ARTICLE TYPE

Numerical Considerations for Advection-Diffusion Problems in Cardiovascular Hemodynamics

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Summary

Numerical simulations of cardiovascular mass transport pose significant challenges due to the wide range of Péclet numbers present in cardiovascular flows and backflow at outlet (Neumann) boundaries. In this paper we present and discuss several numerical tools to address these challenges in the context of a stabilized finite element computational framework. To overcome numerical stability issues when backflow occurs in Neumann boundaries we propose an approach based on the prescription of the total flux. In addition, we propose a consistent flux boundary condition at the outlet boundaries and demonstrate its superiority over the traditional zero diffusive flux boundary condition in preserving the physical accuracy of the solution. Lastly, we discuss Discontinuity-Capturing (DC) stabilization techniques to address the well-known oscillatory behavior in the solution near the advancing wavefront in advection-dominated flows. We present numerical examples in both idealized and patient-specific geometries to demonstrate the efficacy of the proposed formulation. The proposed numerical framework represents a powerful computational tool to investigate mass transport in cardiovascular processes.

KEYWORDS:
backflow stabilization, cardiovascular simulation, Neumann inflow boundary condition, discontinuity-capturing operator, scalar advection diffusion, consistent boundary condition

1 INTRODUCTION

Mass transport plays an important role in numerous cardiovascular pathologies including thrombosis and atherosclerosis. Computational mass transport models offer the unique capability to study the influence of various biochemical parameters that are otherwise difficult to measure in vivo but are essential to gain an insight into various biochemical processes. However, cardiovascular mass transport is characterized by the presence of highly advection-dominated flows (with Péclet numbers of up to $10^7$) that make obtaining an accurate numerical solution challenging. Furthermore, since computational analyses are typically limited to a small region of interest, they inevitably lead to the introduction of artificial boundaries in the computational model. The boundary conditions that are prescribed at these boundaries form a crucial component of any computational model and need to be chosen carefully to preserve the accuracy of the computational model.

A number of outflow boundary conditions have been proposed to simulate blood flow in arteries. Here, the prescription of Neumann conditions at boundaries that exhibit partial or complete inflow is known to lead to the divergence of simulations.
Similar scenarios can arise in scalar advection-diffusion systems, such as those considered for the modeling of thrombus formation for cardiovascular mass transport. Despite the numerous reports on outflow stabilization for flow problems, these strategies have not been adopted for scalar advection-diffusion systems. Instead, to circumvent the issue of backflow divergence in scalar advection-diffusion systems, current mass transport models have resorted to a number of unphysical approaches such as the imposition of arbitrary Dirichlet boundary conditions at the outlet face, artificial extension of the computational domain, or artificial increase in the diffusivity of the scalar. Furthermore, while there have been a number of reports on identification of appropriate outflow boundary conditions for flow problems, little work has been done in this regard for scalar advection-diffusion problems.

Another important issue concerning the modeling of scalar transport in cardiovascular systems is the occurrence of high Péclet number flows in large arteries. These advection-dominated flows lead to the development of steep concentration gradients, thereby necessitating the need of stabilization techniques to avoid unphysical oscillations in the numerical solution. To address this issue, a number of discontinuity capturing methods have been proposed.

In this work, we present a stabilized finite element framework that incorporates three salient features: (i) a backflow stabilization technique to obtain stable solutions with Neumann outflow boundaries for scalar advection-diffusion problems, (ii) a consistent boundary condition that preserves the local physics of the problem despite the introduction of artificial computational boundaries; and (iii) stabilization techniques including SUPG and DC operator to address the numerical oscillations in the solution. We present numerical results in both the idealized and patient-specific geometries to demonstrate the efficacy of the proposed computational framework. These results demonstrate that the proposed computational framework offers the capability to obtain accurate, stable numerical solutions for three-dimensional transient cardiovascular mass transport systems.

