

Article

Topology Optimization of Hydrodynamic Grooves for Gas-Liquid Two-Phase Mechanical Face Seals in Liquid Oxygen Medium

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Abstract

Conventional parametric optimization of groove geometries for mechanical face seals is inherently constrained by predefined groove configurations, offering limited design flexibility, especially under complex gas–liquid two-phase lubrication conditions. To overcome this limitation, this study proposes a topology optimization framework specifically developed for gas–liquid two-phase lubricated turbopump mechanical face seals using liquid oxygen (LOX) as the working fluid. A finite element-based topology optimization model is established to systematically design hydrodynamic grooves under various geometric parameters and operating conditions. Numerical results demonstrate that the proposed framework exhibits strong robustness, with the optimized groove topologies being largely insensitive to the initial design guess. The final groove morphology and resulting sealing performance are governed by five key factors: groove-to-dam ratio, groove depth ratio, circumferential angle of the design domain, sealing pressure, and rotational speed. Parametric analysis indicates that the optimal groove-to-dam ratio lies in the range of 0.7–0.8, while the favorable groove depth ratio falls between 3.0 and 3.5. Compared with conventional spiral grooves having identical circumferential angles and depth ratios, the topology-optimized grooves yield significantly improved overall sealing performance, with the average liquid film opening force increased by 17.80–20.67%. The findings provide reliable theoretical foundations and practical parametric design guidelines for high-performance face seals operating under gas–liquid two-phase lubrication.

Keywords: design optimization; gas-liquid two-phase flow; topology optimization; mechanical face seal; liquid oxygen; turbopump

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1. Introduction

As indispensable core components in rotating fluid machinery, mechanical face seals are widely employed in the petrochemical, aerospace, new energy, nuclear power, and other industrial sectors. Their primary function is to reliably contain high-temperature, high-pressure, hazardous, flammable, or explosive process fluids, thereby preventing leakage-induced equipment failure, environmental contamination, and safety risks. A

typical mechanical seal consists of a rotating ring and a stationary ring that form a tribological contact interface. During operation, the contact pressure at the mating faces generates interfacial friction, which restricts medium leakage and ensures stable equipment performance.

However, under extreme service conditions—such as ultra-high rotational speeds, elevated pressures, cryogenic temperatures, and highly corrosive environments—the contacting face pairs of conventional mechanical seals suffer from insufficient lubrication, accelerated wear, and excessive heat generation. These drawbacks significantly shorten seal service life, degrade sealing efficiency, and increase leakage rates, severely compromising the reliability and operational safety of rotating fluid machinery. In contrast, non-contacting mechanical seals feature machined hydrodynamic grooves on the sealing faces. As the rotating ring spins, the fluid wedging effect creates a continuous and stable lubricating liquid film that physically separates the two rings and eliminates direct solid-solid contact. This design substantially improves interfacial lubrication, reduces friction and wear, and enhances both load-carrying capacity and sealing performance, making it particularly suitable for harsh operating environments. Consequently, non-contacting hydrodynamic mechanical seals have become a prominent research focus in tribology and sealing engineering.

Extensive studies have confirmed that the geometric configuration and dimensional parameters of hydrodynamic grooves are decisive factors influencing the performance of non-contacting seals. Key geometric variables—including groove shape, depth, width, number, and groove-to-dam ratio—directly modulate the integrity of liquid film, hydrodynamic pressure buildup, volumetric leakage, and film load-bearing capacity. Hence, the optimization of hydrodynamic groove structures is a critical pathway for improving overall sealing performance, and this has motivated considerable research efforts worldwide using various optimization approaches. Wang et al. (2021) optimized composite outer-spiral inner-herringbone grooves via orthogonal experiments and identified a balanced parameter set that reconciles sealing tightness with lubrication performance [1]. Li et al. (2023) developed a spiral-groove optimization scheme based on axiomatic design theory to reduce design randomness and uncertainty [2]. Chen et al. (2026) established a multi-objective response surface optimization model for liquid hydrogen turbopump seals to suppress medium phase transition and enhance sealing efficiency [3]. Chen et al. (2020) verified that the NSGA-II genetic algorithm outperforms exhaustive enumeration in multi-condition groove optimization [4]. Ma et al. (2020) and Xu et al. (2022) respectively optimized spiral groove geometric parameters using orthogonal arrays and genetic algorithms to restrain fluid vaporization and reduce leakage flux [5,6].

Despite the performance gains achieved through these parametric strategies, nearly all existing studies rely on predefined fixed groove topologies (e.g., spiral, herringbone, or T-shaped textures) and merely fine-tune their geometric dimensions. This paradigm inherently limits design freedom and fails to fully exploit the load-bearing potential of the sealing face surface.

As an advanced generative design technique, topology optimization fundamentally differs from parametric optimization: it iteratively determines the optimal material or fluid distribution within a prescribed design domain without requiring a predefined structural layout. Since Michell pioneered truss topology optimization theory in 1904 [7], mature algorithms such as SIMP [8], level-set [9], and ESO [10] have been widely adopted in structural mechanics and fluid lubrication design, achieving remarkable results. Fesanghary et al. (2012) optimized thrust bearing groove depths using SQP gradient-based optimization [11], while Waseem et al. (2016) realized high-precision micro-texture design through homogenization-driven topology optimization [12]. Ostayen (2010) and Codrignani et al. (2020) incorporated adjoint sensitivity analysis and cavitation models to

improve the accuracy of hydrodynamic groove design [13,14]. Kong et al. (2025) and Zhang et al. (2025) separately optimized sliding bearing surface textures using SIMP and MMV topology optimization frameworks [15,16]. Kalliorinne et al. (2020, 2021) investigated the parametric dependence of bearing performance via MMA-based topology optimization for compressible and incompressible flow regimes [17–19].

Meng's research group pioneered the integration of reaction-diffusion equation-based topology optimization into mechanical seal groove design, offering an innovative technical route for texture generation on sealing faces [20–22]. Meanwhile, Wang et al. (2014) and Meng et al. (2021, 2025) developed a homogeneous two-phase phase-change model to characterize the vaporization-condensation behavior of liquid oxygen (LOX), providing a robust numerical tool for gas–liquid two-phase seal simulations [23–25].

Liquid oxygen readily vaporizes under low local pressure, resulting in coexisting gas and liquid phases across the sealing interface. However, most existing seal groove studies adopt parametric optimization with fixed groove geometries and lack the flexibility for free-form design under cryogenic two-phase conditions; moreover, traditional two-phase seal models do not account for the coupling between phase transition and topology evolution. Targeting turbopump mechanical face seals using LOX as the working medium, this paper establishes a topology optimization model that maximizes the load-carrying capacity of the two-phase liquid film while accounting for LOX phase transition effects. This study innovatively couples reaction-diffusion topology optimization with a homogeneous gas–liquid phase-change model for LOX, enabling adaptive generation of optimal groove topologies under two-phase lubrication and providing quantitative parametric design guidelines for cryogenic seal grooves. The novelty is clearly distinguished from previous works. Finite element simulations quantitatively evaluate the individual influences of geometric parameters (groove-to-dam ratio, groove depth ratio, circumferential design angle) and operating conditions (sealing pressure, rotational speed) on the optimized groove configurations. Finally, the sealing performance of the topology-generated grooves is benchmarked against that of conventional spiral grooves to validate the superiority of the proposed design.

2. Mechanical Calculation Model

2.1. Geometric Model

Figure 1 depicts the geometric model adopted in this study. Figure 1a presents the full three-dimensional assembly of a representative hydrodynamic mechanical seal, comprising a rotating ring, a stationary ring, and an ultrathin liquid film confined between the two mating faces. Shallow hydrodynamic grooves are machined on the end face of the rotating ring. The fluid wedging effect within these grooves enhances the film load capacity, mitigates interfacial friction and wear, and simultaneously reduces medium leakage. Consequently, the geometric morphology and dimensional parameters of the shallow grooves on the rotating face are dominant factors governing the overall sealing performance of hydrodynamic non-contacting seals.

The hydrodynamic grooves are periodically arranged along the circumferential direction on the rotating ring face. To streamline topology optimization computations and improve numerical efficiency, a single fan-shaped periodic sector (Figure 1b) is extracted as the design domain. In this schematic, r_o , r_g , and r_i denote the outer seal radius, groove root radius, and inner radius, respectively; ω indicates the rotational direction of the rotating ring. Boundary Γ_1 is subjected to the high sealing pressure, while Γ_2 corresponds to atmospheric backpressure. Periodic boundary conditions are imposed on Γ_3 and Γ_4 to replicate the circumferentially repeated groove layout.

