

Computational flow modeling of Triply Periodic Minimal Surfaces as feed channel spacers in Ultra-High Pressure Reverse Osmosis Applications

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Abstract

Triply periodic minimal surfaces (TPMS) are a special class of mathematical surfaces characterized by a high surface area-to-volume ratio. They have generated considerable interest in fields such as acoustics, heat transfer, and membrane-based filtration processes. This study evaluates the performance of four different TPMS designs—Schoen Gyroid, Schoen Crossed Layers of Parallels (CLP), Schoen Transverse Crossed Layers of Parallels (tCLP), and Schwarz-Primitive—when used as feed channel spacers under ultra-high pressure reverse osmosis (UHPRO) conditions, at approximately 200 bar. Our experimentally validated computational fluid dynamics model reveal different flow patterns within the feed channels for each of the four TPMS designs, leading to varying hydrodynamic and permeation properties. Under the simulated UHPRO conditions, the Gyroid and tCLP designs yield up to a 23% increase in average permeate velocity and a 14% reduction in average membrane-surface concentration relative to a non-woven spacer of the same porosity. The enhanced performance comes with an increased feed channel pressure drop, although it only constitutes less than 4% of the operating pressure when extrapolated for a meter-long membrane module. Additionally, the study analyzes the effects of varying inlet velocity and spacer porosity on membrane performance. Overall, this research provides valuable insights into the potential use of TPMS spacers in UHPRO applications.

Keywords: Ultra-High Pressure Reverse Osmosis, Triply Periodic Minimal Surfaces, Membrane Spacers, Schoen Gyroid, Schwarz Crossed Layers of Parallels, Schoen Primitive, Computational Fluid Dynamics,

Nomenclature

General notation

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2D	two-dimensional
3D	three-dimensional
CAD	Computer Aided Design
HEI	Hydraulic Efficiency Index
MLD	Minimal liquid discharge
NF	Nanofiltration
OCT	Optical Coherence Tomography
RANS	Reynolds Averaged Navier-Stokes
S-CLP	Schwarz Crossed Layers of Parallels
S-Gyroid	Schoen Gyroid
S-Primitive	Schwarz Primitive
S-tCLP	Schwarz Transverse Crossed Layers of Parallels
STL	StereoLithography
TPMS	Triply periodic minimal surfaces
UHPRO	Ultra-high pressure reverse osmosis
ZLD	Zero liquid discharge

Subscripts

ch	channel
f	feed channel
m	membrane side
p	permeate side
sp	spacer

Variables

$\mathbf{n}$	Surface normal vector
c_{inlet}	Solute concentration at channel inlet (m/s)
D_h	Hydraulic diameter of spacer-filled feed channel (mm)
f_{os}	Osmotic coefficient, (Nm/kg)
u_{inlet}	Component of velocity normal to channel inlet (m/s)
$\bar{\bar{\tau}}$	Viscous stress tensor of fluid (Pa)

$\bar{I}$	Unit matrix
$\Delta\pi$	Trans-membrane osmotic pressure difference (Pa)
ΔP_f	Feed channel pressure drop (Pa)
ϵ	Porosity of the spacer
$\mathbf{Q}$	Volumetric flow rate of feed solution through channel (m^3/s)
$\mathbf{U}$	Fluid velocity vector (m/s)
$\mathbf{v}_p$	Membrane-normal component of permeate velocity vector (m/s)
μ	Viscosity of feed solution ($Pa \cdot s$)
$\bar{c}_m$	area weighted average of solute concentration on membrane, (kg/m^3)
$\bar{v}_p$	area weighted average of permeate velocity on membrane, (m/s)
π	Osmotic pressure (bar)
ρ	Density of feed solution (kg/m^3)
A	Total surface area of empty channel (mm^2)
c	Solute concentration in feed channel (kg/m^3)
D	Mass diffusion coefficient of solute in water (m^2/s)
h	Feed channel height (mm)
P	Absolute hydrodynamic pressure in feed channel (bar)
R_m	Membrane resistance (m^{-1})
r_s	Solute rejection coefficient
R_w	Water recovery rate
SF	Solid fraction of spacer-filled feed channel (%)
V	Volume of feed channel without spacers (mm^3)
x, y	x,y coordinates

1. Introduction

The rapid growth of the human population has led to the depletion of freshwater resources and increased demand for freshwater. The United Nations World Water Development Report 2024 [1] states that as of 2022, 2.2 billion people lack access to safely managed drinking water. This situation has sparked growing interest in technologies for improved brine and industrial wastewater management, such as zero liquid discharge (ZLD) and minimal liquid discharge (MLD) methods. These methods typically employ single or multiple reverse osmosis (RO) membranes operating at high pressures (up to 80 bar) or ultra-high pressures (up to 300 bar) [2].

The commercial implementation of ultra-high-pressure reverse osmosis (UHPRO) membranes poses several technical challenges. These include the need to redesign modules to withstand high operating pressures and corrosive feed water. Additionally, membrane compaction can lead to deteriorated performance [3], which needs to be addressed. Also, the increased concentration polarization at UHPRO conditions leads to a higher propensity for scaling and fouling in feed channels. Concentration polarization refers to the buildup of dissolved solutes on the membrane surface as they are rejected during filtration. The high solute concentration results in low permeate flow due to higher osmotic pressures and a higher solute flux through the membrane, caused by a larger trans-membrane concentration difference [4]. As a result, these effects lead to lower overall water recovery and higher brine management costs. Compared to conventional RO methods, the detrimental effects of concentration polarization are severe in UHPRO due to inorganic scaling caused by the precipitation of rejected salts at the membrane [5]. Methods to mitigate concentration polarization effects include using improved membrane materials and novel feed channel spacer designs.

Feed channel spacers are static-mixing elements placed in the space between two consecutive membrane leaves (the feed channel). Most commercially available feed channel spacers comprise a layer of net-shaped filament units repeated in two dimensions. The purpose of the spacers is twofold: to provide structural support for the feed channel and to enhance the mass transfer through membranes by acting as static mixers that generate vorticity in the flow. These benefits come at the expense of increased feed channel pressure drop due to flow obstruction [6]. Also, spacers create stagnant flow zones, which can exacerbate biofouling, especially under high-flux conditions [7]. Until recently, spacers were manufactured using methods such as extrusion and molding processes. These traditional manufacturing methods limited spacer designs to simple, net-like shapes. However, new additive manufacturing techniques are beginning to overcome these limitations.

Additive manufacturing refers to the process of manufacturing products from digital design data by depositing materials in successive layers. Among the many additive manufacturing methods available, the most common for spacer production are digital light processing (DLP), selective laser sintering (SLS), powder bed fusion, and photopolymerization [8]. Recently, these methods have been used to produce spacers with complex shapes. Li et al. [9] used SLS to develop modified spacer filaments and twisted tapes. They found that multi-layered spacers outperformed the best available single-layered, non-woven spacers. Building on this, Balster et al. [10] studied single and multi-layered spacers manufactured using SLS and reported that single-layered spacers with twisted tapes enhanced mass transfer due to the swirling nature of the flow. A study of other novel spacer shapes [11] also showed that ladder, asymmetric herringbone, and helical

spacers (manufactured using fused deposition modeling) increased mass transfer through flow swirling. A similar conclusion was also reported by Fritzmann et al. in [12], where doubly helical spacers were found to not only improve mass transfer but also to improve the solute selectivity in ultrafiltration (UF) applications. Some of the other novel spacer designs explored recently include perforated net-like spacers ([13]), wave or hill-like spacers ([14]), column-type spacers ([15]), and 3-D printed turbulence promoters ([16]), with all of the designs exhibiting enhanced permeate flux when compared to conventional spacers. The feasibility of manufacturing complex spacer designs using additive manufacturing techniques has recently sparked interest in a new class of geometries known as triply periodic minimal surfaces (TPMS).

TPMS are geometric surfaces that are characterized by smooth, edge-free surfaces with a mean curvature of zero at every point on the surface. As their name suggests, these surfaces minimize the total surface area for a given boundary curve and are periodic in all three spatial directions. Due to these unique characteristics, TPMS are highly suitable as feed channel spacers and have already attracted widespread interest across various desalination technologies. Al-Ketan et al. [17] studied the mechanical properties of sheet and skeletal TPMS designs and established that sheet diamond TPMS structure showed a stiffness behavior independent of relative density, making it suitable as high-pressure filtration spacers. In a similar study, Femmer et al. [18] studied different TPMS designs for heat transfer applications and found that the Schwarz-D configuration performed the best for heat transfer enhancement. Drawing a comparison between heat and mass transport, their conclusions indicate enhanced mass transfer in membrane applications. Sreedhar et al. [19] demonstrated proof of concept for applying TPMS designs for RO and UF applications. They showed 15.5% and 38% increase in permeate flux for RO and UF applications, respectively. The pressure drop and fouling propensity were also reportedly lower than those of commercial spacers. Sreedhar et al. [20] also studied TPMS designs with varying void fraction and directionality for UF applications and demonstrated that while all TPMS designs showed improved mass transfer, the Gyroid design with 84% void fraction showed the best performance with a 67% increase in Sherwood number and 8% enhancement in the critical flux. TPMS designs were also studied by Thomas et al. [21], and a 60% increase in water flux was reported for the best TPMS design when compared to commercial spacers in membrane distillation applications. Experimental [22] and numerical [23] studies (although with different TPMS designs) on direct contact membrane distillation (DCMD) showed enhanced flux and reduced fouling propensity for TPMS designs due to higher membrane and spacer wall shear stresses. A key challenge in extending TPMS-based experimental studies to UHPRO conditions is the development of testing facilities capable of operating at these high pressures. However, numerical methods can be used to substitute such experiments.

Computational fluid dynamics (CFD) applied to flow in feed channels has evolved considerably over the years. Early CFD studies were largely 2D, laminar, and limited to truncated domains. They often treated the feed as pure water and membranes as impervious walls. These works examined transition to turbulence ([24]), spacer shape ([25], [26]) and configuration ([27]) effects, and turbulence modeling ([26], [28]). Sitaraman and Battiatto [29] extended this by performing 2D axisymmetric, full-length RO simulations, showing non-monotonic permeation behavior along the channel and highlighting the limits of truncated domains. Three-dimensional simulations (earlier examples include [30], [31]) later became common, typically using periodic unit cells to study

curvature ([32, 33]), spacer geometry [34, 35], and flow angle effects ([36]). With advancements in computing power, more realistic commercial spacer designs such as woven ([37, 38, 39]), non-woven ([40, 41]), pillar [42, 43], TPMS ([23]) and biomimetically inspired ([44]) spacer designs were simulated, although on truncated domains. High fidelity CFD simulations at the module scale that resolve flow around complex three dimensional spacers at sub-millimeter scale are still beyond current computational capabilities.

In summary, additive manufacturing, along with advanced simulation capabilities, can enable the adoption of TPMS spacers for UHPRO applications. TPMS spacers have been extensively studied in heat transfer applications and have demonstrated enhanced heat transfer performance. However, there is a significant knowledge gap regarding the impact of TPMS spacer designs on fluid dynamics and mass transfer in UHPRO systems. No numerical studies as far as the authors know, despite recent advances, have yet examined how TPMS geometries influence hydrodynamics, concentration polarization, and permeation in UHPRO feed channels, while experimental investigations are confined to measuring averaged flow parameters. In membrane-based mass transfer applications,

TPMS designs have demonstrated (under UF, NF, and RO conditions) several positive attributes, such as enhanced permeation, improved fouling resistance, and reduced pressure drop, making them strong candidates for UHPRO applications. A particularly relevant property of TPMS spacer designs for UHPRO applications is their high strength-to-porosity ratio, which is expected to reduce membrane compaction under ultra-high pressure conditions. This absence of systematic analysis albeit TPMS' several advantages represents a critical gap, given the growing importance of UHPRO in desalination technology. We address this gap through this study that evaluates four distinct TPMS configurations as spacers in UHPRO applications through high-fidelity numerical simulations. To our knowledge, this is the first systematic numerical study of TPMS spacers under UHPRO conditions. The paper is organized as follows. Section 2 lists the aim, scope, and assumptions used in this study. Section 3 introduces the mathematical concept of TPMS and explains the various TPMS designs considered in this work. Section 4 then describes the governing equations, boundary conditions, and numerical methods. The numerical methodology is validated and verified against previously published results, as detailed in Section 5. The spacer flow simulation results are discussed in Section 6, and the major conclusions from this study are reported in Section 7.

2. Aim, Scope and Assumptions of this Study

2.1. Aim

The goal of this study is to assess the effect of TPMS spacer designs on membrane performance in UHPRO-based desalination applications using high-fidelity numerical simulations. This work is the first to systematically compare multiple sheet TPMS spacer geometries in UHPRO channels, linking detailed flow physics to permeation performance.