2 | METHODS

2.1 | Strong form and boundary conditions

The strong form of the governing equation for the transport of a scalar in an incompressible flow is given as

$$\frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c - \nabla \cdot (D \nabla c) = R \quad \text{in} \quad \Omega,$$

where $c$, $\mathbf{u}$, $D$, $R$, and $\Omega$ denote the concentration of the scalar, flow velocity, diffusion coefficient, source (or reaction) terms, time, and the domain respectively. For the prescription of boundary conditions, we consider a unique, disjoint decomposition of the boundary, $\Gamma$ into two parts defined as:

$$\Gamma^{\text{in}}(t) = \{x \in \Gamma | u_n(x, t) \leq 0\},$$

$$\Gamma^{\text{out}}(t) = \Gamma - \Gamma^{\text{in}}(t),$$

where $u_n$ is the dot product of the velocity with the outward unit normal to the boundary, $x$ is the position vector, $\Gamma^{\text{in}}(t)$ is the inflow boundary, and $\Gamma^{\text{out}}(t)$ is the outflow boundary. We remark here that the inflow and outflow boundaries are functions of time owing to the time dependence of the velocity field. Furthermore, each of these boundaries can be decomposed into their Dirichlet component, $\Gamma_D$ and Neumann component, $\Gamma_N$ such that

$$\Gamma_D^{\text{in/out}}(t) = \Gamma_D \cap \Gamma_D^{\text{in/out}}(t),$$

$$\Gamma_N^{\text{in/out}}(t) = \Gamma_N \cap \Gamma_N^{\text{in/out}}(t).$$

It is customary in finite element simulations to handle the inlet boundaries via strongly imposed Dirichlet boundary conditions. In contrast, outflow boundaries are described via weakly imposed Neumann boundary conditions. The issue of divergence of scalar transport simulations arises due to the presence of a backflow at a Neumann boundary such that $\Gamma_N^{\text{in}}(t) \neq \emptyset$. Specifically, the prescription of diffusive flux at a face exhibiting inflow fails to guarantee stable energy estimates and leads to the divergence of numerical simulation. To mitigate this issue, it is recommended to prescribe the total flux at a Neumann inlet boundary while only the diffusive component of flux is specified at the Neumann outlet boundary, such that

$$D \nabla c \cdot \mathbf{n} = h^{\text{out}} \quad \text{on} \quad \Gamma_N^{\text{out}}(t),$$

$$-c \mathbf{u} \cdot \mathbf{n} + D \nabla c \cdot \mathbf{n} = h^{\text{in}} \quad \text{on} \quad \Gamma_N^{\text{in}}(t).$$
where \( h^{in} \) and \( h^{out} \) denote the prescribed flux data on the Neumann inlet and outlet boundaries.\(^\text{[1]}\) As will be described in Section 2.2, this distinction in prescription of Neumann boundary conditions at inlet and outlet boundaries results in a term in the weak form of the governing equation that is typically ignored and causes the numerical simulation to diverge.

### 2.2 Weak form

The weak form for the scalar advection-diffusion problem governed by Eq. [1] is given in three-dimensional form as follows: Given a bounded domain \( \Omega \subset \mathbb{R}^3 \) and the corresponding velocity field \( \mathbf{u} \), find \( c \in H^1(\Omega) \) such that

\[
\int_{\Omega} \left[ \delta_c \frac{\partial c}{\partial t} + \delta_c \mathbf{u} \cdot \nabla c + \nabla \delta_c \cdot D \nabla c \right] dV - \int_{\Gamma_N} \delta_c (D \nabla c) \cdot \mathbf{n} dA = \int_{\Gamma_t} \delta_c \mathbf{r} dV \quad \forall \delta_c \in H^1_0(\Omega) \tag{8}
\]

where \( \delta_c \) is the weighting function, \( H^1(\Omega) \) is the solution function space consisting of once-differentiable functions that satisfy the Dirichlet boundary conditions on \( \Gamma_D \) while \( H^1_0(\Omega) \) is the weighting function space consisting of once-differentiable functions that vanish on the Dirichlet boundary \( \Gamma_D \). Since cardiovascular mass transport problems are characterized by high Péclet number, we utilize a stabilized finite element framework using the SUPG formulation.\(^\text{[10]}\) This stabilization involves the addition of an extra term to the weak form such that the stabilized weak form for scalar advection-diffusion problems is given as

\[
\int_{\Omega} \left[ \delta_c \frac{\partial c}{\partial t} + \delta_c \mathbf{u} \cdot \nabla c + \nabla \delta_c \cdot D \nabla c \right] dV - \int_{\Gamma_N} \delta_c (D \nabla c) \cdot \mathbf{n} dA + \sum_{i=1}^{n_{el}} \int_{\Omega_i} \nabla \delta_c : \mathbf{u} \mathbf{r} dV = \int_{\Omega} \delta_c \mathbf{r} dV \quad \forall \delta_c \in H^1_0(\Omega) \tag{9}
\]

where \( n_{el} \) denotes the number of elements in the discretized domain, \( \Omega_i \) is the domain of the \( i \)-th element, \( \tau \) is the stabilization parameter, and \( \mathbf{r} \) is the weak residual given as

\[
\mathbf{r} = \frac{\partial c}{\partial t} + \mathbf{u} \cdot \nabla c - D \nabla^2 c
\]