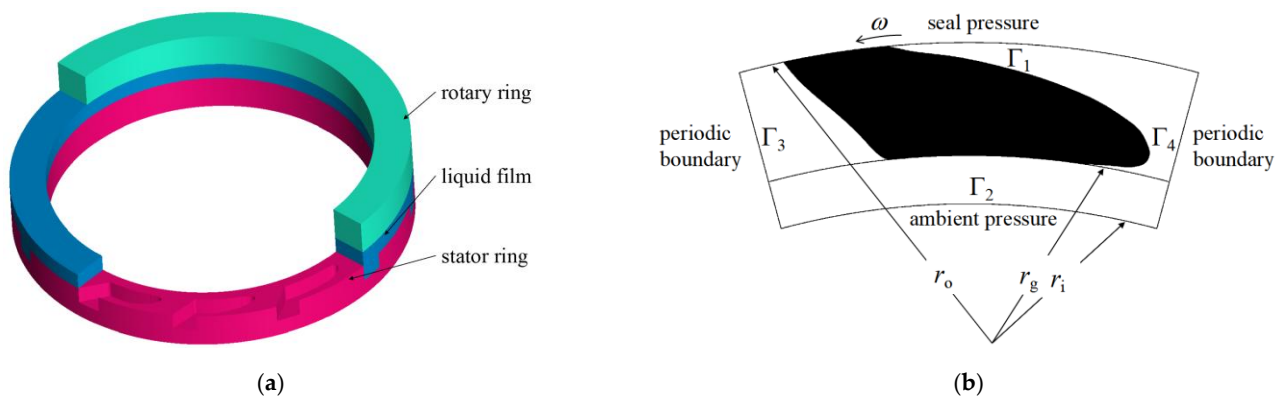


Figure 1. Schematic of the seal geometric model. (a) Three-dimensional full assembly model. (b) Single fan-shaped periodic design domain.

2.2. Topology Optimization Formulation

To facilitate a concise mathematical description of the groove profile evolution, the following physical assumptions are introduced:

1. The seal mating faces are perfectly flat and axially aligned;
2. The liquid film thickness is negligibly small, and pressure and fluid property gradients across the film thickness are neglected;
3. The fluid film maintains steady, isothermal, laminar flow;
4. No velocity slip occurs at the gas–liquid interface; gaseous oxygen is treated as an ideal compressible fluid;
5. Viscous heat dissipation within the thin film is disregarded.

Based on the homogeneous two-phase lubrication framework proposed by Wang et al. [23], a topology optimization model for hydrodynamic seal grooves is established with the design variable ϕ , and the optimization objective is to maximize the liquid film opening force. The mathematical statement is formulated as follows:

$$\min_{\phi} J(\phi) = -F_{\text{open}} = -\iint_{\Omega} p d\Omega, \quad \phi \in [0,1] \quad (1)$$

where F_{open} is the liquid film opening force that separates the seal faces; p is the local fluid film pressure; $\Omega = 2D$ denotes the two-dimensional computational domain of the interfacial liquid film; and ϕ is the continuous design variable that modulates the local film thickness, bounded between 0 and 1.

A rational material property interpolation scheme [25] is adopted to correlate the design variable ϕ with the physical liquid film thickness h :

$$h = h_0 + h_g \frac{\phi}{1 + m(1 - \phi)} \quad (2)$$

where h_0 is the nominal baseline film thickness over the non-grooved land regions (i.e., the clearance between the rotating and stationary rings); h_g is the physical groove depth; and m is a penalty coefficient fixed at $m = 5$.

Equation (2) yields clear binary physical interpretations: $\phi = 1$ corresponds to full-depth groove zones with a film thickness of $h_0 + h_g$, whereas $\phi = 0$ represents flat land regions with a thickness of h_0 . During iterative optimization, the penalty term m drives intermediate design states ($0 < \phi < 1$) to converge asymptotically toward either 0 or 1, ultimately yielding manufacturable groove topologies with distinct and smooth boundaries upon convergence.

2.3. Gas–Liquid Two-Phase Reynolds Governing Equation

Under the aforementioned model assumptions, the interfacial fluid flow is governed by a coupled system comprising the homogeneous Reynolds equation (Equation (3)) and the two-phase mass transfer equation (Equation (4)):

$$-\nabla \cdot \left(\frac{\rho h^3}{12\mu} \nabla p \right) + \frac{1}{2} \mathbf{U} \cdot \nabla (\rho h) = 0 \quad (3)$$

$$\nabla \cdot \left[F_l \left(\frac{h^2}{12\mu} \nabla p - \frac{1}{2} \mathbf{U} \right) \right] - \frac{F_l(1-F_l)}{p} \left[\nabla p \cdot \left(\frac{h^2}{12\mu} \nabla p - \frac{1}{2} \mathbf{U} \right) \right] = - \left(\frac{1-F_l}{\rho_l} + \frac{F_l}{\rho_g} \right) S \quad (4)$$

where $\mathbf{U}$ is the fluid velocity vector; ρ is the mixture fluid density; μ is the dynamic viscosity of the gas–fluid mixture; and F_l is the liquid volume fraction.

The effective density and viscosity of the homogeneous two-phase mixture are weighted by the liquid fraction:

$$\rho = F_l \rho_l + (1 - F_l) \rho_g \quad (5)$$

$$\mu = F_l \mu_l + (1 - F_l) \mu_g \quad (6)$$

where the subscripts l , and g denote the liquid oxygen and gaseous oxygen phases, respectively.

The gas density obeys the ideal gas equation of state: $\rho_g = p/(RT)$. The source term S quantifies the volumetric mass transfer rates induced by LOX vaporization and condensation, characterizing the intensity of interphase mass exchange within the thin film. For vaporization (liquid-to-gas phase transition), the mass source term driven by bubble growth is formulated as:

$$S = -C_1 N \rho_g 4\pi R_b^2 |\dot{R}_b| \quad (7)$$

For condensation (gas-to-liquid phase transition):

$$S = C_2 N \rho_g 4\pi R_b^2 |\dot{R}_b| \quad (8)$$

where $R_b = 10^{-6}$ m is the characteristic bubble radius; C_1 and C_2 are empirical vaporization and condensation rate coefficients, set equal via:

$$C_1 = C_2 = C = 0.05 \frac{|p - p_{\text{sat}}|}{p_{\text{sat}}} \quad (9)$$

Neglecting surface tension and viscous damping terms and applying a first-order approximation to the Rayleigh–Plesset bubble dynamics equation yields the bubble growth rate $\dot{R}_b$:

$$\dot{R}_b = \sqrt{\frac{2|p_{\text{sat}} - p|}{3\rho_l}} \quad (10)$$

where p_{sat} is the saturation vapor pressure of liquid oxygen at the specified operating temperature. The instantaneous bubble number density N is defined piecewise based on the local liquid fraction and pressure:

$$N = \begin{cases} \frac{3F_l}{4\pi R_b^3}, p < p_{\text{sat}} \\ \frac{3(1-F_l)}{4\pi R_b^3}, p > p_{\text{sat}} \end{cases} \quad (11)$$

Dirichlet boundary conditions for pressure and liquid volume fraction are imposed at the seal inner and outer radii:

$$\begin{cases} r = r_i, p = p_a, F_l = \begin{cases} 1, p_a > p_{\text{sat}} \\ 0, p_a \leq p_{\text{sat}} \end{cases} \\ r = r_o, p = p_s, F_l = \begin{cases} 1, p_s \geq p_{\text{sat}} \\ 0, p_s < p_{\text{sat}} \end{cases} \end{cases} \quad (12)$$

Under the present LOX operating conditions, the mass transfer equation (Equation (4)) is convection-dominated, with large convective flux magnitudes that introduce severe numerical oscillations during finite element solution. To stabilize the discretized system, the Streamline Upwind/Petrov–Galerkin (SUPG) method is implemented to suppress spurious oscillations arising from phase-change gradients. Since both the Reynolds and mass transfer equations exhibit strong nonlinearity, the Newton–Raphson iterative scheme is adopted for their coupled solution. The complete numerical solution workflow is outlined in Figure 2, with key steps summarized as follows:

1. Discretize the fan-shaped design domain (Figure 1b) using triangular finite element meshes;
2. Initialize the liquid film pressure field p and liquid volume fraction F_l over the entire domain;
3. Solve the coupled Reynolds and mass transfer equations via Newton iteration to update the distributions of pressure and liquid fraction;
4. Recalculate the mixture density ρ and viscosity μ using Equations (5) and (6);
5. Evaluate the relative iterative errors for the pressure and liquid fraction fields to check convergence. If the convergence criteria are satisfied, terminate computation; otherwise, return to Step 3 for subsequent iterations.