2.2. Scope

This study focuses on results obtained from unsteady, three-dimensional simulations of feed channel flows with TPMS spacers. To maintain computational tractability, the scope of this work is limited by the following aspects:

- **Membrane compaction:** is excluded to focus on TPMS spacer-driven hydrodynamics and permeation effects. Membrane compaction is material- and history-dependent, involves nonlinear poroelastic deformation, and requires fluid–structure interaction physics, which adds significant modeling complexity and uncertainty. Treating membrane interfaces as rigid and non-deforming provides a stable baseline for comparing TPMS designs and interpreting flow physics. Future work will extend the present framework to incorporate membrane compaction effects through coupled fluid–structure interaction models, enabling evaluation of spacer hydrodynamics under realistic deformation conditions.
- **Fouling:** Organic and inorganic fouling are not modeled. Fouling processes demand multiphysics coupling of deposition, film growth, and scaling kinetics with evolving surface properties, which are system-specific and computationally intensive. Excluding fouling allows clear attribution of performance changes to spacer geometry under idealized conditions. In subsequent studies, we aim to extend the current modeling framework to include fouling effects and assess TPMS spacer performance including these effects.
- **Domain size:** Simulations are restricted to truncated domains representing portions of the feed channel, rather than full meter-scale modules, to enable high-resolution modeling within current computational limits to provide insights on the coupling between fluid flow and concentration polarization effects.
- **Manufacturability:** In this study, manufacturability and mechanical considerations are treated as design-space constraints that ensure the geometries are physically realizable, while the analysis focuses on the hydrodynamic and mass-transfer mechanisms that govern spacer performance under UHPRO conditions.

2.3. Assumptions

The following modeling assumptions are adopted:

- The feed fluid is single-phase, Newtonian, and isothermal. Density, viscosity, and solute diffusion coefficient vary with solute concentration and are modeled in the simulations.
- The solute is treated as a single, non-reactive species. Precipitation, adsorption, or chemical reactions are not modeled.
- The membrane is represented by a boundary condition using the solution-diffusion model. Membrane permeability, hydraulic resistance, and solute rejection coefficients are constant in space and time.
- Natural convection and buoyancy effects are negligible. The ratio of Grashof number to Reynolds number is less than 1 (estimated values range from $7e-4$ to 0.04), justifying this assumption.
- Periodic boundary conditions are applied in the lateral direction, consistent with repeating spacer units of membrane modules.

- At the operating Reynolds numbers (less than 460) considered in this work, the vortical structures from spacer-induced mixing are resolved to the smallest possible scale; coupling of turbulence models are therefore not warranted for the fluid flow equations.

3. TPMS Spacer Designs

Mathematically, a minimal surface is defined as a surface that locally minimizes surface area while maintaining mean zero curvature at every point on it. Triply periodic minimal surfaces (TPMS) are minimal surfaces that are continuous, infinite, and periodic in all three directions and are characterized by smooth, edge and corner-free surfaces. They can be used to build crystalline structures by repeating the basic periodic unit in all three dimensions. The cellular structure of TPMS provides desirable mechanical and physical characteristics such as high stiffness-to-weight ratio, high surface area-to-volume ratio, and enhanced mechanical energy absorption that make them suitable for thermal [45, 46], mechanical [47], and acoustic applications [48].

The high surface area-to-volume ratio of TPMS is expected to reduce concentration polarization and fouling mitigation in addition to providing mechanical strength to counter the high feed channel pressure in UHPRO applications. The complex geometry is also expected to enhance fluid mixing through vorticity generation. TPMS surfaces are generated mathematically using level-set equations of the form $\phi(x, y, z) = C$. The spacer volumes around these surfaces are generated by one of the two methods: skeletal-based or sheet-based. In the skeletal-based methods, the spacer volume is defined as that region enclosed within these surfaces. The sheet-based method generates volume by thickening the level-set surface by a specific amount. For this study, we have selected the sheet TPMS spacers due to their high stiffness [49], which is advantageous for UHPRO conditions. Of the numerous sheet TPMS designs available, we chose the following TPMS surfaces for this study: Schoen Gyroid (S-Gyroid), Schwarz crossed layers of parallels (S-CLP), Schwarz transverse crossed layers of parallels (S-tCLP) and Schwarz Primitive (S-Primitive). The level-set equations for these surfaces are given by:

Schoen Gyroid (S-Gyroid):

$$\sin y \cos x + \sin z \cos y + \sin x \cos z = C$$

Schwarz CLP (S-CLP) and Schwarz tCLP (S-tCLP):

$$\sin z \sin y - 0.4 \sin(1.2x) \cos z \cos y = C$$

Schwarz-Primitive (S-Primitive):

$$\cos x + \cos y + \cos z = C$$

where x , y , and z are the Cartesian coordinates at a point on the surface, and C is a constant controlling the porosity of the spacer. All four designs are generated using the TPMS tool [50] with a porosity value ranging between 87%-88%. The CAD geometry (in triangulated stereolithography (STL) format) is generated using the tool with triangulations of 60 cells per unit. The feed channel height (and hence the periodic unit size) is set to be 0.87mm, as is representative of typical commercial systems. The feed-channel

height of 0.87 mm (34 mil) corresponds to the natural periodic length scale of the TPMS geometries generated in this work and provides sufficient sheet thickness for structural stability in additively manufactured prototypes. Note that many commercial SWRO elements employ thinner 28-mil spacers. TPMS structures can be manufactured to be scaled proportionally to these smaller channel heights. The current thickness, therefore, serves as a representative geometry for assessing the hydrodynamic behavior of TPMS spacers. The four TPMS spacer designs generated are shown in Figure 1[a-d]. It should be noted that the S-CLP and S-tCLP designs are the same, except for their alignment with respect to the incoming feed flow.

In order to have a fair comparison of the TPMS designs against commercial spacers, a non-woven type spacer design (hereafter referred to as Non-Woven) is also considered in this study. The Non-Woven spacer design consists of two rows of parallel, cylindrical spacers embedded in the feed channel. To be consistent with the TPMS designs, the feed channel height for this design is also fixed to 0.87 mm. The mesh angle between the cylindrical axes of the two rows of spacers is kept as 90° and the incoming flow angle is chosen to be 45°. The diameter of the cylindrical spacers is fixed as 0.20 mm so that the net solid-fraction (or porosity) is similar to that of the TPMS designs. The Non-Woven spacer design is shown in Figure 1(e).

The geometric characteristics of the spacers are provided in Table 1. The hydraulic diameter D_h is defined as,

$$D_h = 4 \frac{(V_{ch} - V_{sp})}{(A_{ch} - A_{sp})}$$

where V_{ch} and A_{ch} refer to the empty channel volume and surface area, respectively. Also, V_{sp} and A_{sp} denote the spacer volume and spacer area, respectively. The porosity of the feed channel ϵ is calculated as,

$$\epsilon = 1 - \frac{V_{sp}}{V_{ch}}$$

The spacer volumes and areas are measured from the CAD modeling software and are reported in Table 1.

Table 1: TPMS spacer designs and their geometric characteristics used in this study

TPMS Designs	Feed channel height, h [mm]	Volume of spacer in unit cell, V_{sp} [mm ³]	Surface area of spacer, A_{sp} [mm ²]	Porosity, ϵ	Hydraulic diameter, D_h [mm]
S-Gyroid	0.87	0.1063	2.2720	0.88	0.972
S-CLP	0.87	0.0746	1.8545	0.88	1.259
S-tCLP	0.87	0.0746	1.8545	0.88	1.259
S-Primitive	0.87	0.0804	3.6472	0.87	2.58
Non-Woven	0.87	0.0773	1.5004	0.88	0.764

The curvature of the spiral wound module is neglected, and the computational domain is chosen to be a channel with a rectangular cross-section. The computational domain is constructed such that there are 18 periodic spacer units in the direction of the incoming

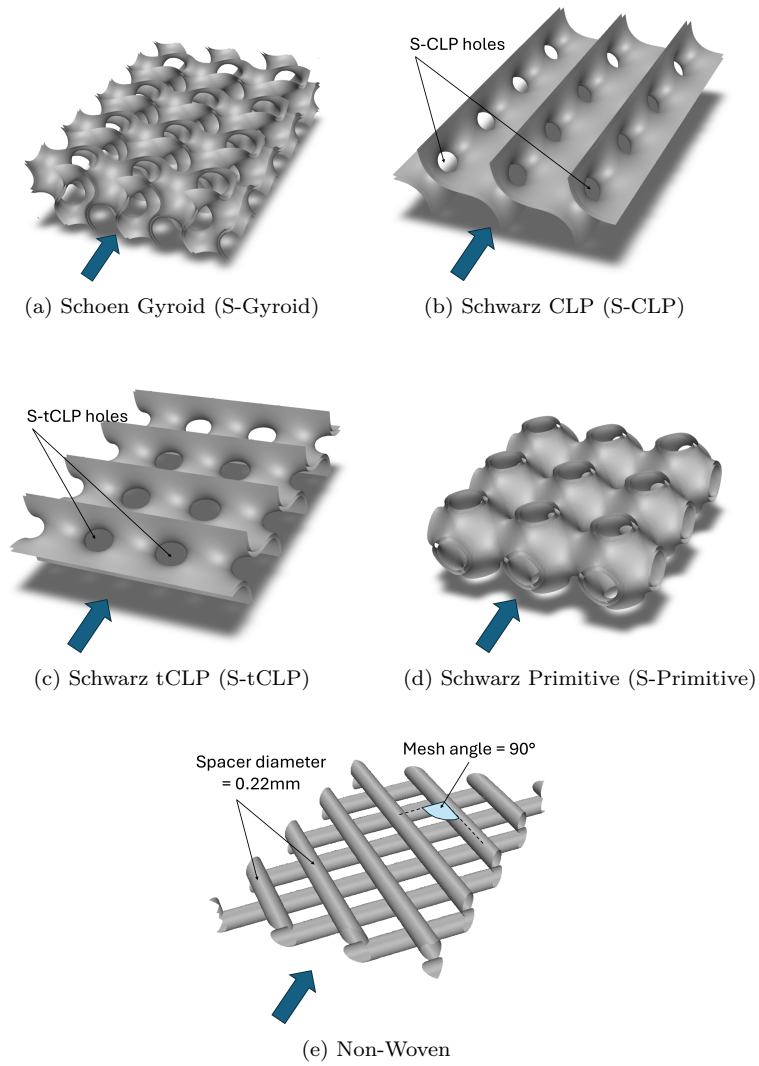


Figure 1: The various TPMS spacer designs considered in this study. Arrows indicate the direction of feed flow

flow and three units in the lateral direction. As a result, the total dimensions of the computational domain are $15.87\text{mm} \times 2.61\text{mm} \times 0.87\text{mm}$. The four different TPMS spacer designs are expected to produce distinct flow features. To capture and analyze these effects, the next section introduces the governing equations and numerical framework used in this study.

4. Governing Equations, Boundary Conditions, and Numerical Methods

A 3D Cartesian coordinate system is used to describe the computational domain. The incoming flow direction is indicated as the x -direction while the membrane normal direction is denoted by the z -direction. The fluid considered in this study is a solution of NaCl in water with a concentration of 100 kg/m^3 , and at a temperature of 298 K , representative of hypersaline brines. To account for the density variation with solute concentration, the solution is modeled as weakly compressible fluid. The unsteady, compressible, Navier-Stokes equations are used as the governing equations in this study and are given as follows.