(10)

We remark here that due to the use of linear finite element basis functions in our implementation, the last term in above expression vanishes. For our implementation, we choose the stabilization parameter given as

\[
\tau = \frac{1}{\sqrt{\tau_1 + \tau_2 + \tau_3}}, \quad \tau_1 = \left( \frac{2}{\Delta t} \right)^2, \quad \tau_2 = \mathbf{u} \cdot \mathbf{g}, \quad \tau_3 = 9D^2 \mathbf{g}, \quad \mathbf{g} = \left( \frac{\partial \xi}{\partial x} \right) \frac{\partial \xi}{\partial x}
\]

(11)

where \( \Delta t \) is the time step size and \( \mathbf{g} \) is the metric tensor based on the Jacobian of the mapping between the barycentric coordinates \( \xi \) and the physical coordinates \( \mathbf{x} \).

### 2.3 Backflow stabilization technique

Having presented the weak form of the governing equations with SUPG stabilization, we turn our attention to the prescription of Neumann boundary conditions. Using Eq. [6] and [7], the boundary term in Eq. [9] at a Neumann face can be reformulated as

\[
\int_{\Gamma_N} \delta_c (D \nabla c) \cdot \mathbf{n} dA = \int_{\Gamma_N} \delta_c (D \nabla c) \cdot \mathbf{n} dA + \int_{\Gamma_N} \delta_c (D \nabla c) - \mathbf{c} \cdot \mathbf{u} \cdot \mathbf{n} dA + \int_{\Gamma_N} \delta_c \mathbf{u} \cdot \mathbf{n} dA
\]

(12)

As indicated earlier, typically Dirichlet boundary conditions are prescribed on inlet faces while Neumann boundary conditions are prescribed at outlet faces such that \( \Gamma_D(t) = \emptyset \) and \( \Gamma_N(t) = \emptyset \), resulting in a null contribution from the last term in Eq. [13].
However, in cases where a Neumann face is associated with an inflow i.e. $\Gamma_{\text{in}}^N(t) \neq \emptyset$, the last term in Eq. 13 results in a non-trivial contribution and must be included in the implementation to obtain a stable solution. We remark here that the analogous term for the Navier-Stokes equation is typically multiplied by a scaling factor $\beta$ and different studies have employed different values of $\beta$ in the context of Navier-Stokes equation. However, owing to the lack of mathematical rigor justifying the introduction and choice of such a scaling factor, we do not consider any scaling factor for the scalar advection-diffusion problem.

### 2.4 Consistent flux boundary condition

The boundary conditions imposed at artificial boundaries generated due to the truncation of a physical domain form a crucial component of the corresponding computational model. Since the physics of the problem is unknown at such artificial boundaries, the task of identifying appropriate boundary conditions that preserve the physics of the problem remains challenging. With a view to keep the local physics unaltered despite the introduction of artificial boundaries, various boundary conditions have been proposed in the literature in the context of Navier-Stokes equations. Among these, the most common boundary conditions for the outlet boundaries are the Neumann boundary conditions that impose a prescribed value of diffusive flux at the outlet boundary, as in Eq. 6. An alternative to this choice, proposed in the context of Navier-Stokes equations by Papanastasiou and Malamataris, is to avoid prescription of any arbitrary boundary condition on such boundaries and instead extend the validity of the weak form of the governing equations to the Neumann boundaries. This approach is particularly useful when analytic or asymptotic techniques cannot predict the physics downstream from the artificial outflow, making it challenging to formulate appropriate boundary conditions at the artificial outlet boundaries. In the context of Navier-Stokes equations, these boundary conditions have been referred in the literature using different terminologies such as ‘no boundary condition’, ‘free boundary condition’. However, owing to the fact that these boundary conditions are consistent with the weak form of equation, we will refer to them as ‘consistent boundary condition’. This approach amounts to treating the boundary term in the weak form given by Eq. 8 as being unknown. For finite elements of degree $p$, this approach has been shown to be equivalent to imposing a boundary condition of the form

$$\nabla^{p+1} c = 0.$$  \hspace{1cm} (14)