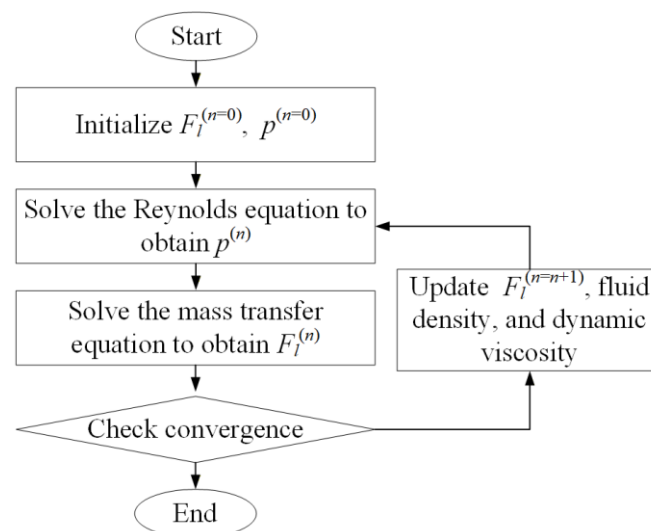


Figure 2. Flowchart of the coupled solution algorithm for gas–liquid two-phase Reynolds equations.

2.4. Adjoint Equations and Design Sensitivity Analysis

To solve the constrained minimization problem stated in Equation (1), a Lagrangian functional $L(\phi, p, v)$ is constructed to transform the equality-constrained optimization into an unconstrained formulation:

$$L(\phi, p, v) = - \iint_{\Omega} p d\Omega + \iint_{\Omega} v \left[-\nabla \cdot \left(\frac{\rho h^3}{12\mu} \nabla p \right) + \frac{1}{2} U \cdot \nabla(\rho h) \right] d\Omega \quad (13)$$

where v denotes the adjoint state variable.

The Fréchet derivative of L with respect to the primal pressure p yields the variational residual that serves as the starting point for deriving the adjoint system:

$$\left\langle \frac{\partial L}{\partial p}, \delta p \right\rangle = - \iint_{\Omega} \delta p d\Omega + \iint_{\Omega} v \cdot \left[-\nabla \cdot \left(\frac{h^3}{12\mu} \delta(\rho \nabla p) \right) + \frac{1}{2} U \cdot \nabla(\delta \rho h) \right] d\Omega \quad (14)$$

Applying integration by parts together with the divergence theorem converts Equation (14) into a volume integral supplemented by boundary flux terms, as shown in Equation (15):

$$\begin{aligned} \left\langle \frac{\partial L}{\partial p}, \delta p \right\rangle = & \iint_{\Omega} \left[-1 + \frac{h^3}{12\mu} \frac{\partial \rho}{\partial p} \nabla p \cdot \nabla v - \nabla \left(\frac{\rho h^3}{12\mu} \nabla v \right) - \frac{1}{2} \frac{\partial \rho}{\partial p} U h \nabla v \right] \delta p d\Omega \\ & + \int_{\Gamma_1 \cup \Gamma_2} \left[\nabla v \frac{h^3}{12\mu} \rho + \frac{1}{2} U v h \frac{\partial \rho}{\partial p} - v \frac{h^3}{12\mu} \nabla p \frac{\partial \rho}{\partial p} \right] \delta p \cdot n ds - \int_{\Gamma_1 \cap \Gamma_2} v \frac{h^3}{12\mu} \rho \nabla(\delta p) \cdot n ds \end{aligned} \quad (15)$$

Substituting the partial density derivative $\frac{\partial \rho}{\partial p} = \frac{F_g}{RT} = \frac{1-F_l}{RT}$, which follows from the

ideal gas law and Equation (5), into the residual leads to Equation (16):

$$\begin{aligned} \left\langle \frac{\partial L}{\partial p}, \delta p \right\rangle = & \iint_{\Omega} \left[-1 + \frac{h^3}{12\mu} \frac{1-F_l}{RT} \nabla p \cdot \nabla v - \nabla \left(\frac{\rho h^3}{12\mu} \nabla v \right) - \frac{1}{2} \frac{1-F_l}{RT} U h \nabla v \right] \delta p d\Omega \\ & + \int_{\Gamma_1 \cup \Gamma_2} \left[\nabla v \frac{h^3}{12\mu} \rho + \frac{1}{2} U v h \frac{1-F_l}{RT} - v \frac{h^3}{12\mu} \nabla p \frac{1-F_l}{RT} \right] \delta p \cdot n ds - \int_{\Gamma_1 \cap \Gamma_2} v \frac{h^3}{12\mu} \rho \nabla(\delta p) \cdot n ds \end{aligned} \quad (16)$$

Setting this variational residual to zero and imposing homogeneous Dirichlet adjoint boundary conditions on $\Gamma_1 \cup \Gamma_2$ yields the strong-form adjoint governing system:

$$\begin{cases} -1 + \frac{h^3}{12\mu} \frac{1-F_l}{RT} \nabla p \cdot \nabla v - \nabla \left(\frac{\rho h^3}{12\mu} \nabla v \right) - \frac{1}{2} \frac{1-F_l}{RT} U h \nabla v = 0 & \text{in } \Omega \\ v = 0 & \text{on } \Gamma_1 \cup \Gamma_2 \end{cases} \quad (17)$$

Once the primal and adjoint solutions have converged, the total derivative of the Lagrangian with respect to the design variable ϕ is evaluated to extract the design sensitivity information, which quantifies how small perturbations in ϕ affect the objective function:

$$\frac{\partial L}{\partial \phi} = \left[-\frac{h^2}{4\mu} \rho \nabla p \cdot \nabla v + \frac{1}{2} U \rho \nabla v \right] \frac{h_g(1+m)}{[1+m(1-\phi)]^2} \quad (18)$$

2.5. Reaction-Diffusion Topology Update Equation

Equation (18) clearly confirms the strong coupling between the groove topology and the continuous design field ϕ . The evolution of ϕ over successive optimization iterations is governed by reaction-diffusion partial differential equations that incorporate the computed sensitivity field. Two variants of the reaction-diffusion formulation are implemented to accommodate distinct groove manufacturing requirements for the grooves: a classical single-well formulation for variable-depth groove generation, and an improved double-well potential formulation for uniform-depth, sharp-boundary grooves.

The classical reaction-diffusion equation is expressed as

$$\begin{cases} \frac{\partial \phi}{\partial t} = \kappa \nabla^2 \phi + \frac{1}{c} \frac{\partial L}{\partial \phi}, & \text{in } \Omega \\ \frac{\partial \phi}{\partial n} = 0, & \text{on } \Gamma_1 \cup \Gamma_2 \end{cases} \quad (19)$$

where t is a pseudo-time variable tracking the topology evolution, κ is the diffusion coefficient controlling interface smoothness, and $c = L_2$ denotes the norm of the sensitivity field for numerical normalization. The reaction term drives the topology toward higher load capacity under the guidance of sensitivity gradients, while the diffusion term regularizes irregular groove boundaries and suppresses numerical noise. The magnitude of κ is mesh-dependent: finer discretization requires smaller diffusion coefficients to preserve fine topological features.

Although Equation (19) efficiently evolves groove layouts, it inherently produces spatially varying groove depths because of unconstrained intermediate values of ϕ . To satisfy the stringent uniform-depth manufacturing requirements for LOX turbopump seals, we adopt a modified reaction-diffusion equation that incorporates a double-well potential [26]:

$$\begin{cases} \frac{\partial \phi}{\partial t} = \kappa \nabla^2 \phi - b g'(\phi) + 30 \cdot g(\phi) \cdot \frac{1}{c} \frac{\partial L}{\partial \phi} & \text{in } \Omega \\ \frac{\partial \phi}{\partial n} = 0 & \text{on } \Gamma_1 \cup \Gamma_2 \end{cases} \quad (20)$$

with the double-well potential function defined as $g(\phi) = \phi^2(1 - \phi)^2$. This function attains its global minima at $\phi = 0$ (land zones) and $\phi = 1$ (groove zones). The coefficient b amplifies the penalization of intermediate design states ($0 < \phi < 1$), forcing the ϕ field to converge sharply toward binary values. This formulation delivers two critical improvements: it homogenizes the groove depth across all grooved regions and narrows the transitional zones between land and groove, yielding crisp binary topologies with uniform machining depth that are ideal for seal fabrication.

