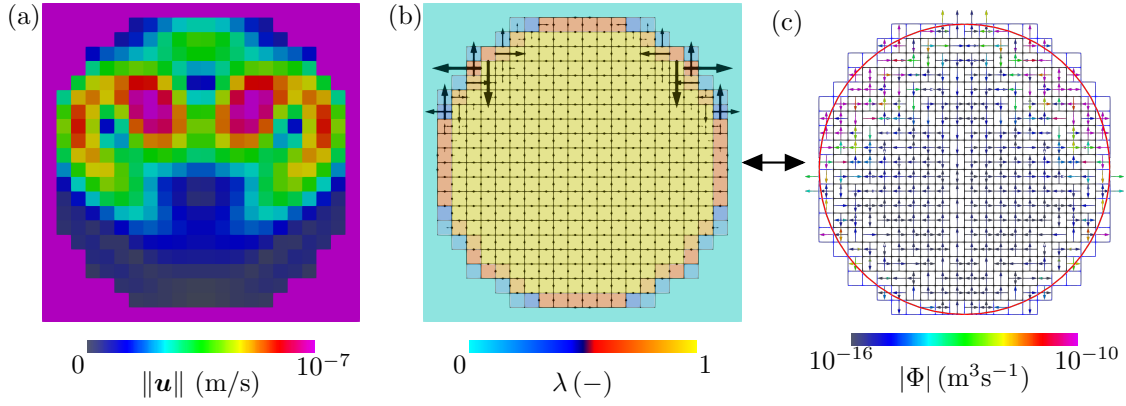


Figure 4: Residual velocity values within the obstacle with the magnitude value below 10^{-10} m/s (a), display of face fluxes scaled by magnitude (b) and colored by magnitude (c)

Figure 4a. However, the fluxes created by this velocity field are not restricted to the interior of the obstacle, but points both outside and inside, as visible in Figures 4b and c. This leads to the observed effects, since the advection term is coupled with the flux values. This is best visible in the rewritten form of species balance (6) in OpenFOAM implementation,

$$\text{fvm}::\text{ddt}(c_T x_i) + \text{fvm}::\text{div}(\Phi, c_T x_i) = \text{fvm}::\text{laplacian}(D_i, c_T x_i), \quad (7)$$

where $\text{fvm}::\text{ddt}$, $\text{fvm}::\text{div}$, $\text{fvm}::\text{laplacian}$ are OpenFOAM's implementation of time derivative, divergence, and Laplacian operators applied for terms in brackets respectively, see [15] for details.

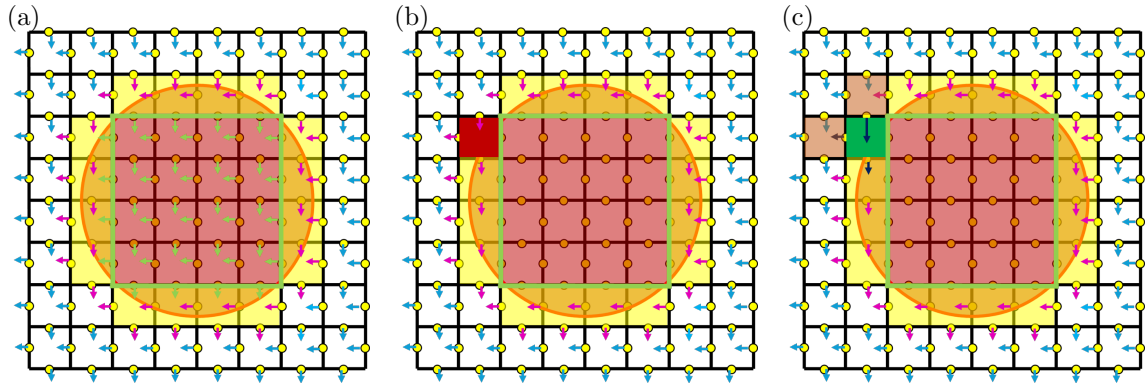


Figure 5: Flow correction algorithm outline. (a) Identified fluxes to be switched off (in green), and directly affected fluxes (in pink). (b) Exemplary cell with broken local balances. (c) Imbalanced flux redistribution and creation of new imbalanced cells.

In summary, IB, while maintaining both the global and local mass, momentum, and species balances, breaks the physics of the solution in Ω_{sf} and in Ω_{s} , where it creates spurious fluxes. To overcome this feature, we propose to locally break the species balance in Ω_{sf} to promote the solution physicality, i.e., to disallow any nonphysical species transfer across Γ_{sf} or, at least, across Ω_{sf} . In particular, a correction to the species transport is proposed that is based on setting the fluxes for all faces in Ω_{s} and faces in Ω_{sf} that are within the solid to zero. The switched off fluxes are colored green in Figure 5a.