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{U}) = 0 \quad (1)$$

$$\frac{\partial}{\partial t}(\rho \mathbf{U}) + \nabla \cdot (\rho \mathbf{U} \otimes \mathbf{U}) = -\nabla P + \nabla \cdot \bar{\bar{\tau}} \quad (2)$$

$$\frac{\partial c}{\partial t} + \nabla \cdot (c \mathbf{U}) = \nabla \cdot (D \nabla c) \quad (3)$$

Here ρ , $\mathbf{U}$, P , and c refer to the fluid density, velocity, hydrodynamic pressure, and solute concentration, respectively. The matrix $\mathbf{U} \otimes \mathbf{U}$ in the momentum equation above refers to the dyadic product of the velocity vector with itself. To close the momentum equation, the viscous stress tensor $\bar{\bar{\tau}}$ is defined assuming Newtonian flow behavior as,

$$\bar{\bar{\tau}} = \mu \nabla \mathbf{U} + \nabla \mathbf{U}^T - \frac{2}{3} \mu (\nabla \cdot \mathbf{U}) \mathbf{I} \quad (4)$$

In Eqn. 4, μ denotes the dynamic viscosity of the solution and $\mathbf{I}$ refers to the identity matrix of rank equal to the spatial dimension (3 in this study). In Eqn. 3, D refers to the solute diffusion coefficient. Since we assume isothermal conditions for the feed flow, the energy equation is not considered. However, the fluid properties such as density, viscosity, and diffusion coefficient are strongly dependent on the local solute concentration. This strong dependence is incorporated into the simulations by expressing these properties as polynomial functions of the local concentration, as given below.

$$\rho = -2.179 \times 10^{-4} c^2 + 0.692 c + 997.99 \quad (5)$$

$$\mu = -6.196 \times 10^{-10} c^2 + 1.968 \times 10^{-6} c + 9.885 \times 10^{-4} \quad (6)$$

$$D = 2.811 \times 10^{-20} c^4 - 2.645 \times 10^{-17} c^3 + 7.021 \times 10^{-15} c^2 - 1.458 \times 10^{-13} c + 1.477 \times 10^{-9} \quad (7)$$

These concentration-dependent properties (Eqns. 5–7) are taken from Sitaraman and Battiato [29], and are derived from the work by Bartholomew and Mauter [51]. Here,

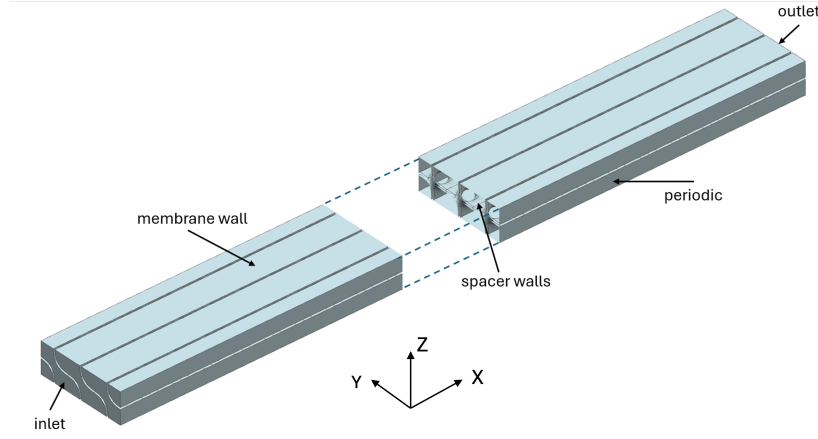


Figure 2: Schematic of the 3D computational domain along with the boundary conditions used in this study. The dotted lines are fictitious and included to hide membrane walls and periodic boundaries, so that spacer walls are visible.

the solute concentration and fluid density are expressed in kg/m^3 , viscosity in $\text{Pa}\cdot\text{s}$, and solute diffusion coefficient in m^2/s . These concentration-dependent properties capture how saline brines deviate from ideal water behavior, directly affecting flow resistance and solute transport.

With the governing equations established, appropriate boundary conditions are required to simulate the feed flow in the channel. These are summarized in Figure 2. At the inlet to the computational domain, a time-invariant, Dirichlet boundary condition for velocity (u_{inlet}) and solute concentration ($c_{inlet} = 100 \text{ kg/m}^3$) is specified. Spatially uniform profiles of velocity and concentration are specified at the inlet, and a Neumann boundary condition is used for the hydrodynamic pressure. Homogeneous Neumann conditions for velocity and concentration are specified normal to the outlet plane. A Dirichlet condition for hydrodynamic pressure is imposed at the outlet. The pressure is kept constant (200 bar) at the outlet boundary for all the simulations in this study to simulate UHPRO conditions. Periodic boundaries (along the y -direction) are used to simulate a large domain in the lateral direction.

Membrane wall boundary conditions need specific mention here. The membrane surfaces are modeled as porous walls based on the solution-diffusion model. They allow the flow of water through the porous surface while providing a higher resistance to the flow of solute through them. The permeate velocity v_p , which is defined as the volumetric flux of permeate water, is given by the following relation.

$$\mathbf{n} \cdot \mathbf{U} = v_p = \frac{1}{\mu R_m} (\Delta P_{fp} - \Delta \pi) \quad (8)$$

In the above equation, $\mathbf{n}$ is the normal vector to the membrane wall, and R_m denotes the membrane resistance. ΔP_{fp} is the trans-membrane pressure difference, which is defined as the hydrodynamic pressure difference between the feed and the permeate sides. Since the feed pressure is much larger than the permeate pressure, it is common to assume that $\Delta P_{fp} = P$, where P is the local feed channel pressure [37]. $\Delta \pi$ refers to the osmotic pressure difference between the feed and permeate sides and is calculated as,

$$\Delta\pi = f_{os}(c - c_p) \quad (9)$$

where f_{os} is the osmotic coefficient and c_p is the solute concentration at the permeate side. Similar to density and transport coefficients mentioned previously, the osmotic coefficient is also calculated as a polynomial function of solute concentration [51] as given below:

$$f_{os} = 8.48 \times 10^4 - 3.141 \times 10^{-6}c^2 + 2.13 \times 10^{-4}c + 0.917 \quad (10)$$

Under a steady-state assumption, the solute conservation equation across the membrane wall is given by,

$$\mathbf{n} \cdot \mathbf{U}(c_m - c_p) - D\nabla c|_m = 0 \quad (11)$$

where c_m is the solute concentration at the membrane wall. The effect of permeate concentration is taken into account in the simulation through the solute rejection coefficient, r_s . The solute rejection coefficient is expressed as,

$$r_s = \frac{c_m - c_p}{c_m} \quad (12)$$

The value of r_s is fixed as 99% uniformly in all simulations consistent with prior CFD studies [37, 52, 29]. While it is true that local solute and permeate flux varies across the membrane length, high-flux RO membranes show only modest dependence of permeate flux on solute rejection coefficient [53, 54].

Substituting Eqn. 12 in Eqn. 11, one obtains,

$$\mathbf{n} \cdot \mathbf{U}rc_m - D\nabla c|_m = 0 \quad (13)$$

Eqn. 8, along with Eqn. 13, are solved at the membrane walls to obtain the permeate velocity and solute concentration. The TPMS spacer surfaces are simulated as no-slip walls.

The above governing equations and boundary conditions were solved using the commercial CFD solver ANSYS Fluent 2023 R1 (hereafter referred to as Fluent). Unsteady, laminar, pressure-based solver is chosen for all the studies, and the energy equation is not invoked. The solute concentration c is modeled as a user-defined scalar (UDS) in the solver. The generic, UDS transport equation framework provided in Fluent solves for the product of density and the UDS and is different from Eqn. 3. This framework is transformed into a form similar to Eqn. 3 by explicitly incorporating a source term in the UDS transport equation. The density and transport properties, namely, viscosity and diffusion coefficient, are specified as polynomial functions of the UDS using the built-in ‘DEFINE PROPERTY’ functionality in Fluent.

The Reynolds numbers (based on the integral length scale) studied in this work are in the range 20-460. The turbulent length scales based on these Reynolds numbers are well resolved using the grid generated in this study. Hence, turbulent eddy viscosity models are not included in the momentum equation (Eqn. 2).

The implicit, first-order, dual-time stepping scheme is used for time integration, with the maximum number of inner iterations fixed as 20. A time-step of 0.1 ms is used in all

the simulations. By monitoring the boundary fluxes and volume-averaged solute concentration over time, it was observed that the flow-through time for any of the simulations was not more than 0.25 seconds in physical time. Hence, unsteady simulations of four flow through times (1.0 seconds) were used for all cases, and assumed to thoroughly flush out the initial transients. The unsteady statistics of the simulations were then gathered using data based on continuing these simulations for an additional five flow-through times (1.25 seconds). Thus, all simulations were evolved for approximately 2.25 seconds of physical time. The unsteady statistics were calculated by averaging flow quantities at each time-step.

Spatial discretization of the momentum and solute concentration equations is carried out using a second-order upwind scheme, whereas the pressure is discretized using the standard scheme. Under-relaxation factors of 0.7, 0.99, 0.8, and 0.3 are specified for momentum, UDS, density, and pressure, respectively, to ensure solution stability and numerical convergence.

Since the membrane boundary condition discussed earlier is not readily available in the commercial software, a custom boundary condition is implemented using the in-built ‘DEFINE PROFILE’ functionality. The membrane boundary is defined as a velocity inlet condition, although with the outward-bound permeate velocity. The solute concentration at the membrane surface is computed internally using Eqn. 13. The entire framework for performing these simulations, along with the custom membrane wall boundary condition and solute transport treatment, is available online as open-source files [55]. Finally, numerical accuracy was ensured through a grid independence study, which identified an optimum resolution of 0.029 mm. The details of this study are provided in Appendix A.

5. Validation and Verification

The numerical solution strategy outlined in the previous section is validated and verified using both experimental data and computational results from previous studies, using two different test cases. The first test case, described in Section 5.1, is specifically designed to demonstrate the accuracy of the numerical schemes and the effectiveness of the membrane boundary modeling approach. In contrast, the second test case, detailed in Section 5.2, aims to show the numerical method’s ability to accurately simulate complex hydrodynamic properties within a feed channel containing 3D spacers. These test cases not only demonstrate the accuracy of the modeling method but also highlight its robustness when applying it to realistic membrane-spacer designs.

5.1. Flow through 2D open channel

This verification case aims to evaluate the accuracy of the numerical model in simulating and predicting the concentration polarization that develops on membrane surfaces. For this study, a two-dimensional rectangular channel is considered, measuring 7.62 cm in length and a 1 mm in height. The left face of the channel simulates the flow inlet, while the right boundary simulates the outlet. The bottom surface is treated as an impermeable wall, while the top surface represents the membrane. A schematic of the domain is shown in Figure 3(a). The feed solution enters the domain with a velocity of 0.2 m/s ($Re = 400$) and a concentration of 32 kg/m³. A simplified membrane boundary condition is employed, with a uniformly imposed permeate velocity of 4 μ m/s, consistent with previously published literature [56].

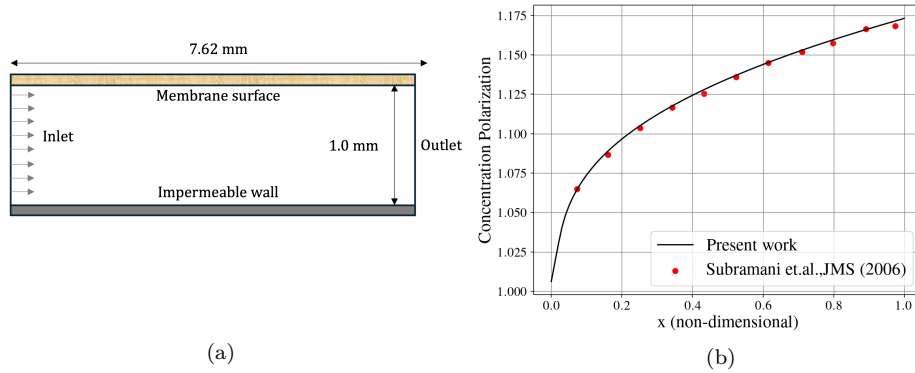


Figure 3: Verification case taken from [56] (a) Schematic of the computational domain and boundary conditions used (b) Comparison of the axial variation of concentration polarization modulus from the present work against that published in [56]

Subramani and Hoek [56] simulated this domain using FEMLAB and reported excellent agreement with finite difference [57] and film theory results.

In our present work, the 2D rectangular channel, is discretized using 100 rectangular cells in both the flow and wall-normal directions with finer meshes near the wall and membrane surfaces to accurately capturing the velocity and concentration boundary layers. In the predominant flow direction (x direction), the cell sizes are uniform. The inlet is specified as a Dirichlet boundary where the normal velocity (0.2 m/s) and solute concentration (32 kg/m^3) are specified. A Neumann boundary condition for pressure is also imposed at the inlet. At the outlet, a Dirichlet condition for pressure (set at 1 bar) is applied. The permeate velocity through the membrane surface is not calculated as a part of the solution; instead, its value ($4 \mu\text{m/s}$) is uniformly imposed, and the solute concentration at the membrane is calculated using Eqn. 13. Unsteady simulations are then carried out using the numerical strategy described earlier.