From a physical perspective, this is same as the prescription of a zero diffusive flux for the case of linear finite elements ($p = 1$), as considered in this study. However, from a numerical perspective, this approach of handling outlet boundary leads to lower errors of $\mathcal{O}(h + 1/Pe)^{p+1}$ than the traditional approach of imposition of zero diffusive flux which results in errors of $\mathcal{O}(h^{p+1} + 1/Pe)$, where $h$ is the maximum element size and $Pe$ is the Péclet number.

In this work, we employ both the zero diffusive flux boundary condition, as described by Eq. 6, and the consistent boundary condition for the scalar advection-diffusion problem and compare their performance in preserving the local physics in the computed solution.

### 2.5 Discontinuity capturing operator

In the context of high Péclet number flows, SUPG stabilized formulations for scalar advection-diffusion problem fails to resolve the steep gradients in the solution near the scalar concentration wavefront, resulting in numerical undershoot/overshoot in concentration near the wavefront. Therefore, in addition to SUPG stabilization, we implemented a DC operator to resolve steep gradients in the solution near the scalar concentration wavefront. This approach introduces an additional term of the form $\nabla \delta \mathbf{v} \cdot \nabla c$ to the left hand side of Eq. 8 with

$$v_2 = \max[0, \tau_{\text{DC}}] \tilde{g},$$  \hspace{1cm} (15)

where $\tilde{g}$ is the contravariant counterpart of the metric tensor introduced in Eq. 12 and

$$\tau_{\text{DC}} = f_{\text{DC}} \sqrt{\frac{(\mathbf{u} \cdot \nabla c - R)^2}{\nabla c \cdot \tilde{g} \nabla c}} - \tau_s \frac{(\mathbf{u} \cdot \nabla c - R)^2}{\nabla c \cdot \tilde{g} \nabla c},$$  \hspace{1cm} (16)

We remark here that the inclusion of DC scheme makes the scalar advection-diffusion problem nonlinear. Therefore, the resolution of gradients near the concentration wavefront is obtained at the cost of an increase in computational expense.
NUMERICAL EXAMPLES

In this section, we present numerical results to illustrate the suitability of the proposed computational framework. The following applies to all the numerical examples presented in this section:

- A flow solution is first obtained by solving the stabilized Navier-Stokes equations using the cardiovascular hemodynamics modeling environment, CRIMSON (www.crimson.software). Here, blood is modeled as a Newtonian fluid with a density of $1060 \text{ kg/m}^3$ and a dynamic viscosity of $0.004 \text{ Pa.s}$. All walls are modeled as rigid, with a homogeneous Dirichlet boundary condition for the velocity.
- For scalar advection-diffusion equation, a constant concentration of $c = 10 \text{ mol/m}^3$ is prescribed at the inlet face and a zero flux boundary condition is applied to all walls.

3.1 Idealized geometries

To provide a better understanding of specific numerical challenges, we first present results for cases where idealized geometries and problem parameters are chosen to isolate specific numerical challenges. Here, we present results for three specific cases that highlight the effectiveness of the different components of the proposed computational framework.