Let us now focus on a cell $\Omega_P \in \Omega_{\text{sf}}$ with faces $\{f\}_P = \{f\}_P^{\text{int}} \cup \{f\}_P^{\text{ext}}$, where $f \in \{f\}_P^{\text{int}}$ if most of it lies within the solid and $f \in \{f\}_P^{\text{ext}}$ otherwise. Such a cell is colored red in Figure 5b. Prescribing $\Phi_f = 0 \forall f \in \{f\}_P^{\text{int}}$ breaks the local mass and species balance as $\sum_{f \in \{f\}_P^{\text{ext}}} \Phi_f = 0$ is not enforced. Now, after this flux adjustment, two possible situations may occur in any $\Omega_P \in \Omega_{\text{sf}}$.

First, there are both inflow ($\Phi_f > 0$) and outflow ($\Phi_f < 0$) faces in $\{f\}_P^{\text{ext}}$. Second, only the inflow or outflow faces remain in $\{f\}_P^{\text{ext}}$.

The correction for the first case is achieved by rescaling the remaining fluxes Φ_f , $f \in \{f\}_P^{\text{ext}}$ to compensate for the flux imbalance in Ω_P . In this case, the rescaling is based on the original flux magnitude. In the second case, rescaling the available fluxes cannot resolve the flux imbalance as their sum will always be either positive or negative. In any case, the imbalanced fluxes are transferred to the "plus one" neighbor of Ω_P as indicated in Figure 5c. Although this flux transfer corrects Ω_{sf} , it breaks the balance of mass and species in its outer neighbors. However, because there are more outer neighbors to Ω_{sf} than there are cells within it¹ and the mean flow velocity can be expected to increase with distance from Γ_{sf} , the newly created imbalances are in relative terms significantly smaller than the original ones.

Finally, note that the ordering of flux correction in Ω_{sf} is a factor that should be taken into account. In particular, optimal correction ordering is such that the most possible imbalanced fluxes are transferred streamwise along Γ_{sf} . However, to find such an ordering for a general flow field and solid geometry is non-trivial. Simultaneously, using the same non-optimal ordering repeatedly will lead to accumulation of errors in only a small number of cells. In the proposed implementation, we use stochastic ordering for flux correction at any time step to prevent the accumulation of any residual error.

4 Results

To verify the results of the proposed correction, the initial test for advective tracer transport is re-evaluated; its results are summarized in Figure 6. The initial and final distribution of the tracer around the obstacle are displayed in Figure 6a. The suppressed internal fluxes within the particle scaled and colored by their magnitude are given in Figures 6b and c, respectively. Comparing Figures 2 and 6 showcases the functionality of the proposed correction that mitigates the influence of the spurious cross-IB fluxes on the species transport.

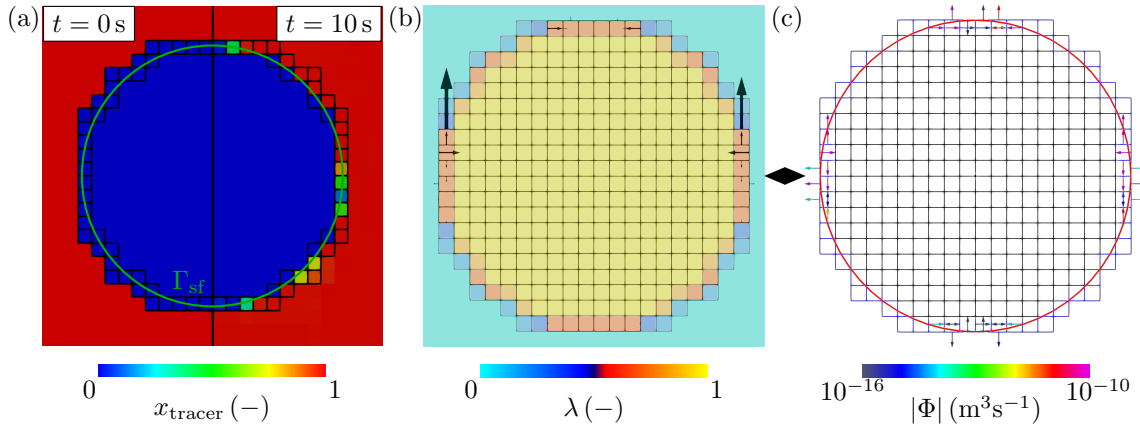


Figure 6: Results of re-evaluation of the initial test case displayed in Figures 2 and 4 with the described transport correction applied.

Moreover, to demonstrate the general applicability of the proposed correction, the original simplified test is modified as follows. A three-dimensional case with the geometry of dimensions $30 \times 100 \times 30$ FV cells $\sim 0.3 \times 0.3 \times 1.0$ m. A spherical obstacle with a diameter of 20 cells ~ 0.2 m is projected in the center of the domain. The inlet, outlet, and wall boundaries are prescribed with boundary conditions for $\mathbf{n}_{\text{inlet}} \cdot \nabla p_{\text{inlet}} = 0$, $p_{\text{outlet}} = 0$, $\mathbf{n}_{\text{wall}} \cdot \nabla p_{\text{wall}} = 0$ for the pressure and $\mathbf{u}_{\text{inlet}}^T = (0, -0.5, 0) \text{ m/s}$, $\mathbf{n}_{\text{outlet}} \cdot \nabla(\mathbf{u}_{\text{outlet}}) = \mathbf{0}$ and for the wall boundaries we prescribe the slip condition for velocity.