2.6. Full Topology Optimization Workflow

Triangular meshes discretize the fan-shaped periodic domain (Figure 1b). The finite element framework sequentially solves the Reynolds equation, mass transfer equation, adjoint equation, and reaction-diffusion update equation. The complete two-loop iterative optimization pipeline is visualized in Figure 3:

Loop 1: Variable-depth groove topology optimization via classical reaction-diffusion (Equation (19)):

1. Initialize the design variable field ϕ over the entire design domain Ω ;
2. Solve the coupled primal flow equations (Reynolds + mass transfer) and the adjoint Equation (17);
3. Compute the objective function sensitivity $\partial L / \partial \phi$ from Equation (18);
4. Discretize Equation (19) using implicit Euler time integration and finite elements to update ϕ ; clamp all design variables within $[0,1]$ via $\phi = \max(0, \min(1, \phi))$;
5. Repeat iterations until the relative change in the ϕ field between successive steps drops below 0.1%. Upon convergence, exit Loop 1.

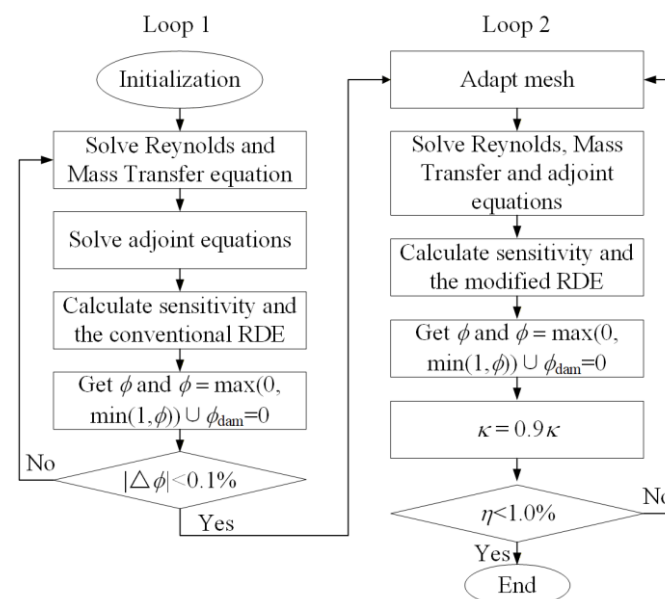


Figure 3. Integrated flowchart of gas–liquid two-phase hydrodynamic groove topology optimization.

Loop 2: Uniform-depth groove refinement via double-well reaction-diffusion (Equation (20)). The main calculation steps are as follows:

1. Apply adaptive local mesh refinement along predicted groove boundaries and reduce the diffusion coefficient κ to resolve fine topological features;
2. Resolve the flow, adjoint, and sensitivity fields;
3. Update ϕ via Equation (20) and re-clamp variables to the interval $[0,1]$;
4. Calculate convergence metric η :

$$\eta = \frac{\iint_{\Omega} \phi(1 - \phi) d\Omega}{\iint_{\Omega} d\Omega} \times 100\% \quad (21)$$

Terminate iterations when $\eta < 1\%$. Smaller η indicates fewer intermediate design states, more uniform groove depth, and sharper land-groove interfaces.

3. Results and Discussion

Numerical parametric studies are conducted on LOX turbopump seals, which are susceptible to significant vaporization, to systematically evaluate the proposed topology optimization framework. Table 1 summarizes the baseline geometric dimensions, operating parameters, finite element mesh settings, diffusion coefficient, and thermophysical properties of liquid and gaseous oxygen. Subsequent subsections quantitatively investigate the influences of initial topology guesses, geometric design parameters, and operational conditions on the optimized groove morphology and sealing performance. Orthogonal array experiments are additionally employed to identify optimal combined parametric schemes, followed by a direct performance comparison with conventional spiral grooves.

Table 1. Baseline geometric dimensions, operating parameters, and fluid thermophysical properties.

Parameter	Symbol (Unit)	Value	Parameter	Symbol/Unit	Value
Sealing supply pressure	p_s (MPa)	3.0	Back atmospheric pressure	p_a (MPa)	0.1
Seal outer radius	r_o (mm)	55	Seal inner radius	r_i (mm)	45
Nominal baseline film thickness	h_0 (μm)	2.5	Groove physical depth	h_g (μm)	7.5
Groove-to-dam ratio	ζ	0.7	Groove depth ratio	ξ	3.0
Sector circumferential angle	α	$\pi/6$	Rotational speed	n (r/min)	30,000
LOX Saturation vapor pressure	p_{sat} (MPa)	1.75	Liquid oxygen density	ρ_g (kg/m^3)	902.48
LOX dynamic viscosity	μ_l (Pa·s)	77.56×10^{-6}	Gaseous oxygen viscosity	μ_g (Pa·s)	10.45×10^{-6}
Operating temperature	T (K)	130	Gas constant for oxygen	R (J·kg·T)	260
Total triangular mesh count	-	45431	Diffusion coefficient	κ	0.005

3.1. Verification of the Proposed Method

To validate the governing equations and the optimization algorithm developed in this paper, the infinite-width bearing example reported in Ref. [17] is selected as a benchmark for topology optimization verification. The reference employs the Method of Moving Asymptotes (MMA) in conjunction with the built-in optimization module of COMSOL 6.3 Multiphysics for numerical computation. For groove-to-dam ratios of 0.4, 0.5, 0.6, and 0.7, the bearing opening forces obtained in Ref. [17] are 12.355 kN, 14.001 kN, 14.937 kN, and 15.538 kN, respectively. In comparison, the opening forces predicted by the proposed approach are 12.185 kN, 13.797 kN, 14.731 kN, and 15.324 kN, yielding a maximum relative error of only 1.48%. These comparative results confirm that the proposed algorithm provides reliable prediction accuracy, thus rendering it suitable for topology optimization of end-face groove configurations in gas-lubricated mechanical seals.

3.2. Mesh Density Selection

In finite element simulation, the discretization scale of triangular meshes (i.e., the total number of elements) exerts a decisive influence on both the accuracy of structural optimization results and the numerical computational efficiency. Figure 4 illustrates the performance response of the optimized grooves under varying mesh densities. The results show that the gas film opening force F_{open} and the groove area ratio AR increase monotonically with a gradual rise in the total element count, while the computation time t increases correspondingly. Once the number of mesh elements exceeds 45,431, the rate of

change of the key output parameters (including F_{open} and AR) decreases markedly with only mild fluctuations, indicating that the computational results have entered a stable convergence regime. At this stage, further mesh refinement yields only marginal gains in precision but substantially raises the computational cost. Therefore, after a comprehensive trade-off between computational accuracy and operational efficiency, the mesh discretization scheme with 45,431 elements is ultimately adopted as the standard computational domain for the present model [27].

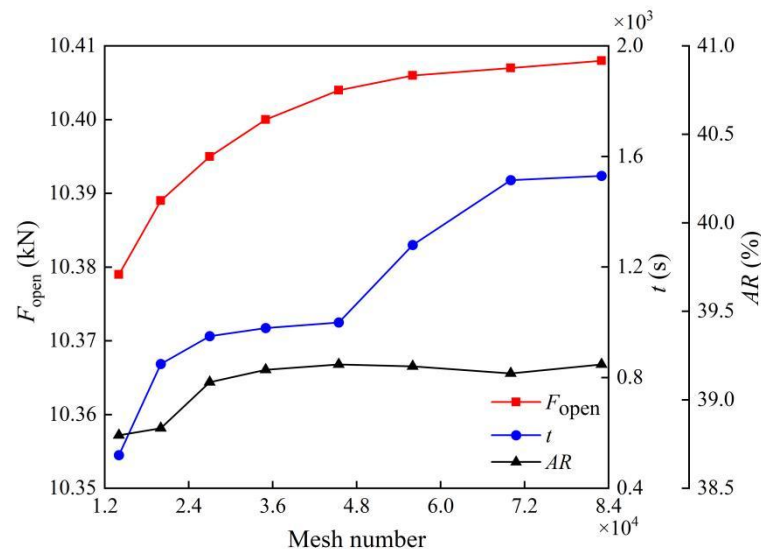


Figure 4. Effect of mesh number.

3.3. Effect of Initial Topology Structure

Six distinct initial design configurations (Cases 1–6) are examined to assess the robustness of the proposed framework against different starting topologies under gas–liquid two-phase LOX conditions: Cases 1 and 2 adopt uniform global guesses of $\phi = 0.5$ and $\phi = 1.0$, respectively, while Cases 3–6 embed localized subdomains shaped as semi-circular, right triangular, linear strip, and circular holes. Figure 5 tracks the topology evolution for all six initializations. Regardless of the starting layout, all cases converge to groove structures with highly consistent macroscopic geometric features: an inclined straight segment on the upstream side, a concentric arc near the inner seal radius, and an irregular curved contour along the outer radius. Minor local density discrepancies exist between the globally uniform initial guesses (Cases 1–2) and the patterned local initializations (Cases 3–6), yet all optimized layouts align closely after circumferential periodic assembly.