3.1.1 Backflow stabilization

To illustrate the numerical issues caused by backflow at a Neumann boundary, we consider a T-Bifurcation domain obtained via a union of two cylinders, as shown in Figure 1 with associated geometrical dimensions. This choice of geometry exhibits backflow at outlet faces even under the steady flow conditions. First, we obtain a steady flow field solution by prescribing a constant parabolic flow profile at the inlet with a flow rate of $196 \text{ mm}^3/\text{s}$ resulting in a maximum velocity of $v_{\text{max}} = 2000 \text{ mm/s}$ and a mean velocity of $v_{\text{mean}} = 1000 \text{ mm/s}$. This results in Reynolds number, $Re_{\text{mean}} = 66.25$ based on the mean velocity and the inlet radius. A zero-pressure boundary condition is applied at both outlet faces. For the scalar advection-diffusion problem,
a zero diffusive flux is prescribed at the outlet faces. A constant value of diffusion coefficient, \( D = 10^{-2} \text{ mm}^2/\text{s} \) is chosen, resulting in a corresponding Péclet number of \( \text{Pe}_{\text{mean}} = 2.5 \times 10^4 \). This choice of a moderately high value of Péclet number allows us to illustrate the issue of simulation divergence due to backflow. Numerical experiments with lower value of Péclet numbers have revealed that for higher amount of diffusion, one can obtain a stable solution even without any backflow stabilization technique. This is expected since the contribution of the advective flux to the total flux decreases with decrease in Péclet number and therefore one can obtain a stable solution even without the inclusion of the last term in Eq. 13. This observation reveals the reason behind the ability to achieve a stable solution without any additional stabilization when the diffusion coefficient is artificially increased, as done in prior computational models.\textsuperscript{11,12} However, as mentioned earlier, such an artificial increase in diffusion coefficient is difficult to justify on physical grounds.

The domain is spatially discretized using linear tetrahedral elements with an approximate elemental length of \( 10^{-2} \text{ mm} \) resulting in a total mesh size of around 11.3 million elements. This large mesh size was chosen to ensure that the scalar solution is accurately captured near the outlet boundary. A constant time-step size of \( \Delta t = 10^{-5} \text{ s} \) is used. The scalar simulation is carried out for 8000 time steps corresponding to a physical time of 0.08 s.

Figure 2(A) shows the velocity contours of the steady flow profile plotted at the mid-plane of the T-Bifurcation geometry along the \( Z \) direction. As expected, the velocity profile at the outflow exhibits backflow, indicated by the negative values of the velocity along \( Y \) direction in Figure 2(B). Using this flow field as input, we solve transient scalar advection-diffusion problem with the aforementioned parameters and boundary conditions. Figure 3(A) shows the scalar concentration solution at \( t = 0.036 \text{ s} \) obtained without the inclusion of backflow stabilization technique. The scalar solution is characterized by numerical pollution at the outflow boundaries arising due to the backflow at these boundaries, leading to eventual divergence of the numerical solution. In contrast, the incorporation of the proposed backflow stabilization technique yields a stable solution for scalar concentration as shown in Figure 3(B). We remark here that the solution in Figure 3(B) does show numerical oscillations in the interior of the domain. These oscillation that are observed in the interior of the domain will be discussed in more detail in Section 3.1.3.
FIGURE 3 Scalar contours at time = 0.036s in the T-Bifurcation. A) No backflow stabilization resulting in an unstable solution, and B) With backflow stabilization resulting in a stable solution in the presence of backflow.

3.1.2 Consistent flux boundary condition

Next, we turn our attention to the task of identifying appropriate boundary condition at the outflow face. Here, we compare the performance of consistent boundary condition and zero diffusive flux boundary condition in preserving the local physics of the solution despite the introduction of artificial outlet boundary. To this end, we first consider a larger domain which is subsequently truncated to obtain a smaller domain with an artificial boundary. This allows us to consider the solution in the larger domain as the true solution and study the effect of the boundary condition applied at the artificial boundary via a comparison of the solution in the smaller and larger domain. An ideal boundary condition should preserve the accuracy of the solution in the smaller domain despite the introduction of artificial boundary. Noting this, we first consider a larger cylindrical domain with a radius of \( r = 0.5 \) mm and a length of \( l_1 = 10 \) mm. We obtain a steady flow field solution by prescribing a constant parabolic flow profile at the inlet with a flow rate of \( 196 \) mm\(^3\)/s resulting in a maximum velocity of \( v_{\text{max}} = 2000 \) mm/s and a mean velocity of \( v_{\text{mean}} = 1000 \) mm/s. This results in Reynolds number, \( \text{Re}_{\text{mean}} = 265 \) based on the mean velocity and the inlet radius. A zero-pressure boundary condition is applied at the outlet face. For the scalar advection-diffusion problem, we choose a constant value of diffusion coefficient, \( D = 10^2 \) mm\(^2\)/s, resulting in a corresponding Péclet number of \( \text{Pe}_{\text{mean}} = 10 \). This relatively low value of Péclet number is chosen since it allows us to best illustrate the differences between the two boundary conditions. As mentioned earlier in Section 2.4, the primary difference between the two choices of boundary condition concerns with the lower errors of \( \mathcal{O}(h + 1/\text{Pe})^{p+1} \) for consistent boundary condition as opposed to the errors of \( \mathcal{O}(h^{p+1} + 1/\text{Pe}) \) for zero diffusive flux boundary condition. Therefore, a lower value of Péclet number results in more significant differences in the solutions obtained with these two boundary conditions.