The purpose of this simulation is to confirm the numerical strategy's accuracy and the membrane boundary modeling approach. Therefore, only the comparison of the concentration polarization (CP) modulus is discussed here. The CP modulus at a specific x -location is defined as the ratio of the membrane solute concentration at that location to the bulk solute concentration (32 kg/m^3 in this study). The CP modulus, computed from the steady-state solution as a function of non-dimensional x -location (non-dimensionalized by the channel length of 7.62 cm), is plotted in Figure 3(b). This plot also includes computational results reported in [56]. Good agreement is achieved between the present work and that reported in [56] with the root mean square (RMS) deviation and the maximum absolute deviation in CP calculated as $1.69e-3$ and $3.03e-3$ respectively. These very small errors confirm that the boundary condition reproduces CP behavior with high fidelity. The authors in [56] report that their results perfectly match the values predicted by film theory and the finite difference solver results published in [57]. Thus, the numerical approach presented here is also shown to be in close agreement with the predictions from film theory. Other hydrodynamic properties of the flow, including the wall-normal velocity gradient and pressure drop, also align with the

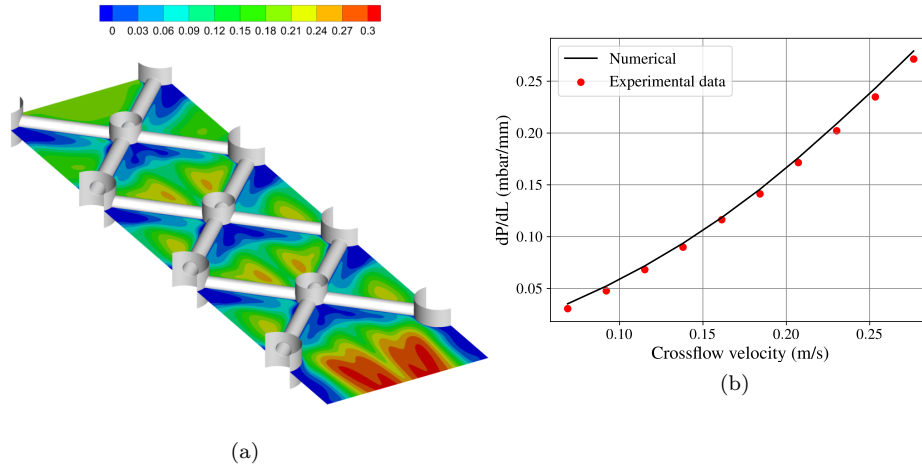


Figure 4: Validation test case taken from [42] (a) Contours of axial velocity (in m/s) at the mid-plane of the channel for $u_{inlet} = 0.185$ m/s (b) Total feed channel pressure drop (in mbar) for various cross-flow velocities compared against experimental data published in Ghaffour et al. [42].

findings in [56], although they are not shown here for brevity. This verification test demonstrates that the current numerical and membrane modeling approach accurately matches previously published results.

5.2. Flow through feed channel with 3-dimensional spacers

The purpose of this test case is to demonstrate the accuracy of the numerical strategy in predicting hydrodynamic phenomena in 3D, complex and spacer-filled channel geometries. A rectangular feed flow channel of height 1.2 mm is considered for this study. The channel houses a 3D, column-type spacer. The spacer consists of horizontal, non-woven type and cylindrical filaments with a strand angle of 90 degrees. The vertical cylindrical columns centered at the intersection of the horizontal filaments support the membrane from being compressed onto the horizontal filaments. The diameter of the horizontal filament is 0.5 mm, and that of the vertical column is 1.0 mm. The height of the column is fixed as the height of the channel (1.2 mm).

This channel-spacer configuration has been investigated both experimentally and numerically by Ghaffour et al. [42] for its effectiveness in permeation and biofouling mitigation. The authors measured pressure drop and fouling development in column-spacer modules across a range of feed velocities.

Ghaffour et al. [42] also carried out Direct Numerical Simulations (DNS) of the channel-spacer configuration. Their computational domain included four spacer units arranged in the flow direction, with periodic boundaries in the lateral direction. The DNS results revealed a complex flow pattern behind the horizontal filaments and the vertical column. Notably, the column spacer exhibited lower membrane shear stress compared to the commercial spacer, suggesting that it has reduced biofouling properties.

The numerical strategy discussed in the previous section is utilized to simulate the experiments, aiming for a quantitative comparison with feed channel pressure drop measurements. In alignment with the DNS simulations conducted by Ghaffour et al. in [42],

we consider a rectangular domain comprising four spacer units in the flow direction and one unit in the lateral direction. The feed solution, approximated as pure water, enters the domain through the inlet, where the normal component of velocity is specified. At the outlet, the pressure is maintained at atmospheric levels. The lateral sides of the domain are treated as translationally periodic. The membrane surfaces are modeled as impervious walls, reflecting the low permeate velocity observed in the experiments and ensuring consistency with the numerical modeling by Ghaffour et al. in [42].

Figures 4(a) display the contours of axial velocity and static gauge pressure at a horizontal plane that intersects the middle of the channel height. The axial velocity contours reveal significant flow features within the spacer channel. The flow obstruction caused by the horizontal filaments and the column leads to the development of a recirculation zone downstream of the column, as indicated by the negative axial velocity values shown in Figures 4(b). Additionally, flow acceleration can be observed upstream of the horizontal filaments and near the columns, where the flow expands as it passes over the filaments. These axial velocity contours are quite similar to those reported in [42]. Figure 4(b) illustrates the total pressure drop in the feed channel for various inlet velocity values. A near-quadratic relationship is observed between pressure drop and inlet velocity, with higher inlet velocities resulting in greater pressure drops. Furthermore, the computed pressure drop aligns well with the experimentally measured values, featuring a maximum relative error of 0.008 Pa and RMS error of 0.005 Pa thereby confirming quantitative accuracy.

Together, the verification and validation cases demonstrate that the numerical framework accurately reproduces both fundamental concentration polarization behavior and complex spacer-induced hydrodynamics. Agreement with film theory, prior simulations, and experimental pressure drop data confirms the robustness of the membrane boundary condition and CFD implementation, providing confidence in applying this approach to TPMS spacer designs.

6. Results and Discussions

Numerical simulations of spacer-filled channels are performed using the previously described framework on the National Laboratory of the Rockies supercomputer *Kestrel* [58]. *Kestrel* computing nodes are equipped with dual-socket Intel Xeon Sapphire Rapids 52-core processors per node panel. Each simulation was run on 2 nodes (104 processor cores) and consumed a peak memory usage of 30 GB.

This section is organized as follows. Sub-section 6.1 examines spacer geometry effects, focusing on TPMS spacers alone. The hydrodynamic and solute concentration behavior of Non-Woven spacers have been extensively characterized in prior studies [38, 59]. The present analysis, therefore, focuses on isolating the topology-driven mechanisms associated with TPMS geometries under UHPRO conditions, with the reported global membrane performances compared with the corresponding computed values of the Non-Woven spacers in Sub-section 6.2. Sub-section 6.2 also describes how inlet velocity affects hydrodynamic and membrane permeation properties. Sub-section 6.3 discusses porosity effects on membrane performance. Finally, sub-section 6.4 compares present results with prior studies.

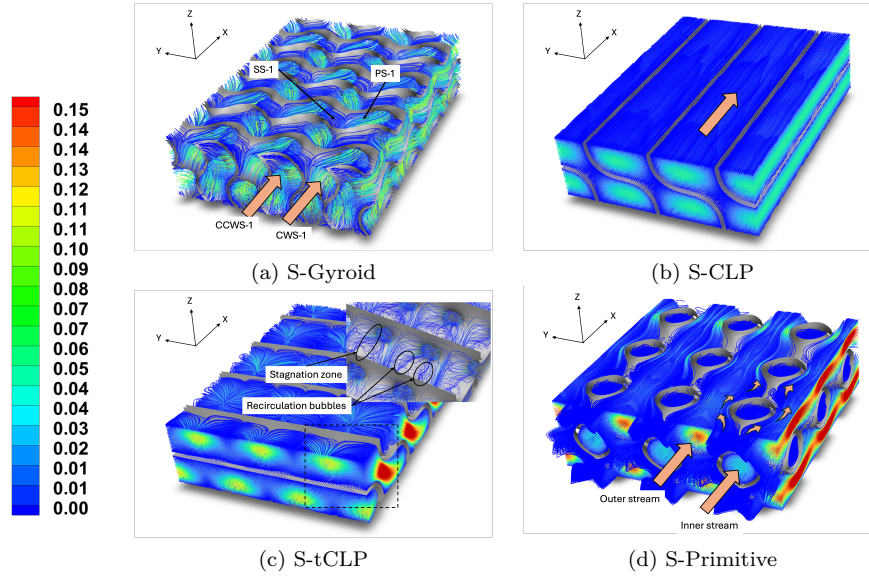


Figure 5: The streamlines passing through various spacer designs colored by velocity magnitude in m/s. Grey surfaces indicate the spacer walls surfaces. The orange, filled arrows indicate the bulk flow direction.

6.1. Effect of TPMS spacer geometry

To compare different spacer designs, flow simulations are conducted using the same inlet velocity ($u_{inlet} = 0.025$ m/s) for each design. We analyze flow streamlines, pressure drops, shear stress, and solute concentration distributions with the different spacer designs in the upcoming sub-sections.

6.1.1. Flow field

Figure 5 illustrates the streamlines through the feed flow channel for all the TPMS spacer designs. For the sake of clarity, only the three periodic spacer units closest to the outlet boundary, with fully developed flow profiles, are shown.

The streamlines for the S-Gyroid spacer are depicted in Figure 5(a). This design creates six pairs of alternate co-rotating and counter-rotating flow streams. These streams (for example, CCWS-1 and CWS-1 shown in the figure) follow helical trajectory through the channel and bifurcate into high-velocity and low-velocity sub-streams post each periodic unit. The primary stream (PS-1) continues the helical path, while the secondary stream (SS-1) merges with the counter-rotating stream, leading to a complex flow pattern. In contrast, the S-CLP spacer results in a simpler flow field. The bulk flow is predominantly unidirectional, traveling parallel to the spacer walls. Low-velocity, cross-streams that emerge transverse to the CLP holes (shown in Figure 1(b)) do provide occasional, albeit negligible, flow deviations. In contrast to these designs, S-tCLP maximally obstructs flow and has no ‘line-of-sight’ from the inlet to the outlet. Feed is forced through the tCLP holes, where it splits into two sub-streams that turn about 90° and then meet adjacent sub-streams. This interaction produces a pair of counter-rotating vortices beneath the membrane and a stagnation zone between them (see inset of Figure 5(c)). The S-Primitive design splits the incoming flow into two separate paths: an

inner stream through the central channel and an outer stream along the membrane walls. Although there is a line of sight from inlet to outlet, the outer stream follows a tortuous route with repeated contractions and expansions, producing complex local flow patterns (Figure 5(d)). It is worth noting that the peak velocity magnitudes vary across designs. The peak velocity magnitude is higher for the S-tCLP and S-Primitive designs (approximately 0.2 m/s) when compared to the S-Gyroid and S-CLP designs (approximately 0.08 m/s).

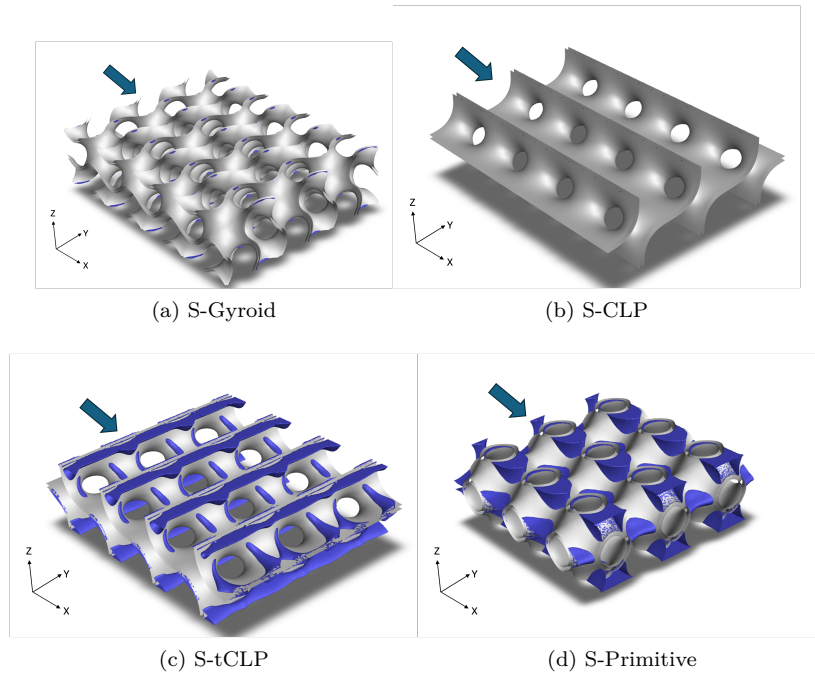


Figure 6: Recirculation zones (colored in blue) developed in the feed channel. Green arrows indicate the flow direction.

The flow fields around the spacers create distinct flow structures inside the feed channel, notably the recirculation and stagnation zones. Recirculation zones can disrupt the concentration boundary layer growth by frequent back flow and the transport of solute concentration away from the membrane walls. In contrast, stagnation zones have low fluid movement and can promote bio-fouling. In this study, a simple postprocessing approach to the CFD solution is adopted to identify these zones. Grid cells with zero or negative x -velocity are identified and tagged. The zone volume is then computed by summing up the element volumes of all such tagged cells.

Figure 6 shows such zones (colored in blue) for the designs. The S-CLP spacer shows almost no recirculation or stagnation zones due to its unidirectional flow. Similarly, the S-Gyroid spacer also shows small recirculation zones downstream of the transverse spacer walls. The cumulative volume of these zones is only 0.04% the total feed channel volume. In contrast, the S-tCLP and S-Primitive spacers exhibit significantly larger recirculation and stagnation zones. The formation of recirculation and stagnation zones in the S-tCLP

design is already evident from the streamline plot in Figure 5(c). These zones are found to occupy 4.73% of the total fluid volume for the S-tCLP spacer. However, the largest recirculation zone is observed for the S-Primitive spacer and occupies 7.4% of the total fluid volume. Interestingly, although the S-tCLP design appears more obstructive, it generates smaller recirculation zones when compared to S-Primitive design. This is because approximately 84.5% of the feed flow passes through the outer stream of the S-Primitive design. This higher flow percentage, combined with the considerable obstruction, creates larger wake regions behind them, causing larger stagnation zones.