Figure 6 quantitatively compares the dimensionless opening force $\bar{F}_{\text{open}}$, the dimensionless volumetric leakage rate $\bar{Q}$, and the grooved area fraction across the six converged topologies, where $\bar{F}_{\text{open}} = F_{\text{open}}/[\pi p_s(r_o^2 - r_i^2)]$, $\bar{Q} = Q/[\frac{1}{2}p_{\text{sat}}n(r_o^2 - r_i^2)h_0]$. The three performance metrics exhibit only marginal deviations among the cases; minor discrepancies arise from the inherent search characteristics of the gradient-based optimization algorithm. In all converged results, grooved regions are localized to high-liquid-fraction zones, where the liquid phase suppresses abrupt geometric distortions induced by gas compressibility and maintains smooth groove boundaries. Low-liquid-fraction regions predominantly concentrate along the seal inner radius. These observations confirm that the developed two-phase topology optimization model possesses excellent robustness with respect to initial guesses, reliably converging to consistent high-performance groove layouts from arbitrarily different starting topologies.

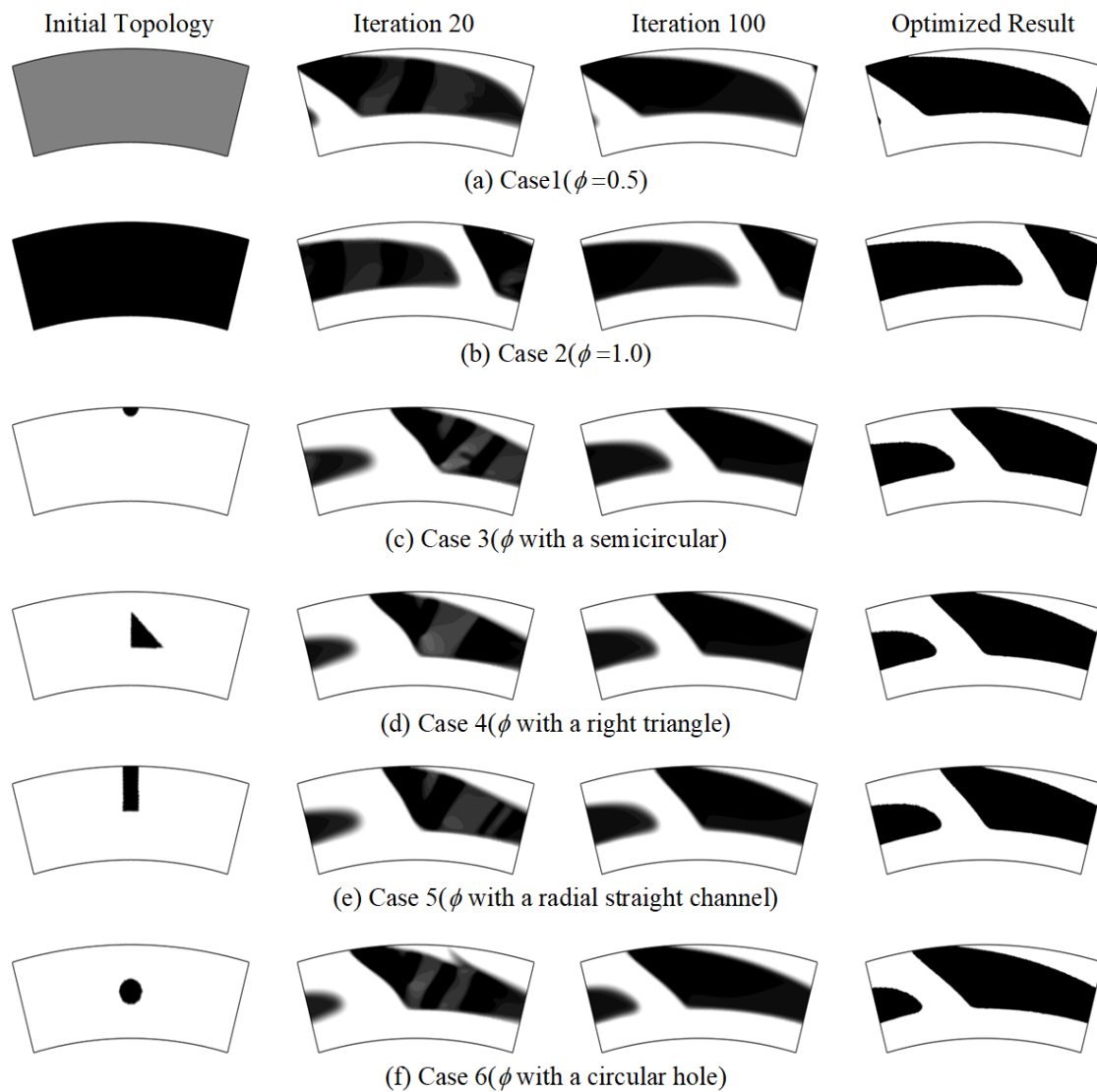


Figure 5. Topology evolution trajectories starting from six distinct initial guess configurations.

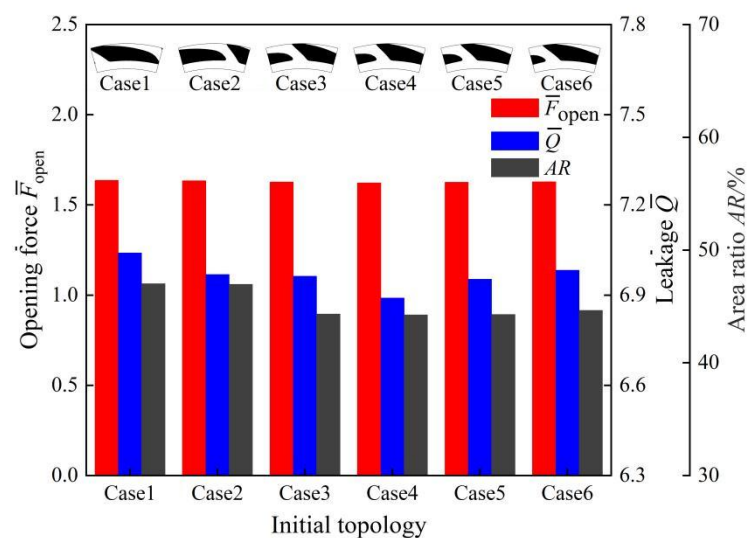


Figure 6. Influence of different initial topology configurations on sealing performance and groove area fraction.

3.4. Influence of Geometric Design Parameters

Figure 7 illustrates how varying the groove-to-dam ratio $\zeta = (r_o - r_g)/(r_o - r_i)$ modulates the optimized groove morphology, opening force, and leakage flux. The liquid film opening force increases monotonically with ζ , yet the growth rate diminishes markedly for $\zeta > 0.8$, and the load capacity plateaus beyond this threshold. Increasing ζ from 0.7 to 0.8 yields negligible opening force improvement, indicating the effective upper bound of usable groove width within the fixed design sector. Volumetric leakage rises continuously with ζ , peaking at $\zeta = 0.9$. Geometrically, discrete multiple grooves within each periodic sector progressively merge into a single continuous groove as ζ increases, accompanied by expanded circumferential groove coverage. These trends demonstrate that the groove-to-dam ratio exerts dominant control over the optimized groove topology, with a clear upper design limit beyond which load capacity saturates.