Using the above-mentioned parameters, we perform two separate simulations for the larger domain: (i) with prescription of consistent boundary condition at the outlet face, and (ii) with prescription of zero diffusive flux boundary condition at the outlet face. Figure 4(A) and 4(B) show the concentration profiles obtained for these two cases. Figure 4(E) shows the corresponding plot of concentration along a line at the midplane in the axial direction. It can be observed that the two solutions overlap with each other, indicating that there is no significant effect of the choice of outflow boundary condition on the scalar concentration at this location. Therefore, either of these solutions can be taken as the true solution in the larger cylindrical domain. Next, we consider the smaller cylindrical domain obtained by truncating the larger domain to a length of \( l_2 = 5 \) mm. Again, we perform two different simulations in the smaller domain with the aforementioned choices of outlet boundary conditions. Figure 4(C) and 4(D) show the corresponding concentration profiles obtained for the two cases. Figure 4(E) shows the corresponding plot of
concentration at the outlet boundary. It can be observed that the prescription of zero diffusive flux at the outlet boundary overestimates the concentration values by approximately 10%. In contrast, the prescription of consistent boundary condition at the outlet boundary yields concentration values that are much closer to the true solution (obtained from the larger domain), with a negligible overestimation of approximately 0.015%. These results illustrate the superior performance of consistent boundary condition as compared to zero diffusive flux boundary condition in preserving the accuracy of the solution in truncated computational domains.

![Figure 4](image-url)

**FIGURE 4** A) Scalar contours for four different cylinders. From top to bottom: 10mm cylinder with Consistent Flux outflow boundary condition, 10mm cylinder with Zero Neumann outflow boundary condition, 5mm cylinder with Consistent Flux boundary condition, and 5mm cylinder with Zero Neumann boundary condition. B) Line plot showing scalar concentration across the cylinder at X = 5mm.

### 3.1.3 Discontinuity capturing operator

Having addressed the numerical issues concerning the outlet boundary, we now focus our attention on the numerical oscillations observed in the concentration solution within the domain for advection-dominated flows. Here, we again consider the shorter cylindrical domain described in the previous section with the corresponding flow solution. To illustrate the numerical oscillations observed in the concentration solution for advection-dominated flows, we now choose a smaller value of diffusion coefficient, $D = 10^{-2}$ mm$^2$/s, resulting in a higher Péclet number of $Pe = 10^4$. For the scalar advection-diffusion problem, we prescribe a consistent boundary condition at the outlet face. Figure 5(A) shows the concentration solution obtained without the incorporation of the discontinuity capturing operator. It can be observed that in the absence of DC operator, the solution is characterized by numerical undershoot/overshoot in concentration profile near the wavefront. This undershoot/overshoot results in unphysical negative values of the scalar concentration as well as a maximum value that is higher than the inlet concentration. Figure 5(C) shows the corresponding plots of the scalar concentration along the axis of the channel at different time instants. It can be observed that the numerical oscillations begin at the first time step and increase in magnitude with time. In contrast, the inclusion of DC operator in numerical scheme results in a smooth solution, shown in Figure 5(B). The corresponding line plots in Figure 5(C) further confirm that the inclusion of DC operator results in a smooth concentration gradient near the wavefront and is devoid of any numerical undershoot/overshoot.
Having demonstrated the capabilities of the stabilized computational framework in resolving numerical issues in idealized geometries with steady flow solution, we examine the same issues in a patient-specific geometry with transient flow solution. To this end, we consider a patient-specific model of a human thoracic aortic aneurysm under transient periodic flow conditions, as observed in cardiovascular hemodynamics.