With respect to species, we assume a mixture of tracer and carrier in a ratio of 1 : 99. All boundaries are set to $\mathbf{n}_{\text{outlet,wall}} \cdot \nabla x_{i,\text{outlet,wall}} = \mathbf{0}$ except for the inlet, where the given ratio is

¹For three dimensional cases, the number of cells in question increases with the second power of the distance from Γ_{sf} .

prescribed. The initial condition corresponds to a fully developed flow and the prescribed tracer to carrier ratio in Ω_f . The test case is evaluated for the simulation time $t = 5$ s both with and without active correction. The test design with the Reynolds number of 10000 aims to create a greater difference in velocity in the vicinity of the obstacle surface. Thus, a greater influence of spurious fluxes is induced, leading to a more severe intrusion of the tracer into the obstacle.

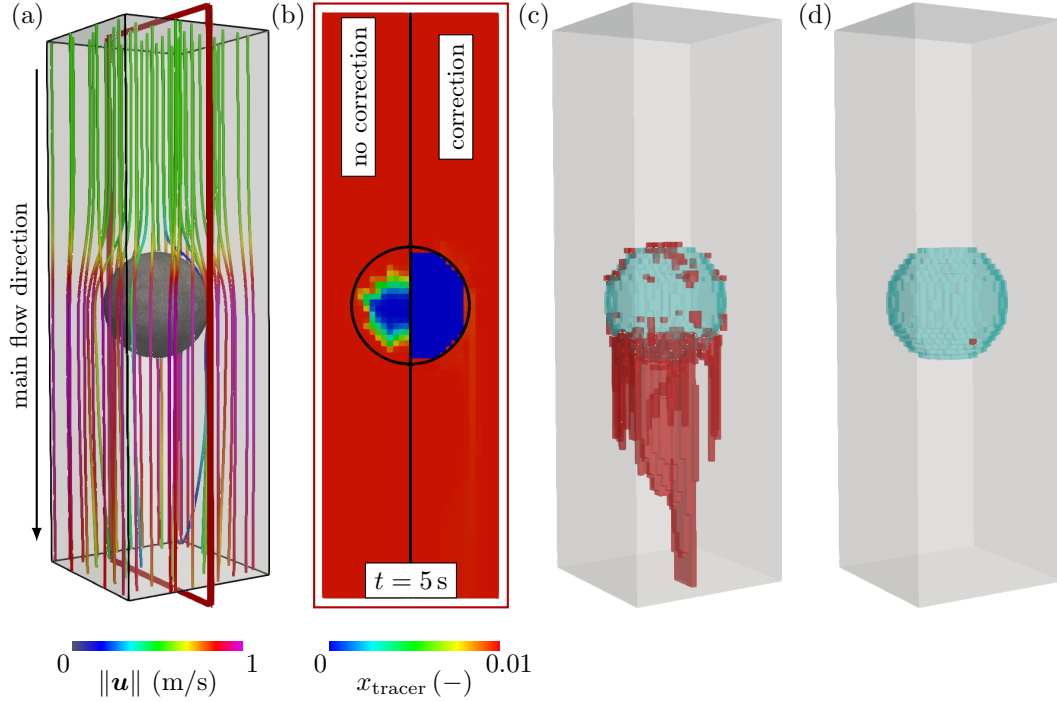


Figure 7: Results of transport correction verification for the 3D case with increased inlet velocity test design and flow visible in (a). The end time distribution of the tracer for configuration with and without correction is displayed in a slice of (a) (b). Distribution of composition error due to transport correction in the surrounding cells with its value above 1% and 10% in (c),(d) respectively.

The new test results are depicted in Figure 7. The interesting feature is the distribution of error in the tracer-to-carrier ratio in the vicinity of the particles, see Figures 7c and d. However, this does not affect the global balance of species in the system and should be further mitigated by enabling a diffusion term. Nevertheless, because of this contribution's limited scope, results with the diffusion term included and showing the application of the proposed correction in the real-life structure of the QCM biosensor will be presented at the conference.

5 Conclusions

The present contribution focuses on the coupling of transient species transport balance with the fluid flow by using the immersed boundary method to define physical obstacles. The main motivation for such solver is the application to model flow and analyte transport in diffusion-limited conditions of QCM biosensors. However, the IBM feature hinders the straightforward implementation with spurious fluxes within the defined obstacle and across its immersed boundary, which leads to the intrusion of the analyte into the defined obstacles. To address this issue, a new transport correction is proposed and verified that suppresses spurious fluxes and, in the end, promotes the physicality of species transport. Correction functionality and properties are demonstrated in the 2D and 3D tests, and residual errors are described and quantified. Overall, the results are promising, enabling the correction to be used in the intended application. Nevertheless, further development is required, namely parallelization to increase overall computational efficiency to allow for simulation of the whole device QCM biosensor.

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