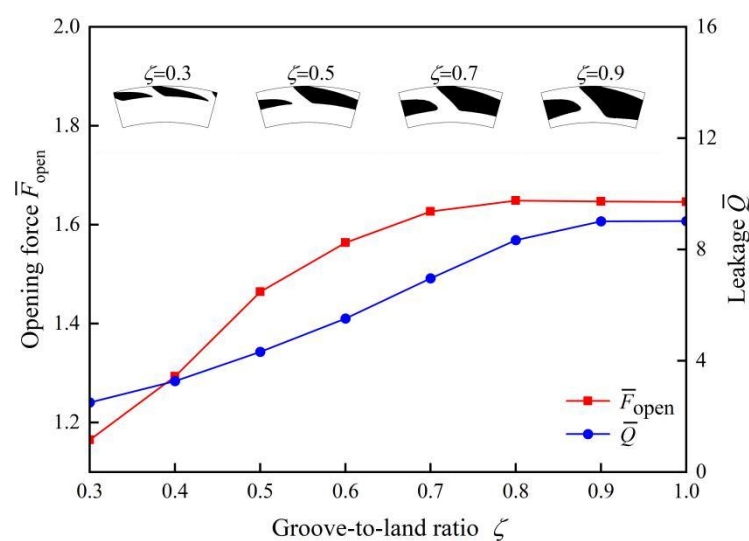
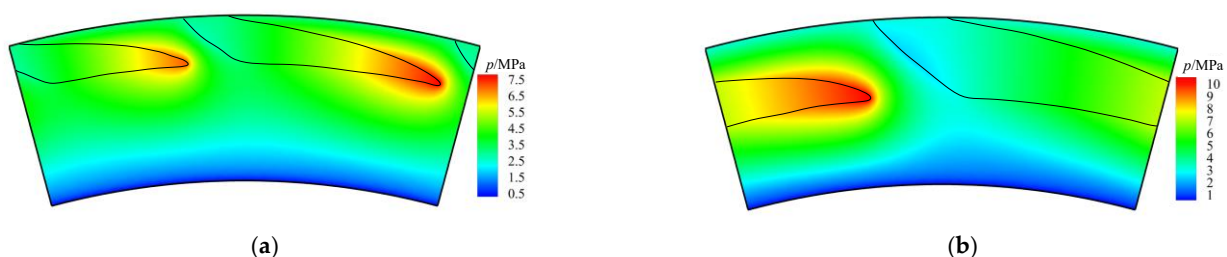


Figure 7. Variation of sealing performance and groove morphology with groove-to-dam ratio ζ .

Figure 8 displays pressure contour maps for four representative groove-to-dam ratios. Under LOX two-phase conditions, fluid pressure naturally decreases radially inward from the high-pressure outer seal radius to the low-pressure inner radius, with peak hydrodynamic pressure concentrated at the trailing edge of the topology-optimized grooves. At low ζ , the optimization algorithm generates two separate narrow grooves per sector to maximize the integrated opening force; cooperative hydrodynamic wedging from dual grooves sustains elevated pressure near the outer radius. Once $\zeta \geq 0.5$, the peak pressure magnitude plateaus, while the overall domain pressure levels continue to rise with larger groove coverage. This transition reveals that low groove-to-dam ratios prioritize peak pressure amplification, whereas higher ratios elevate the average film pressure across the entire sealing face. The groove-to-dam ratio therefore constitutes a critical tuning parameter for both the pressure field distribution and the final groove geometry in two-phase seal topology optimization.



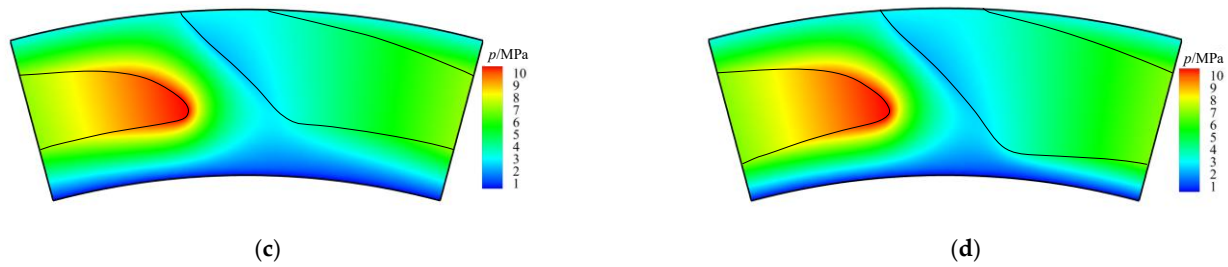


Figure 8. Interfacial liquid film pressure distributions under different groove-to-dam ratios. (a) $\zeta = 0.3$. (b) $\zeta = 0.5$. (c) $\zeta = 0.7$. (d) $\zeta = 0.9$.

Figure 9 quantifies the impact of the groove depth ratio $\xi = h_g/h_0$ on sealing performance and grooved area fraction. Both the opening force and leakage rate rise to distinct maxima within the range $2.5 \leq \xi \leq 3.0$, followed by gradual declines as the depth ratio further increases. As ξ grows, the radial and circumferential groove extents expand steadily, and the grooved area fraction increases at a decelerating rate, signifying groove geometry stabilization above a critical depth threshold. The observed performance trends verify that the groove depth ratio strongly regulates both the load capacity and leakage, as well as the fundamental geometric outline of the optimized textures.

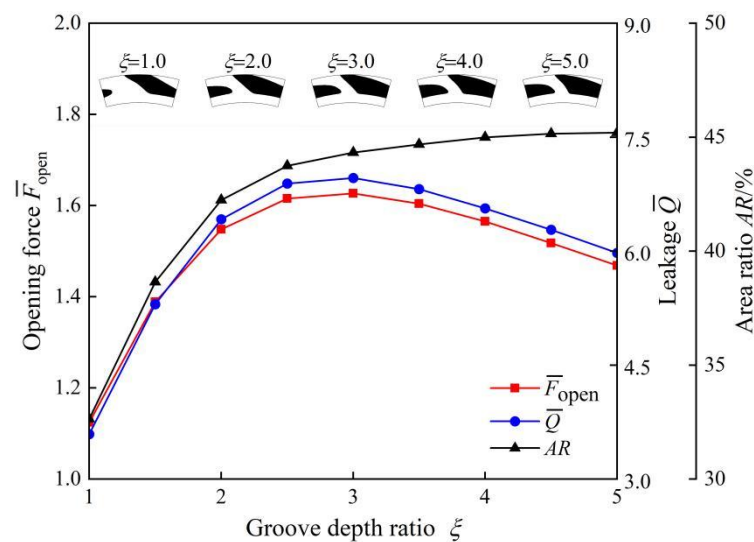


Figure 9. Effect of groove depth ratio ξ on sealing performance and groove area fraction.

Figure 10 presents performance variations with the fan-shaped design domain circumferential angle α ; a larger α corresponds to fewer repeating grooves around the full seal circumference. The opening force exhibits a non-monotonic trend: it first declines, then rises to a global maximum at $\alpha = 2\pi/9$ (equivalent to nine identical circumferential grooves), before decaying again at larger angles. The leakage flux evolves inversely relative to the opening force: small opening force reductions coincide with sharp leakage drops, while major opening force gains accompany mild leakage increases. Geometrically, the optimized grooves transform from slender narrow strips to broad wedge-shaped textures as the sector circumferential angle expands.

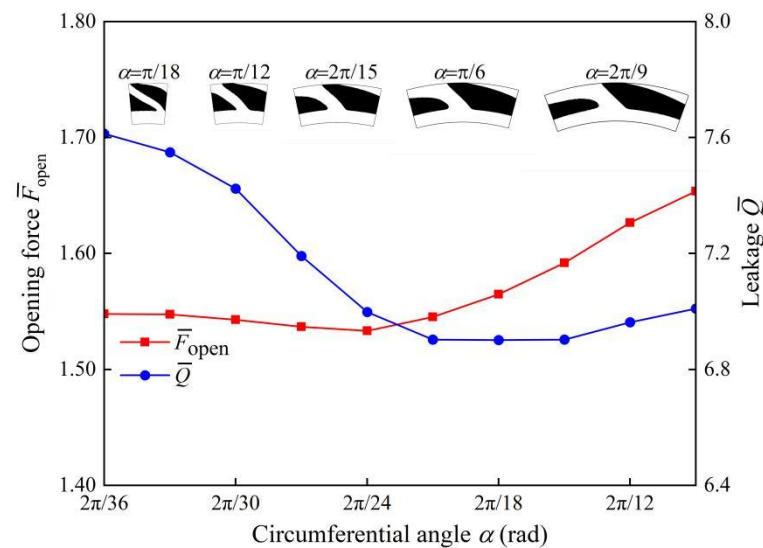


Figure 10. Influence of design domain circumferential angle α on sealing performance and groove layout.

3.5. Influence of Operating Parameters

Figure 11 plots the nearly linear growth of opening force, leakage rate, and grooved area fraction with rising supply pressure, featuring a distinct slope transition at $p_s = 1.5$ MPa. For pressures below 1.5 MPa, the sealing domain is dominated by gaseous oxygen, yielding weak hydrodynamic wedging and low liquid film load capacity. As the supply pressure increases, the optimized grooves extend radially outward to enhance hydrodynamic pressure buildup, directly boosting the overall sealing performance. These results highlight that maintaining a predominantly liquid oxygen film on the mating faces substantially elevates the opening force.