Stagnation zones are potential locations for the onset of fouling, with larger stagnation zones indicating a higher propensity for organic fouling. Based on this observation, the S-tCLP and S-Primitive spacers will have higher fouling propensities when compared to S-Gyroid and S-CLP spacers. Moreover, these zones contribute to increased drag, culminating in elevated pressure drops, which are presented in the next section.

6.1.2. Feed channel pressure drop

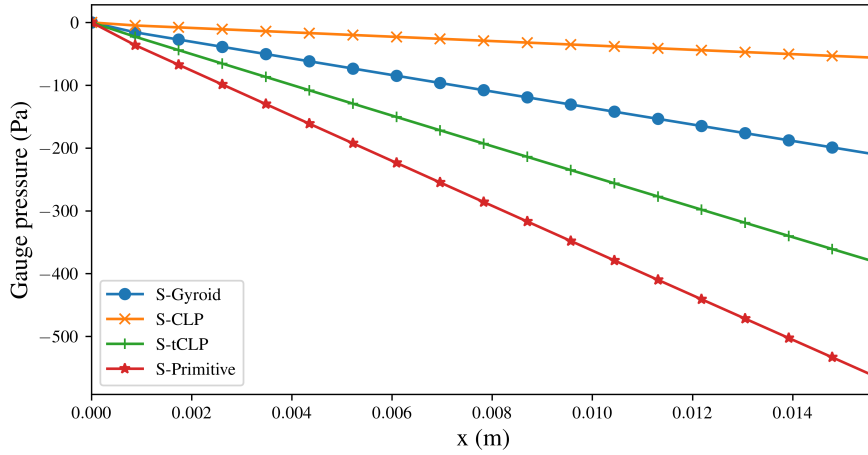


Figure 7: Average gauge pressure along the channel length for various spacer designs for $u_{inlet} = 0.025$ m/s

The area-weighted average of the mean gauge pressure at various longitudinal planes in the feed channel is computed. The gauge pressure is defined such that the inlet pressure is 0 Pa. The axial variation of the mean pressure for all the spacer designs is shown in Figure 7. The pressure is observed to drop linearly along the downstream direction for all the spacer designs, indicating a quick evolution of the flow field in the longitudinal direction into a fully developed regime. The S-CLP spacer results in the lowest feed channel pressure drop. The S-Gyroid spacer follows, but it experiences a pressure drop that is 3.7 times greater than that of the S-CLP design. The S-tCLP and S-Primitive spacers have even higher pressure drops, with values 6.7 and 9.5 times that of the S-CLP spacer, respectively. The differences in pressure drop can be correlated to the size of the recirculation zones, with designs having the smaller recirculation zones (S-CLP) showing the lowest pressure drop and vice versa. Larger recirculation zones increase wake losses also leading to greater effective flow blockage. Interestingly, designs

that experience higher pressure drops are also linked to greater flow velocity magnitudes, as shown in Figure 5. This relationship indicates that there is increased flow restriction due to blockage, even with the same inlet flow velocity and inlet cross-sectional area. This observation aligns with the well-established correlation that the pressure drop in spacer-filled channels is proportional to the square of the characteristic velocity.

6.1.3. Membrane shear stress, solute concentration and permeate velocity

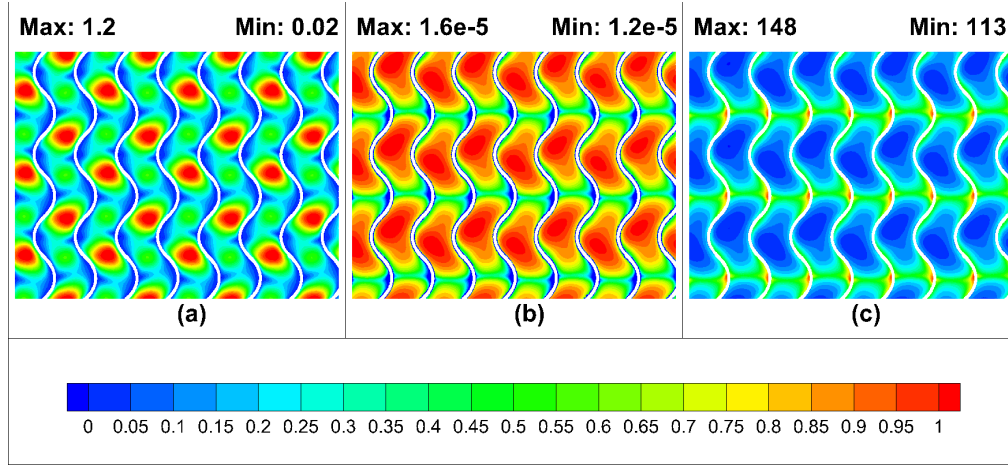


Figure 8: Membrane wall properties plotted for the S-Gyroid spacer. (a) shear stress (b) permeate velocity and (c) solute concentration. All plots are normalized to their respective minimum and maximum values, which are annotated on each sub-figure, and use a common color scale. Units: (a) Pa (b) m/s and (c) kg/m³

The close relationship between membrane shear stress and permeation performance have been reported and discussed previously in multiple articles elsewhere [60, 61]. Spacer geometry alters the flow field inside the feed channel creating velocity gradients and shear stresses on the membrane surfaces. Wall shear stresses play a pivotal role in determining membrane concentration polarization, with higher shear stress values indicating a higher propensity for the solutes to be 'scooped' away from the membrane surface by the flow. This results in lower values of the membrane solute concentration. A lower value of membrane solute concentration results in higher osmotic pressure difference between feed and permeate channel and hence a higher value of permeate velocity. To demonstrate this physics, we show the membrane shear stress, solute concentration and permeate velocity values computed for the S-Gyroid spacer in Figure 8. The three plots show these properties normalized based on the minimum and maximum values annotated on each of the sub-figures. Only the downstream 8 spacers units are shown for clarity. The S-Gyroid spacer and membrane surface intersect creating a wavy pattern as shown the figure. The distinct flow field of the S-Gyroid spacers create alternating zones of high and low shear stresses and is shown in Figure 8(a). It should be noted that the zones of high shear stresses closely coincide with regions of low membrane solute concentration as shown in Figure 8(c). Conversely, higher solute concentration is observed in regions of stagnation zones where the shear stresses are low. The contours of permeate velocity is also shown in Figure 8(b) and a strong correlation between permeate velocity and solute

concentration can be clearly observed with lower solute concentration regions coinciding exactly with higher permeate velocity ones.

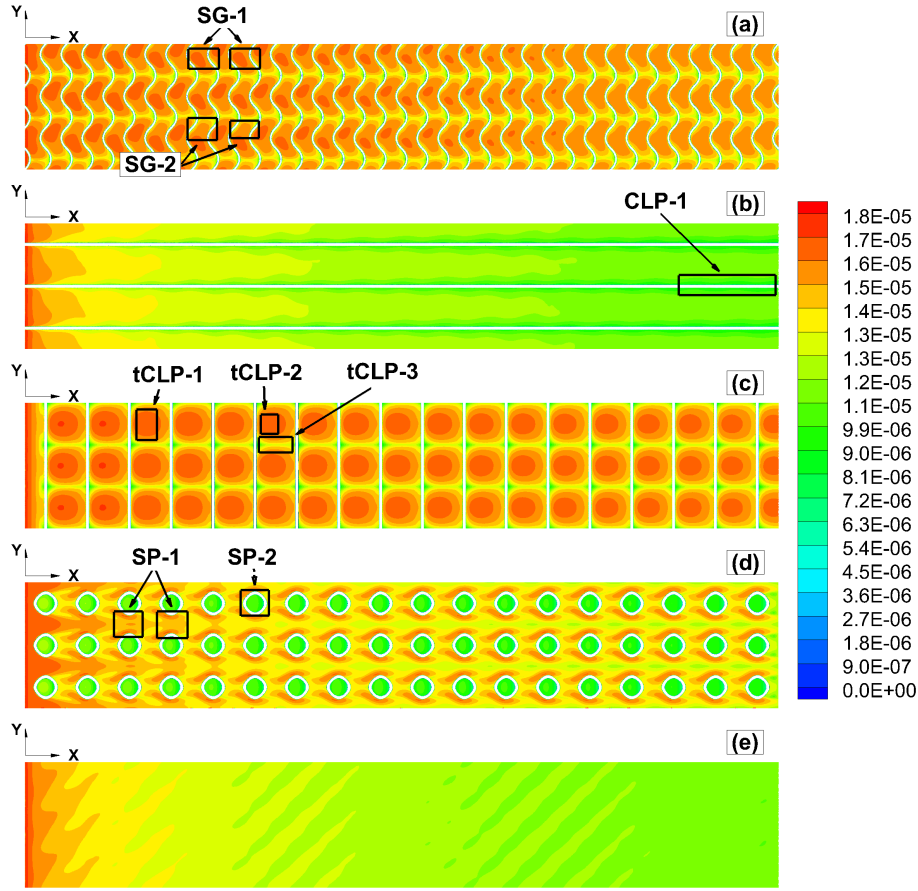


Figure 9: Permeate velocity contours on the top membrane wall. (Units in m/s) (a) S-Gyroid (b) S-CLP (c) S-tCLP (d) S-Primitive and (e) Non-Woven

The close resemblance between solute concentration, shear stress and permeate velocity is also observed for all the TPMS designs. Taking advantage of this, the membrane permeation properties are now discussed using the plots of membrane permeate velocity alone, for all TPMS designs, and are shown in Figure 9. The permeate velocity field of the Non-Woven spacer is shown in Figure 9(e) for comparison. All the spacer designs show a high value of permeate velocity near to the inlet boundary. This is due to the sudden development of the velocity boundary layer near the inlet leading to high shear stress values and low membrane solute concentration. The permeate velocity quickly drops as one moves downstream in the case of S-CLP and Non-Woven spacers. This is because of lack of geometrical features in the spacers that generate high shear stresses on the membrane walls. The parallel array of spacers creates a filament-aligned permeate velocity pattern for the Non-Woven spacer, as can be seen in the Figure 9(e). In the case of CLP spacer, the intersection of the spacer walls with the membrane surface (marked

as CLP-1 in Figure 9(b)), in particular, forms zones of solute deposition leading to high membrane solute concentration and low permeate velocity and shear stress. On the other hand, S-Gyroid and S-tCLP spacers show better consistency in maintaining the permeate velocity values as one moves downstream. This arises because of the unique flow field developed due to both these spacers as explained in the previous sub-sections. In the case of S-Gyroid spacer, the higher permeate velocity zones are located where the helical fluid streams PS-1 and SS-1 (see Figure 5(a)) interact with membrane surface. These zones on the membrane surface are marked as SG-1 and SG-2 in the Figure 9(a). Conversely, the regions of low permeation coincide with the stagnation zone created where spacer walls intersect the membrane walls. Similarly for the S-tCLP spacer, the stream through t-CLP holes intersect the membrane walls creating distinct circular patches of high permeation (marked tCLP-1 and tCLP-2) in Figure 9(c) where as the stagnation zones (shown in Figure 6(c)) create regions of low permeation (and high solute concentration) and is marked as region tCLP-3 in the figure. For the S-Primitive spacers, high permeation regions are created due to the flow constriction created by the outer streams with the spacers (regions marked SP-1 and SP-2) where as the inner streams contribute to solute deposition and hence low permeation.

Table 2: Spacer permeation properties for the $u_{inlet} = 0.025$ m/s case

Spacer design	Inlet volumetric flow rate $\times 10^8$ [m^3/s]	Average permeate velocity [$\mu m/s$]	Osmotic Pressure [bar]
S-Gyroid	5.162	15.25	98.2
S-CLP	5.097	12.00	117.6
S-tCLP	5.318	15.28	98.1
S-Primitive	5.146	13.74	107.2

In summary, this sub-section discusses the hydrodynamic features and permeation properties of membranes with four TPMS spacer-filled channels for the same inlet feed velocity of 0.025 m/s. Each of these spacers, due to its unique geometry, generated a unique flow field inside the feed channel that directly impacted the hydrodynamic and membrane properties. Recirculation and stagnation zone volumes clearly impacted the pressure loss in the membrane modules, with the S-Primitive spacer incurring the highest pressure drop. A comparison of the permeation properties of all spacers for the same inlet velocity (0.025 m/s) is reported in Table 2. The average membrane solute concentration is highest for the S-CLP spacer, followed by the S-Primitive spacer. This causes higher membrane osmotic pressure (Eqn. 9) for these spacers compared to S-Gyroid and t-CLP spacers, as reported in the Table 2. Higher osmotic pressure reduces the net transmembrane pressure difference that drives the permeation through the membrane surfaces. Hence, lower average permeate velocities are observed for the S-CLP and S-Primitive spacers in comparison to S-Gyroid and S-tCLP spacers. It should also be noted that even though the average permeate velocities produced by S-Gyroid and S-tCLP are very close to each other, the inlet volumetric flow rate to S-Gyroid is approximately 4% lower than that to the S-tCLP spacer. This indicates a higher water recovery rate for the S-Gyroid spacer among all the TPMS spacers considered. Higher

water recovery and lower feed channel pressure drop clearly identify S-Gyroid as the best candidate for UHPRO spacer designs among the TPMS surfaces considered in this study.