The computational domain for these test cases is obtained via segmentation from computed tomography angiography (CTA) image data using the cardiovascular hemodynamic modeling environment CRIMSON. Figure 6 shows the computational domain comprising of the ascending aorta and 8 outflow branches to the head and neck resulting in a total of 9 outflow faces. This domain is discretized using linear tetrahedral elements with a total of 6.2 million elements and 1.1 million nodes. A constant time step size of $\Delta t = 10^{-4}$ s is used. A periodic volumetric flow waveform is imposed at the inflow face of the ascending aorta using echocardiography data with a time period of $T = 0.91$ s. For outflow boundary conditions, 3-element Windkessel models are specified on each outflow face, representing the behavior of the distal vascular bed. The numerical values of the Windkessel parameters are tuned to match the clinical measurements from duplex Doppler ultrasonography and cardiac catheterization. To achieve cycle-to-cycle periodicity in the flow solution, we first solve only the flow problem for four cardiac cycles, corresponding to a physical time of $t = 3.64$ s. Subsequently, we solve scalar advection-diffusion problem by introducing a scalar concentration of $c = 10$ mol/mm$^3$ into the domain through the inlet face for $t > 3.64$ s.
3.2.1 Backflow stabilization

We first consider the issue of simulation divergence due to the backflow at a Neumann outflow boundary. To this end, we employ a constant value of diffusion coefficient, $D = 1.0 \text{mm}^2/\text{s}$ and prescribe zero diffusive flux boundary condition to all outflow faces. Figure 7(A) shows the 3D velocity profile at the outlet boundary for $t = 4.39 \text{s}$, corresponding to a time point in the diastolic phase of the cardiac cycle. The flow solution at the outlet boundary is characterized by backflow and leads to numerical pollution in scalar concentration solution obtained without backflow stabilization as shown in Figure 7(B). Figure 7(C) shows the corresponding scalar concentration solution obtained with the inclusion of backflow stabilization. It can be observed that the inclusion of backflow stabilization resolves the numerical instability at the outflow boundary and yields a stable scalar concentration solution.

3.2.2 Consistent flux boundary condition

Next, we consider the effect of the choice of outflow boundary condition on the scalar concentration solution. Here, we compare the results obtained from two different simulations: (i) with consistent boundary condition at outflow faces, and (ii) with zero diffusive flux boundary condition at outflow faces. In both cases, we employ a constant value of diffusion coefficient $D = 100.0 \text{mm}^2/\text{s}$. Figure 8 shows the comparison of scalar concentration profile for the two cases at $t = 6.55 \text{s}$, plotted along four arbitrary locations in the domain. It can be observed that the concentration solution for the two cases agree with each other at locations far from the outflow boundary, as shown in Figure 8(A) and (B). In contrast, Figure 8(C) and (D) show that the solution for the two cases start to differ as one moves closer to the outflow boundary, indicating that the choice of the boundary condition has a significant effect on the local solution near the outflow boundary. In view of the superior performance of consistent boundary condition demonstrated in Section 3.1.2, we believe that the solution obtained with consistent boundary condition represents the true solution more accurately. Regardless, this comparison highlights the importance of choosing appropriate outflow boundary conditions and demonstrates the effect of different choices on the scalar concentration solution.
FIGURE 7 Surface contours of scalar concentration at time $t = 4.39$ s. A) Without scalar backflow stabilization. Numeric instability begins at the thoracic aorta outlet and proceeds to pollute the scalar domain. B) With backflow stabilization. Stable scalar solution in the presence of backflow at an outlet.

3.2.3 Discontinuity capturing operator

In the last example, we demonstrate the efficacy of the DC operator in resolving numerical oscillations in scalar concentration solutions for the patient-specific geometry under transient flow conditions. To this end, we choose a constant value of diffusion coefficient $D = 1.0 \text{ mm}^2/\text{s}$ and apply consistent boundary condition at all outflow faces. Figure 9(A) and (B) show the scalar concentration solution at $t = 4.04$ s obtained without and with the inclusion of DC operator, respectively. Figure 9(C) shows a comparison of the two scalar concentration solutions, plotted along an arbitrary line across the concentration wavefront. It can be observed that the solution without the inclusion of DC operator is characterized by significant numerical undershoot/overshoot near the concentration wavefront. These oscillations result in unphysical minimum and maximum values of the scalar concentration. In contrast, the solution obtained with the inclusion of DC operator shows a smooth variation of scalar concentration across the wavefront with concentration values in physically meaningful range and devoid of any numerical oscillations.