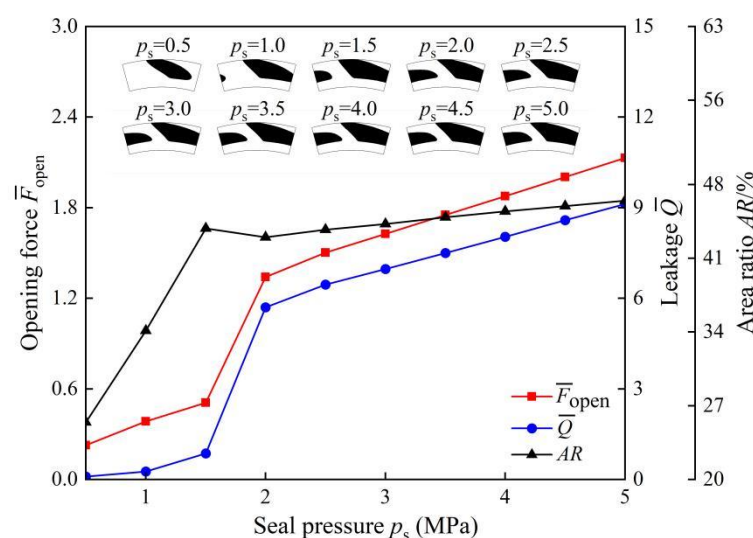


Figure 11. Variation of groove geometry and sealing performance with inlet sealing pressure p_s .

Phase distribution contours at four representative supply pressures are provided in Figure 12. At $p_s = 1.0$ MPa, the entire film domain remains gaseous, with only localized condensation at the groove trailing edges driven by rotational hydrodynamic compression, resulting in very low liquid volume fractions. Elevating p_s expands the condensed liquid zones circumferentially toward the seal inner radius. When $p_s = 2.0$ MPa exceeds the LOX saturation pressure, the film is fully liquid across most of the domain; however,

the convergent-divergent wedge formed by the rotating grooves generates low-pressure recirculation zones upstream of each groove, triggering localized vaporization. Further pressure increments suppress this low-pressure vaporization region by raising the baseline fluid pressure above saturation everywhere on the face. The phase distribution maps confirm strong coupling between the inlet sealing pressure and LOX vaporization-condensation dynamics, with a clear critical pressure threshold governing the bulk phase state.

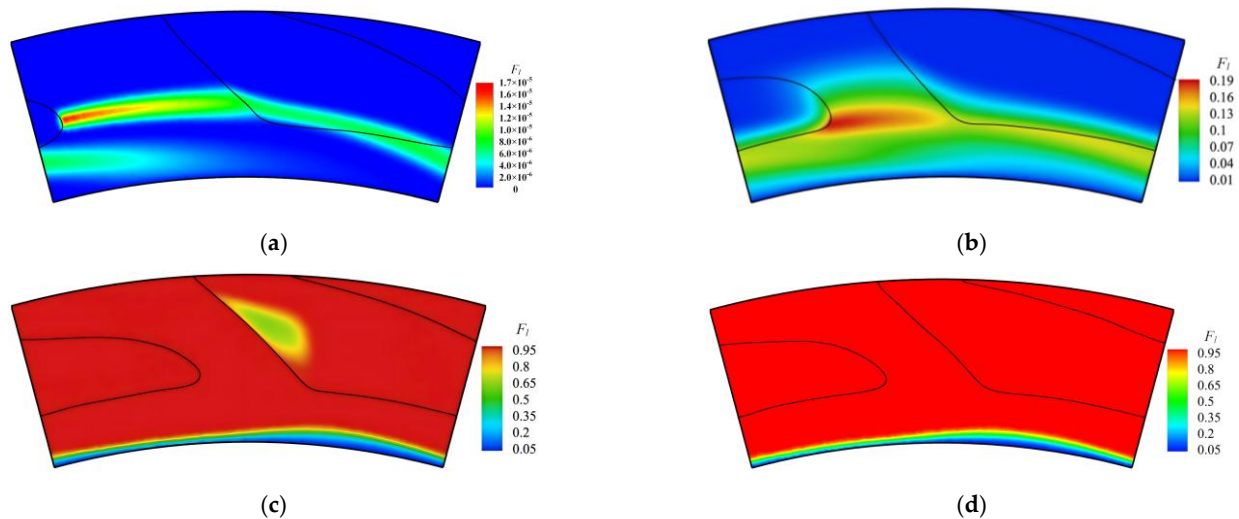


Figure 12. Liquid volume fraction phase contours under varying inlet sealing pressures. (a) $p_s = 1.0$ MPa. (b) $p_s = 1.5$ MPa. (c) $p_s = 2.0$ MPa. (d) $p_s = 2.5$ MPa.

Figure 13 demonstrates the monotonic growth of opening force and leakage flux with increasing rotational speed, a direct consequence of amplified hydrodynamic shear wedging action, which simultaneously augments load capacity and cross-film leakage. The grooved area fraction decreases at a decaying rate with higher rotational speed, reflecting converged, stable groove topologies under ultra-high-speed operating conditions. Multiple discrete narrow grooves emerge at low rotational speeds; as speed rises, separate grooves coalesce into a single broad texture with contracted circumferential and radial extents. This behavior indicates that intense hydrodynamic pressure generation at high rotational speeds eliminates the need for multi-groove layouts to satisfy load capacity targets, proving that rotational speed is a decisive factor governing groove topological evolution.

Liquid film pressure contours across four rotational speeds are visualized in Figure 14, revealing pronounced speed-dependent pressure field modulation arising from coupled hydrodynamic and convergent wedge effects. At low rotational speeds, weak fluid shear yields nearly uniform, low-magnitude pressure distributions without distinct high-pressure zones, where hydrostatic pressure dominates the flow field. As rotational speed increases, intensified viscous shear accumulates fluid at the groove trailing edges, forming concentrated local pressure peaks. Simultaneously, the divergent land-to-groove transition generates expanding low-pressure vaporization zones with rising speed. Rotational speed therefore regulates both the intensity of trailing-edge high-pressure peaks and the spatial coverage of upstream low-pressure regions, dictating the evolutionary trajectory of the topology optimization.

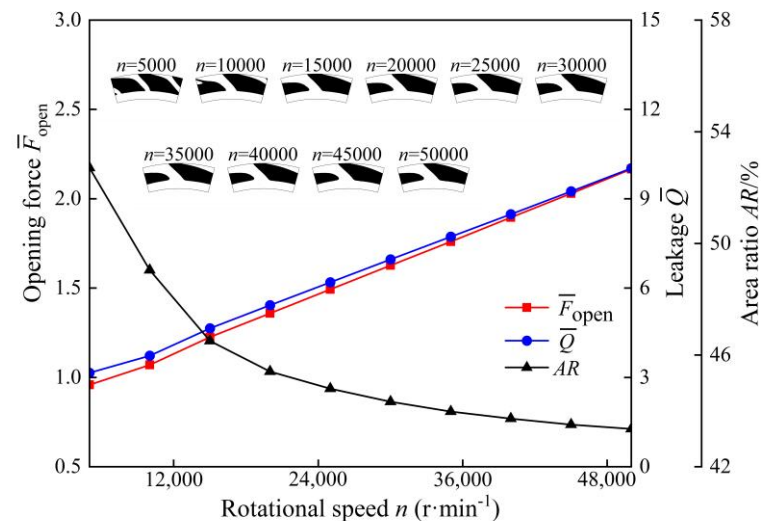


Figure 13. Impact of rotational speed on optimized groove geometry and sealing performance metrics.

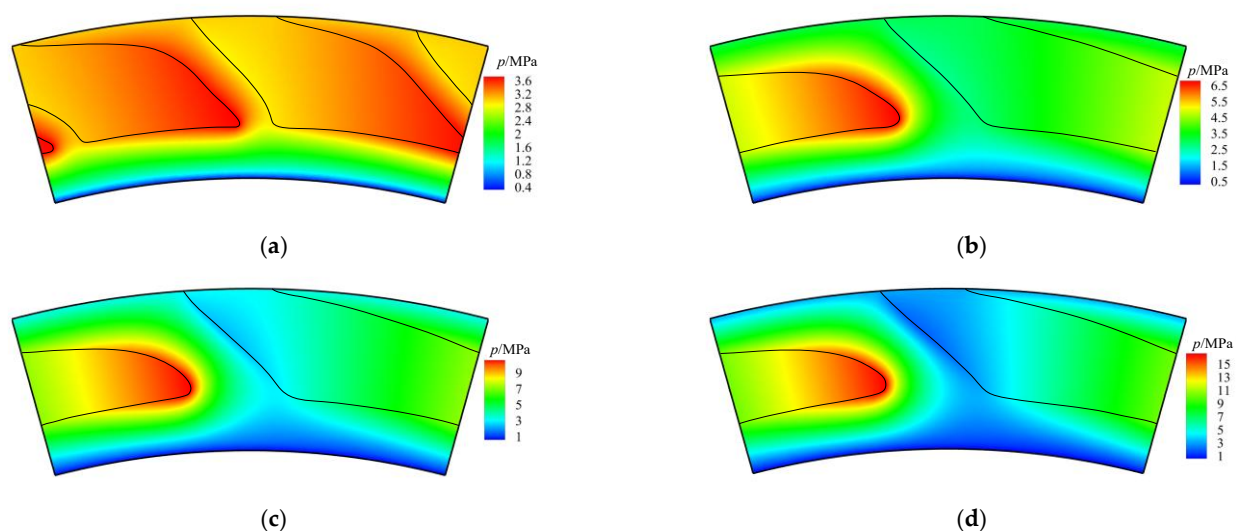


Figure 14. Interfacial pressure contours at four distinct rotational speeds. (a) $n = 5000$ r/min. (b) $n = 15,000$ r/min. (c) $n = 30,000$ r/min. (d) $n = 50,000$ r/min.