6.2. Effect of inlet velocity

This section examines the effect of inlet velocity on membrane performance, specifically considering velocities of $u_{\text{inlet}} = 0.025, 0.05, 0.1$, and 0.2 m/s . While the previous section provided a detailed discussion of the scenario with the lowest inlet velocity ($u_{\text{inlet}} = 0.025 \text{ m/s}$), this section focuses on the highest velocity case ($u_{\text{inlet}} = 0.2 \text{ m/s}$) to highlight the differences. To analyze how varying inlet velocities affect the channel flow field, streamline plots are visualized, as shown in Figure 10. The figure presents the streamlines near the last three spacer units, which are closest to the outlet boundary, in a manner similar to Figure 5.

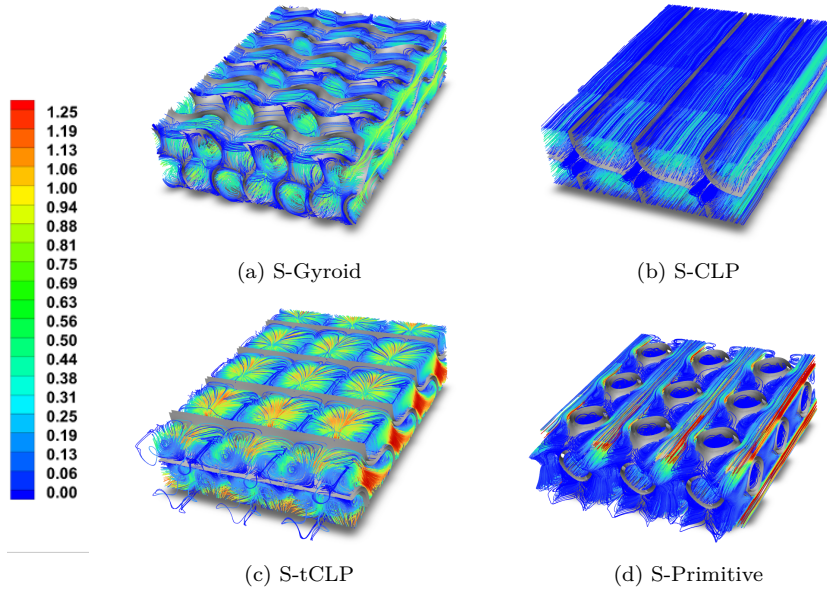


Figure 10: The streamlines passing through various spacer designs for the $u_{\text{inlet}} = 0.2 \text{ m/s}$ case. Streamlines are colored by velocity magnitude and are expressed in m/s.

The streamlines observed are qualitatively similar to those seen previously at $u_{\text{inlet}} = 0.025 \text{ m/s}$. The prominent flow patterns, such as the SS-1 and PS-1 streams in S-Gyroid spacers described earlier, are well-preserved even at the higher inlet velocities. However, the magnitudes of velocity within the flow field have increased in accordance with the increased inlet velocity. A maximum velocity magnitude of 1.25 m/s is recorded for the S-Primitive spacer, followed by 1.0 m/s for the S-tCLP spacer, occurring at the flow constriction and S-tCLP holes, respectively (see Figures 10(c) and (d)).

The increase in flow velocity results in changes that affect the membrane's permeation properties. One noticeable effect is the heightened velocity gradients within the fluid domain and at the membrane walls. The increased velocity gradients at the membrane surfaces lead to higher wall shear stresses, which is consistently observed across all spacer designs. Importantly, the intermittent patterns of low and high shear stress zones,

discussed previously, remain similar to those noted at $u_{inlet} = 0.025$ m/s. However, the magnitudes of shear stress have nearly quadrupled at the highest inlet velocity case. A strong correlation between shear stress, membrane solute concentration and permeate velocity has already been established. Consequently, as the inlet velocity increases, a reduction in membrane solute concentration and an increase in permeate velocity is observed, for all spacer designs.

The increased velocity gradients also lead to earlier flow separation, which in turn creates larger recirculation and stagnation zones. The larger recirculation zone for the S-CLP is now visible in the streamline plot in Figures 10(b).

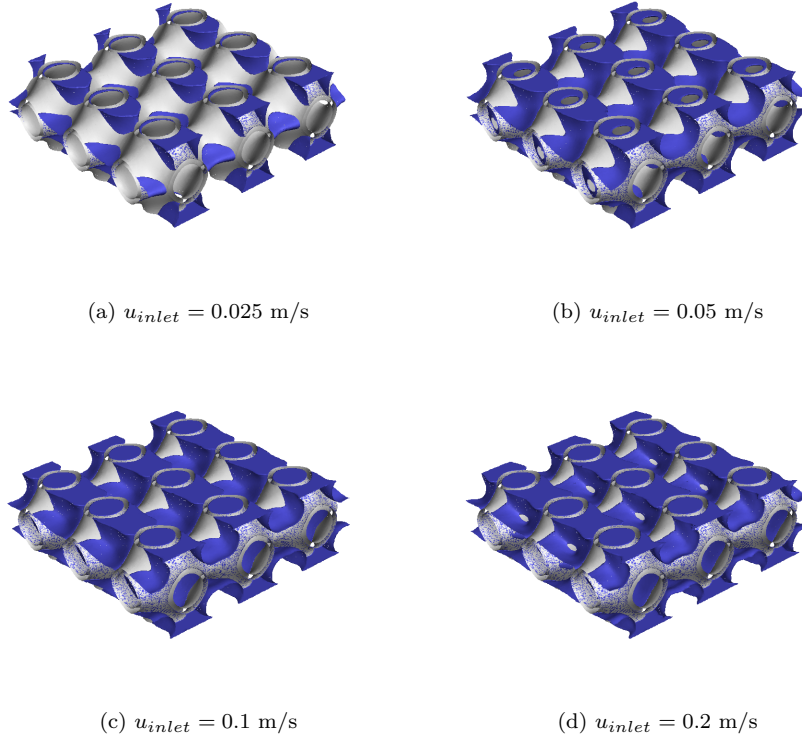


Figure 11: Recirculation zones for the S-Primitive spacer for various inlet velocities

Of particular interest is the case of S-Primitive spacer. Figure 11 illustrates the recirculation zones within the S-Primitive spacer channel for all inlet velocity cases studied. These recirculation zones are identified using the approach mentioned in the previous sub-section. At a low inlet velocity of ($u_{inlet} = 0.025$ m/s), the recirculation zones are relatively small and are primarily located downstream of the outer channel walls, as shown in Figure 11(a). However, as the inlet velocity increases, the size of the recirculation zone also grows. At $u_{inlet} = 0.1$ m/s, the zone completely fills the space between two consecutive outer channels, as depicted in Figure 11(c). Beyond this velocity, further increases in the inlet speed do not significantly change the size of the recirculation zones.

This trend is unique to the S-Primitive spacer and has implications for the total channel pressure drop, as shown in Figure 12(a). The pressure drop for all spacers at all inlet velocities is depicted here. It can be observed that the S-Primitive spacer experiences the highest pressure drop for inlet velocities up to 0.05 m/s. However, further increases in inlet velocity result in a lower pressure drop than anticipated. Thus, at $u_{inlet} = 0.1$ m/s and higher, the S-tCLP spacer appears to incur the highest pressure drop. On the other hand, the lowest pressure drop is observed for the S-CLP and Non-Woven designs due to their minimal flow blockage, while the S-Gyroid shows intermediate pressure drop values.

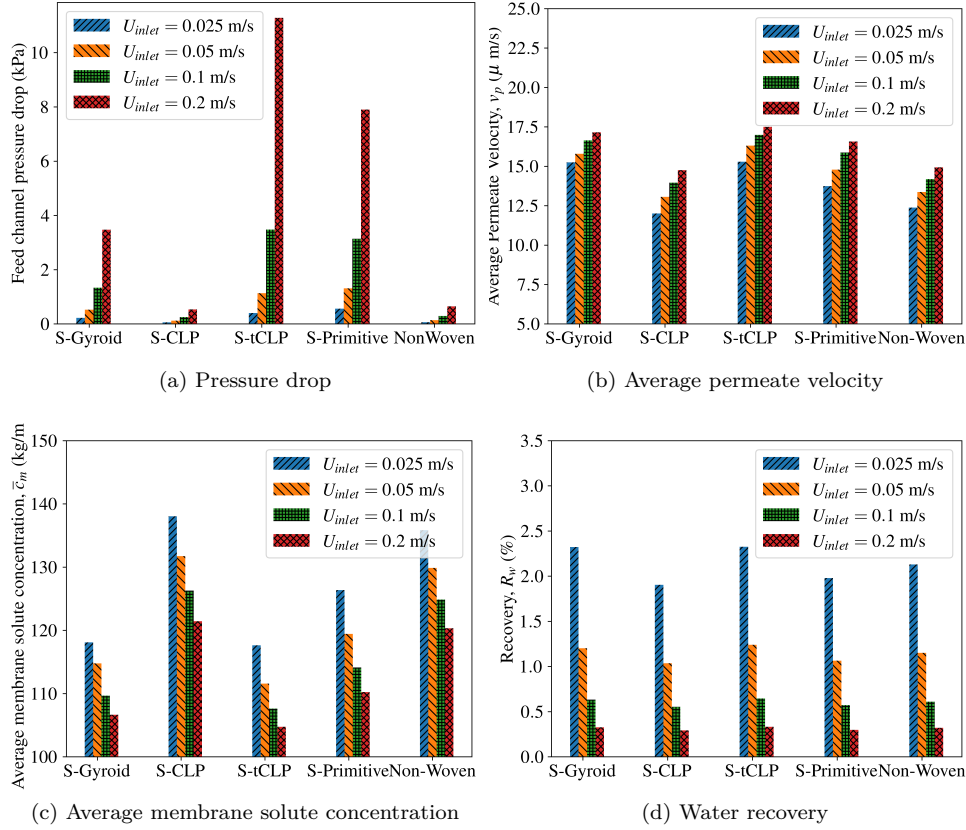


Figure 12: Membrane performance indicators for the four TPMS spacers at different inlet velocities

To analyze the effects of inlet velocity on key membrane permeation properties, two important parameters, namely, the average permeate velocity $\bar{v}_p$ and the average membrane solution concentration $\bar{c}_m$ are defined as,

$$\bar{c}_m = \frac{\text{membrane } \rho c_m \mathbf{v} \cdot \mathbf{dA}}{\text{membrane } \rho \mathbf{v} \cdot \mathbf{dA}} \quad (14)$$

$$\bar{v}_p = \frac{\text{membrane } v_p \cdot \mathbf{dA}}{\text{membrane } \mathbf{dA}} \quad (15)$$

These metrics serve as indicators of mean permeate velocity and solute concentration for the full membrane surfaces and are shown in Figure 12(b) and (c).

A linear relationship between the average permeate velocity, $\bar{v}_p$, and inlet velocity is observed for all the TPMS spacers as well as the Non-Woven spacer. Notably, $\bar{v}_p$ is nearly the same for the S-Gyroid and S-tCLP spacers, which exhibit the highest permeate velocities among all the spacers considered. The S-Primitive spacers yield slightly lower permeate velocities, whereas the S-CLP spacer has the lowest permeate velocity among the TPMS spacers, comparable to that of the Non-Woven spacer.

The relationship between permeate velocity and membrane solute concentration has already been discussed in the previous subsection. Similar conclusions can be drawn about $\bar{v}_p$ and $\bar{c}_m$. The designs with the highest $\bar{v}_p$, specifically the S-Gyroid and S-tCLP, correspond to the lowest values of $\bar{c}_m$, as expected. The S-Primitive spacers have higher $\bar{c}_m$ values compared to S-Gyroid and S-tCLP, while the S-CLP registers the highest values among all the spacers. The Non-Woven design shows $\bar{c}_m$ values that fall between those of the S-Primitive and S-CLP spacers.