4 DISCUSSION AND CONCLUSIONS

Transport problems are of paramount importance in studying cardiovascular pathologies. Diseases such as intimal hyperplasia, atherosclerosis and thrombosis are directly affected by complex transient hemodynamics as well as the transport of numerous chemical species and proteins. The modeling of hemodynamics in cardiovascular systems presents numerical challenges due to the inherently complex, time-dependent flow patterns and vessel geometries. This complexity is further compounded by the presence of large Péclet number mass transport which necessitates the use of stabilization techniques to resolve steep concentration gradients within the flow. The primary aim of this work is to present a stabilized computational framework to study 3D, transient cardiovascular transport problems. This includes the identification of appropriate boundary conditions at the artificial boundaries of the truncated physical domain as well as use of stabilization techniques to avoid spurious numerical oscillations in the computed concentration field.

In the absence of a robust, stabilized computational framework, a number of previous computational models have employed modeling assumptions that are difficult to justify in a general cardiovascular mass transport problem. This includes a global unphysiological increase in diffusivity of species, unrealistic extension of vessel geometry, and the prescription of an
Patient Specific simulations in a human thoracic aneurysm were run with both a zero diffusive flux boundary condition red and a consistent boundary condition black. Comparisons of the scalar profile across the diameter of the model is shown at four locations (A-D). Results show that close to the inflow the scalar profile across the aorta is the same for both outflow boundary conditions. After the thoracic aneurysm the scalar profiles begin to differ and the greatest differences are observed at the outflow boundary.

arbitrarily chosen concentration value at the outlet boundaries. These simplifications severely limit the applicability of such models for general cardiovascular mass transport studies. Furthermore, little attention has been paid to the choice of boundary conditions at the outflow faces and their effect on the computed solution.

In this work, we have presented a general computational framework for cardiovascular mass transport problems. This framework employs SUPG and DC formulation to resolve steep concentration gradients in mass transport characterized by high Péclet numbers. We have also incorporated a backflow stabilization strategy to obtain a stable numerical solution in the presence of flow reversal at outflow boundaries. Furthermore, we have also proposed a novel ‘consistent boundary condition’ and have demonstrated its superiority over the typically used zero diffusive flux boundary condition in preserving the local physics of the computational solution, particularly in cases of low Péclet numbers.

We have demonstrated the application of this framework in two different sets of geometries. Firstly, we chose a set of idealized geometries with steady flow conditions to illustrate the numerical issues associated with backflow and advection-dominated flows. The simplicity of these geometries provide a clear interpretation of different numerical challenges and illustrate the efficacy of the various stabilization techniques reported in this work. Furthermore, we chose an idealized cylindrical geometry that was amenable to the introduction of artificial boundaries via truncation of the domain. This allowed us to compare the performance of different choices of outflow boundary conditions at artificial boundaries against the true solution and demonstrate the superiority of consistent boundary condition in preserving the local accuracy of solution near the outflow boundary. In the second set of examples, a patient specific thoracic aorta model was chosen as the computational domain to illustrate the efficacy of the proposed framework in complex geometries with transient flows.

While the framework presented in this work represents a significant improvement over prior computational models, further work is needed to improve and validate this framework. Firstly, while we have demonstrated the superiority of consistent boundary condition in reducing boundary effects at outflow, small effects were still observed and serve as a limitation to this condition.
FIGURE 9 A) 2D clip of patient-specific geometry with no discontinuity capturing used; oscillations in the scalar solution can be seen near the wavefront. B) 2D clip of patient-specific geometry using the discontinuity capturing; a smooth solution to the scalar problem can be seen throughout the domain. C) 1D scalar solution plotted along the black line seen in A) and B). The use of the DC operator effectively rids the scalar solution of the overshoot/undershoot phenomena seen in the simulation with no DC (red).

Secondly, the nonlinearity introduced in the scalar advection-diffusion problem due to the addition of DC scheme can be avoided by use of a time-lagging DC scheme [citation from Onkar here]. We remark, however, that in presence of nonlinear source terms, the scalar advection-diffusion problem would be nonlinear regardless of DC scheme and therefore incorporating time-lagging may not result in significant computational savings in such scenarios. While the backflow stabilization presented here yields stable solutions, a number of other backflow stabilization methods have been presented for Navier-Stokes equations. It would be worthwhile to adapt these methods for scalar advection-diffusion problems and compare their performance, as done for flow problems. Lastly, benchmark solutions along the lines of those prescribed for flow problems should be attempted to validate the computational framework.

5 | ACKNOWLEDGEMENTS

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