Another key performance indicator examined here is the water recovery rate, R_w , which is defined as,

$$R_w = \frac{\text{membrane } \mathbf{v} \cdot \mathbf{dA}}{\text{inlet } \mathbf{v} \cdot \mathbf{dA}} \quad (16)$$

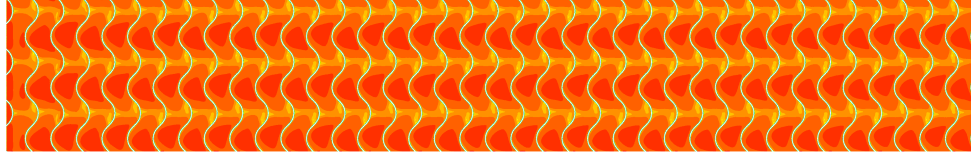
and is the ratio of the total permeate flux produced per unit flux of feed solution supplied. Although $\bar{v}_p$ indicates the mean flux through the membrane for a given inlet feed velocity, R_w provides valuable insights because the membrane and inlet area cross-sections differ for each spacer configuration. Figure 12(d) illustrates the water recovery rate for all spacer designs. Despite having slightly larger inlet cross-sectional areas, both the S-Gyroid and S-tCLP spacers demonstrate the best water recovery rates among all the spacers. Interestingly, although the S-Primitive spacer shows higher $\bar{v}_p$ values than the Non-Woven spacer, the recovery rate is higher for the Non-Woven design due to its lower inlet cross-sectional area (and hence a lower feed flow rate into the feed channel). The S-CLP exhibits the weakest R_w performance among all the spacers.

6.3. Effect of spacer porosity

The previous sub-sections demonstrate that the S-Gyroid spacer outperforms the other TPMS spacers. It achieves the highest permeate flux while maintaining relatively lower feed channel pressure drops and membrane solute concentrations. However, variations in the tolerances of additive manufacturing processes, as well as in operando fouling and solute deposition, can affect or alter the porosity induced by the spacers. In this section, we analyze how varying spacer porosity impacts membrane performance, specifically focusing on the S-Gyroid spacer because of its superior performance compared to

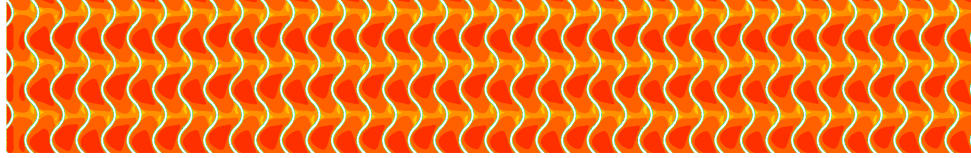
Porosity, $\epsilon = 0.95$

(a)



Porosity, $\epsilon = 0.88$

(b)



Porosity, $\epsilon = 0.75$

(c)

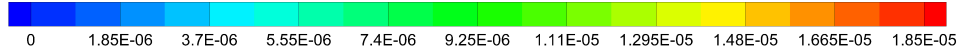
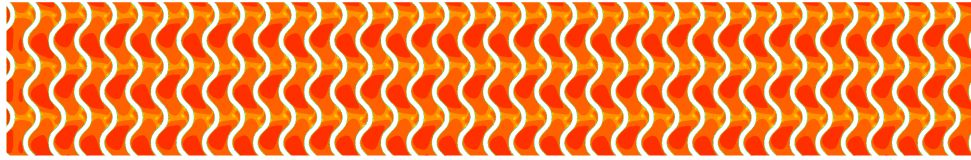


Figure 13: Permeate velocity on top membrane wall for the S-Gyroid spacers with different porosity values. (Units in m/s)

the other spacers. We examine two additional porosity values, 0.95 and 0.75, to explore their effect on membrane performance. These additional porosity levels were selected as idealized bounding cases to assess the sensitivity of hydrodynamic and mass-transfer behavior to porosity, rather than to represent specific manufacturing limits. Adjusting the porosity corresponds to changing the thickness of the surfaces of the S-Gyroid spacer. We generate new CAD geometries for the S-Gyroid spacers using the previously utilized TPMS tool. Subsequently, we conduct CFD simulations with these geometries at various inlet velocities, applying the same numerical approach as in the previous sub-sections.

The permeate velocity contours on the top membrane surface are illustrated in Figure 13 for the three porosity values studied. Notably, the middle figure represents the nominal porosity spacer ($\epsilon = 0.88$) detailed in the previous subsections, whereas the top and bottom figures correspond to porosity values of 0.95 and 0.75, respectively. In all three figures, the inlet velocity is set at 0.2 m/s. It is important to note that, like all TPMS spacers, the spacer surfaces are in direct contact with the membrane surfaces. As porosity decreases, the thickness of the spacer sheet surfaces increases, as seen in Figure 13(c). The permeate velocity patterns across all porosity configurations are remarkably similar, with no significant deviations observed from the nominal porosity configurations. Notably, the high and low velocity zones (SG-1 and SG-2 in Figure 9)

maintain their size and shape across all three porosity configurations. Furthermore, no degradation in permeate velocity values is observed as one moves downstream in the membrane, indicating that changes in porosity do not significantly affect the fluid velocity field within the channel. Although not shown here, the distribution of membrane shear stress and solute concentration also remains consistent across different porosity values. This is not surprising, as previous subsections have demonstrated a strong correlation between membrane shear stress, solute concentration, and permeate velocity.

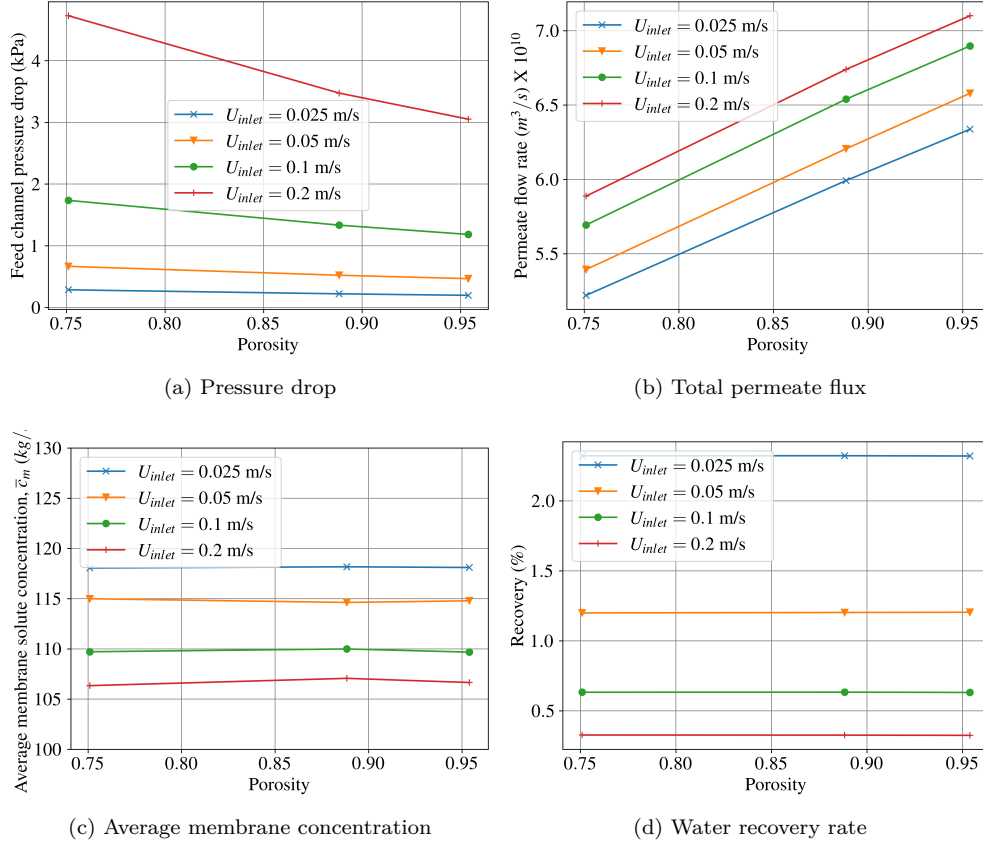


Figure 14: Effect of porosity on membrane performance indicators

The key membrane performance parameters and their relationship with porosity are illustrated in Figure 14. The feed channel pressure drop as a function of porosity is shown in Figure 14(a) for various inlet velocities. Generally, the pressure drop tends to increase as porosity decreases due to the increased flow obstruction caused by the spacer walls. At low inlet velocities ($u_{inlet} = 0.025$ and 0.05 m/s), the variation in pressure drop compared to the nominal porosity case is minimal, resulting in pressure drops of only ~ 65 Pa and ~ 145 Pa for high and low porosity cases, respectively. In contrast, at a higher inlet velocity ($u_{inlet} = 0.2$ m/s), the pressure drop increases non-linearly for decreasing porosity, resulting in a pressure drop difference of 1250 Pa with respect to the nominal porosity case.

Since the permeate velocity variations are already discussed, the total permeate flux through the top membrane is shown in Figure 14(b). The total permeate flux increases linearly with increasing porosity for all inlet velocities. However, the contours of the permeate velocity, illustrated in Figure 13, do not show significant changes with varying porosity. This suggests that the increase in flux is primarily due to the larger membrane surface area resulting from reduced spacer thickness as porosity increases. Additionally, the average membrane solute concentration, $\bar{c}_m$, is plotted as a function of porosity in Figure 14(c). Consistent with the findings regarding permeate velocity, the variations of $\bar{c}_m$ with porosity remain negligible for all inlet velocity values. A similar trend is observed for the water recovery rate, R_w , as depicted in Figure 14(d), which shows almost no variation with porosity. While the total permeate flux exhibits notable changes, the near constant value of R_w can be attributed to variations in the inlet feed flow rate that occur with increasing porosity. These variations are caused due to changes in the inlet cross-sectional areas due to different spacer thicknesses. Consequently, these variations are directly proportional to the total permeate flux, resulting in the consistent value of R_w .

6.4. Prior studies and implications for future membrane module design

There are two reasons why a direct comparison between the results of this study and findings from previously published experimental studies is challenging. Firstly, while there are numerous studies on TPMS designs for heat exchanger applications, research focused on membrane-based desalination methods is comparatively limited. Among these studies, most of the work focus on membrane distillation, with only a few addressing UF and RO applications. Secondly, many studies that utilize TPMS spacers employ skeletal-based designs. In contrast, this study utilizes sheet-based designs due to their superior structural stability, which is essential for operating under UHPRO conditions. Despite these differences, there are shared characteristics across these studies that facilitate qualitative assessments.

Castillo et al. [22], carried out membrane distillation experiments with spacers of comparable porosity, including S-Gyroid, S-tCLP, and a commercial spacer. They reported a higher pressure drop for both TPMS spacers, which aligns with the results of the present study. They also observed the highest permeate flux for the S-tCLP spacer, followed by the S-Gyroid spacer, which is consistent with our findings. On the contrary, Sreedhar et al. [19] performed RO experiments using S-Gyroid, S-Primitive, and S-CLP spacers, reporting flux improvements of 15.5%, 7.8%, and 11.7%, respectively. They noted a lower feed channel pressure drop for all three spacers compared to a commercial spacer tested under similar conditions. A similar trend was observed in another study by Sreedhar et al. [20], where the S-Gyroid, S-Primitive, and S-CLP spacers showed significantly enhanced mass transfer and reduced pressure drop in comparison to a commercial spacer operating under UF conditions. Our study shows a 12% flux enhancement for the S-Gyroid spacer, while the S-CLP and S-Primitive spacers exhibit lower flux when compared to the Non-Woven spacer of equal porosity. Additionally, the results from this study show an increased pressure drop for both the S-Gyroid and S-Primitive spacers. This discrepancy can be attributed to differences in spacer topology and porosity. It is important to note that the S-Gyroid and S-Primitive spacers used in the previous studies ([19], [20]) featured a skeletal-based architecture, whereas the present study employs a

sheet-based topology. Generally, skeletal topology facilitates smoother fluid flow, resulting in a lower pressure drop. Furthermore, the porosity of the commercial spacer used for comparison is not reported in Sreedhar et al. [19] and is considerably lower than that of the TPMS spacers studied in Sreedhar et al. [20]. We hypothesize that the (possibly) lower porosity of the commercial spacer also contributes to its higher pressure drop in comparison to TPMS spacers. These observations highlight the markedly different permeation properties of skeletal and sheet TPMS designs.

Sreedhar et al.[20] investigated the impact of varying porosity in S-Gyroid spacers. Their findings indicated a significant improvement in permeate flux and a reduction in pressure drop as porosity is increased. In contrast, the current study reports that changes to the average permeate velocity of the S-Gyroid spacer with varying porosity are negligible. This disparity can again be attributed to the difference in topologies of the skeletal Gyroid used in [20] and the sheet Gyroid used in the present study. Increasing the porosity in the sheet Gyroid spacer results in thickening the S-Gyroid surface without altering the flow path considerably, resulting in negligible changes to the average permeate velocity. This conclusion is further confirmed by drawing parallels with the convective heat transfer study performed using sheet Gyroid spacer reported by Cheng et.al.[62]. The authors of this study report very minimal changes to the heat transfer coefficient when porosity is higher than 85%.

Due to the limited number of published CFD studies, detailed information about the local flow characteristics in TPMS spacers is scarce. However, a recent study by Swaidan et al.[23] discussed CFD simulations of TPMS spacer-filled channels used in membrane distillation applications, that show similar trends with this work. This study demonstrated that fluid mixing was improved through the generation of vorticity, resulting in higher membrane shear stresses compared to a non-woven spacer. Although the present study uses different TPMS spacers, the salient flow features of TPMS spacers, such as enhanced mixing and increased wall shear stresses, are well captured in the present study as well.

The present study offers numerous insights into the adoption of TPMS spacers for UHPRO membrane module designs. Firstly, three of the four TPMS spacers considered in this study exhibit enhanced permeate velocity when compared to the Non-Woven spacer of the same porosity. Permeate velocity enhancements of 23.5%, 23.2%, and 11.0% are observed for the S-tCLP, S-Gyroid, and S-Primitive spacers, respectively. The S-CLP spacer performs worse than the Non-Woven spacer, producing 3.0% less permeate flux. In terms of water recovery rate R_w , the S-Gyroid and S-tCLP spacers demonstrate superior performance, each achieving a value of 2.38% for the domain size considered. In contrast, the S-Primitive and S-CLP spacers show lower R_w values compared to the Non-Woven spacer.

Secondly, the TPMS spacers exhibiting enhanced permeate velocities also induce increased feed channel pressure drop. The pressure drop is the highest for the S-Primitive spacer at low inlet velocities (0.025 m/s - 0.05 m/s) and S-tCLP spacer for higher inlet velocities (> 0.05 m/s). The feed channel pressure drop is a critical criterion in RO and UF membrane module design as it determines the energy required for operating the pumps that feed these modules. Key performance indicators of RO and UF module operation often employ terms involving the ratio of the permeate flux to the pressure drop to rate different spacer designs. For example, one such performance indicator used to characterize RO and UF membrane modules is the hydraulic efficiency index (HEI),

defined as:

$$HEI = \frac{J_w}{\Delta P} \quad (17)$$

where J_w and ΔP are the total permeate flux and feed channel pressure drop, respectively. HEI is a measure of the permeate flux produced by the membrane module for unit pressure drop, with higher values indicating better performance. However, a direct application of Eqn. 17 to the results of the present study performed for UHPRO applications would yield an HEI value of 0.5 LMH/Pa for the best-performing TPMS spacer, namely, the S-Gyroid. In comparison, the HEI value for the Non-Woven spacer is 1.37 LMH/Pa, and for the poorest permeating TPMS spacer, the S-CLP spacer, is 1.46 LMH/Pa, falsely indicating superior performance for the S-CLP and Non-Woven spacers. This discrepancy arises due to the different rates at which permeate flux and pressure drop scale as the operating pressure is increased. For example, the total channel pressure drop for the S-Gyroid spacer for a one meter long membrane module would be 0.14 bar compared to 0.04 bar for the Non-Woven spacer. This pressure drop value is calculated based on the observation that the pressure gradient in the streamwise direction is nearly constant (see Figure 7). The authors of this study hypothesize that this slight increase in pressure drop (of 0.1 bar) for the S-Gyroid spacer will be less relevant at UHPRO conditions and cannot offset the benefit from the increased (23.2%) permeate flux. In other words, the influence of concentration polarization on local osmotic pressure is strong and reducing concentration polarization has a larger impact on permeate flux than minimizing feed channel pressure drop, since the additional hydraulic loss remains small (~ 0.1 bar) relative to the applied pressure. Since pressure-drop penalties constitute only a small fraction of the total energy input at UHPRO conditions, conventional performance indicators such as HEI become unreliable for ranking spacer performance. The present study, therefore, has focused on local hydrodynamic and mass-transfer behavior rather than proposing a new global energy-efficiency metric; developing such a metric that integrates hydraulic, osmotic, and mechanical considerations is an important direction for future work.

Finally, in practical RO modules, concentration polarization varies along the axial direction and is typically strongest in the upstream high-flux region [29]. Under UHPRO conditions, similar qualitative trends are anticipated, and the solute concentration may exhibit non-monotonic variation due to the combined effects of axial concentration increase and a decline in permeate flux. The spacer-induced mixing mechanisms identified in this study are local in nature and are therefore expected to operate throughout the module, with their relative impact greatest in the upstream, high permeate-flux region. However, full-module simulations, which currently exceed available computational capabilities, are required to confirm this with certainty. Additionally, the numerical simulations used in this study do not consider the effects of membrane scaling and fouling. However, some insights can be drawn from the numerical predictions presented here. It has been observed that the S-tCLP spacer creates a complex flow field featuring two counter-rotating recirculation zones and a stagnation zone located between two adjacent S-tCLP holes. These stagnation zones can function as dead zones where solutes may settle and not be carried away by the flow, leading to inorganic fouling, as noted in previous experimental studies [22]. Additionally, this inorganic fouling can worsen under

UHPRO conditions, resulting in the supersaturation of the solute and potentially blocking fluid paths inside the feed channel. In contrast, the S-Gyroid spacer offers a relatively smoother flow field with smaller recirculation and stagnation zones, which reduces the risk of fouling.

Several important directions for future work arise from the present study. This study employed high-fidelity numerical simulations, and the observed hydrodynamic and permeation trends for TPMS spacers underscore the need for experimental validation using additively manufactured spacer prototypes under UHPRO conditions. Incorporating membrane compaction effects into spacer-resolved numerical simulations is another promising direction to ascertain the effects of membrane deformation and embossing. Additionally, integrating fouling and scaling models would facilitate a more comprehensive assessment of long-term operational behavior, particularly given the distinct recirculation and stagnation patterns associated with various TPMS topologies. Collectively, these extensions would build upon the positive numerical evidence presented and support the translation of TPMS spacer concepts into robust, experimentally validated designs for next-generation UHPRO modules.

7. Conclusions

This study evaluates the performance of four TPMS spacer designs as feed channel spacers under UHPRO conditions, specifically at a pressure of 200bar, with an inlet solute concentration of 100 kg/m³, and varying inlet velocities. The following conclusions are drawn from the numerical simulations conducted in this research:

- The four different spacers create distinctly different feed flow patterns inside the channel. The S-tCLP and S-Primitive spacers generate the most complex flow paths, while the S-CLP spacer results in predominantly unidirectional flow. These unique flow patterns result in varied shear stress distributions, membrane solute concentrations, and permeate velocity fields on the membrane surfaces, leading to differences in permeation and hydraulic properties.
- Under the simulated UHPRO conditions, the S-tCLP and S-Gyroid spacers yield higher permeate fluxes than the Non-Woven reference spacer of the same porosity. The flux enhancement compared to a Non-Woven spacer of the same porosity is 23.5% for the S-tCLP and 23.2% for the S-Gyroid at an inlet velocity of 0.025 m/s. Conversely, the S-CLP spacer yields a permeate flux that is 3% lower than that of the Non-Woven spacer. Additionally, the water recovery rates are highest for the S-Gyroid and S-tCLP spacers.
- Flux gains are offset by higher pressure drops for the S-tCLP and S-Gyroid spacers. The pressure drop associated with the S-tCLP spacer is 17 times that of the Non-Woven spacer, while the S-Gyroid spacer shows a 5-fold increase in pressure drop. Still, the worst-case pressure drop estimated for a 1-meter-long membrane module is less than 4% of the operating pressure. Therefore, further assessment of the impact of increased pressure drop on energy efficiency and operating costs for full membrane modules is necessary.

- The mean membrane solute concentration is observed to be lowest for the S-Gyroid and S-tCLP spacers, which is 17% lower than that of the Non-Woven spacer, indicating improved quality of the permeate. Despite comparable permeation properties of the S-Gyroid and S-Primitive spacers, the lower pressure drop of the S-Gyroid makes it the best performing spacer among those studied.

To our knowledge, this is the first systematic numerical study of TPMS spacers under UHPRO conditions. Due to the high computational costs involved, the numerical experiments are limited to single values of feed channel concentration and UHPRO pressure. Future work will extend the presented modeling framework to include (i) turbulence closure models for solute transport equation, (ii) membrane compaction effects, and (iii) fouling/scaling effects.

Appendix A. Grid Independence Study

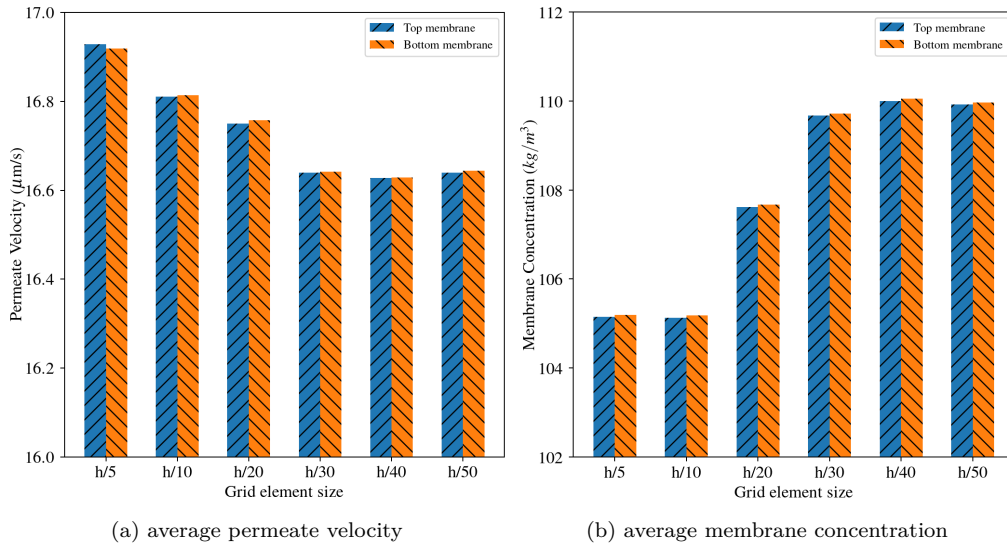


Figure A.15: Results of the grid convergence study. (a) Area-weighted average of the solution concentration on top and bottom membranes for various grids. (b) Average permeate velocity on top and bottom membranes for various grids

Grid generation for performing simulations is carried out using ANSYS Workbench 2023 R1. Tetrahedral elements are used in the core region of the feed channel, while prism cells (also known as inflation layers) are used on the membrane and spacer walls. The global growth ratio for tetrahedral and prism elements are fixed as 1.1 to ensure there are no abrupt grid size transitions. 5 inflation layers are generated to accurately capture the concentration and velocity boundary layers near the walls. The inflation layer growth is defined using the 'smooth transition' algorithm in ANSYS Workbench. The maximum skewness of the tetrahedral-prism mesh is set to 0.7 to ensure there are no bad quality elements. The mesh, consisting of tetrahedral and prism cells, is then converted into polyhedral cells to reduce the total cell count and improve solution accuracy. A grid

independence study was carried out to down-select the optimum grid element size for accurate flow computations. Six different element sizes were evaluated with varying levels of fineness defined as $h/5$ ($= 0.174\text{mm}$), $h/10$, $h/20$, $h/30$, $h/40$ and $h/50$ ($= 0.0174\text{mm}$). The total mesh element counts for these grids ranged from 0.1 million for the coarsest ($h/5$) grid to 20 million for the finest grid ($h/50$). The results of the grid independence study are shown in Figure A.15. Figure A.15(a) shows the average permeate velocity computed for a simulation with inlet velocity of 0.1 m/s and concentration of 100 kg/m^3 at feed pressure of 200 bar. The permeate velocity is seen to be over-predicted for larger element sizes ($h/5$ and $h/10$) and tends to reach an asymptotic value for finer element sizes ($h/30$ and finer grids). Similarly, Figure A.15(b) shows the average solute concentration computed on top and bottom membrane walls for the grids with different mesh element sizes. It can be observed that this value is under-predicted for coarse grids, and accurate values are obtained with finer element sizes. Based on these results, the grid with an element size of $h/30 = 0.029\text{ mm}$ is selected for performing simulations, considering both solution accuracy and computational costs. Details of the computational mesh used for each of the spacer simulations are provided in Table A.3 below.

Table A.3: Details of the spacer grids used in this study

Spacer Design	# of polyhedral cells (in millions)	# of nodes (in millions)	# of prism layers
S-Gyroid	9.59	36.34	5
S-CLP	10.05	44.17	5
S-tCLP	8.77	38.04	5
S-Primitive	13.28	48.84	5
Non-Woven	16.28	74.16	5

Appendix B. Disclaimer and Acknowledgements

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Appendix C. CRediT authorship contribution statement

Sreejith N. A.: Writing - original draft, conceptualization, methodology, validation, investigation, formal analysis. **Jishan Wu:** Writing – review & editing, Investigation **Hariswaran Sitaraman:** Writing – review & editing, Methodology, Investigation, Funding acquisition. **Marc Day:** Writing – review & editing, Supervision, Resources, Project administration, Funding acquisition. **Eric Hoek:** Writing – review & editing, Validation, Supervision, Funding acquisition.

Appendix D. Declaration of competing interests

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

Appendix E. Data availability

Data will be made available on request.

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