3.6. Orthogonal Combined Parameter Optimization

The single-variable parametric analysis identifies three core geometric tuning factors: groove-to-dam ratio, groove depth ratio, and the sector circumferential angle. An orthogonal experimental design is implemented to explore the multi-factor coupling effects and to extract the optimal balanced parameter set for comprehensive two-phase sealing performance. Eighteen distinct structural combinations are constructed by varying the factor levels, with the complete geometric inputs and corresponding sealing performance metrics tabulated in Table 2.

Table 2. Orthogonal array optimization results for combined groove geometric parameters.

Case	ζ	ξ	α (rad)	F_{open} (kN)	Q (g/s)	f	AR (%)
1	0.7	2.5	$2\pi/9$	15.1696	7.32067	0.00075517	41.79
2	0.7	2.5	$2\pi/12$	15.2161	7.53687	0.00076267	43.75
3	0.7	2.5	$2\pi/15$	15.0447	7.64048	0.00077877	44.66

4	0.7	3	$2\pi/9$	15.5788	7.66731	0.00072669	42.98
5	0.7	3	$2\pi/12$	15.3238	7.61554	0.00075093	44.33
6	0.7	3	$2\pi/15$	14.9962	7.55002	0.00077474	45.00
7	0.7	3.5	$2\pi/9$	15.6050	7.69675	0.00072038	43.40
8	0.7	3.5	$2\pi/12$	15.1127	7.45595	0.00075389	44.69
9	0.7	3.5	$2\pi/15$	14.6729	7.27697	0.00078275	45.24
10	0.8	2.5	$2\pi/9$	15.4583	8.55249	0.00072528	46.40
11	0.8	2.5	$2\pi/12$	15.4136	8.90564	0.00073673	48.83
12	0.8	2.5	$2\pi/15$	15.1958	9.09081	0.00075418	50.10
13	0.8	3	$2\pi/9$	15.8763	9.04232	0.00069574	48.09
14	0.8	3	$2\pi/12$	15.5343	9.11546	0.00072171	49.96
15	0.8	3	$2\pi/15$	15.1775	9.18678	0.00074488	51.04
16	0.8	3.5	$2\pi/9$	15.9066	9.22533	0.00068480	49.23
17	0.8	3.5	$2\pi/12$	15.3288	9.07186	0.00072127	50.65
18	0.8	3.5	$2\pi/15$	14.8715	8.94333	0.00074847	51.49

As shown in Table 2, the maximum liquid film opening force is attained at a groove depth ratio of $\xi = 3.5$ with nine circumferential grooves ($\alpha = 2\pi/9$), corresponding to Case 7 ($\zeta = 0.7$) and Case 16 ($\zeta = 0.8$). A modest reduction in depth ratio from 3.5 to 3.0 (comparing Case 4 vs. Case 7, and Case 13 vs. Case 16) entails only marginal losses in opening force while offering substantial leakage suppression. Specifically, relative to Case 7, Case 4 reduces the opening force by merely 0.17% and cuts the leakage by 0.38%; Similarly, compared with Case 16, Case 13 lowers the opening force by 0.19% and the leakage by 1.98%. Overall, a depth ratio of 3.3 delivers a superior balanced performance over 3.5. Furthermore, for two Cases with identical $\xi = 3.0$, Case 4 exhibits a 1.87% lower opening force than Case 13 but achieves a remarkable 15.21% reduction in leakage, offering clear advantages in leakage containment. Consequently, the parametric combination adopted in Case 4 provides the most favorable trade-off between the two core performance indicators: load-carrying opening force and volumetric leakage.

3.7. Performance Benchmarking Against Conventional Spiral Grooves

To quantitatively validate the performance superiority of the topology-optimized groove from Case 4, direct comparative simulations are performed against standard spiral grooves under identical boundary conditions. The baseline geometric parameters (inner/outer radii, groove depth, and sector circumferential angle) are kept exactly the same for both groove types. A matrix of spiral groove variants is generated by sweeping spiral angles (12° , 15° , 18°) and groove width ratios (0.4, 0.5, 0.6), enabling a systematic cross-comparison across a broad conventional spiral design space.

Figure 15 summarizes the performance comparisons under identical operating conditions ($p_s = 3.0$ MPa, $n = 30,000$ r/min, $\alpha = 2\pi/9$, $\xi = 3.0$) for groove-to-dam ratios of 0.7 and 0.8. The topology-optimized groove data correspond to Case 4 ($\zeta = 0.7$) and Case 13 ($\zeta = 0.8$), while the spiral groove results aggregate all 18 parametric combinations. The topology-generated grooves consistently outperform the spiral textures in liquid film opening force, whereas the leakage behavior depends strongly on the groove-to-dam ratio:

- (1) At $\zeta = 0.7$: the average opening force increases by 17.80% relative to the spiral grooves, accompanied by an average leakage rise of 8.02%;
- (2) At $\zeta = 0.8$: the average opening force improves by 20.67%, while the volumetric leakage decreases by 7.87%.

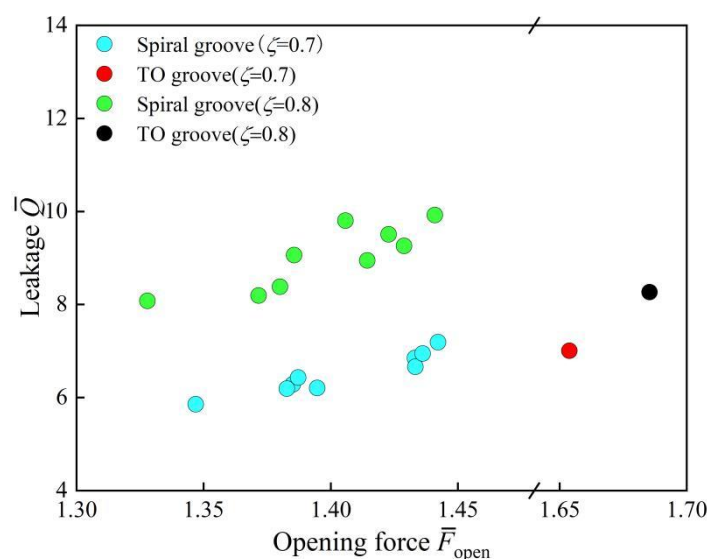


Figure 15. Sealing performance comparison between topology-optimized grooves and conventional spiral grooves.

These results demonstrate that topology-optimized grooves offer significant gains in load-carrying capacity, with leakage characteristics tunable by adjusting the groove-to-dam geometric ratio. In practical seal design, an appropriate value of ζ can be selected to prioritize either maximum opening force or minimum leakage according to the specific operational specifications of the turbopump.

4. Limitations and Future Work

Despite the satisfactory predictive performance of the proposed topology optimization framework under gas–liquid two-phase oxygen conditions, several inherent limitations should be acknowledged, along with corresponding directions for future research. First, all analyses are based solely on numerical simulations without experimental validation; bench tests on LOX turbopump seals are essential to calibrate the model parameters and verify the actual sealing performance of the topology-optimized grooves. Second, the current model relies on simplifying assumptions, including isothermal laminar flow and a homogeneous two-phase formulation, which neglect interphase slip and interfacial tension between liquid and gaseous oxygen. Moreover, viscous shear heating within the ultrathin liquid film is not considered in the governing equations, and surface micro-roughness, structural elastic deformation, and thermoelastic coupling induced by cryogenic temperature gradients are also excluded—factors that may cause deviations from real operating states. In addition, the phase-change source term depends on empirical vaporization and liquefaction coefficients, whose applicability across varying pressure and rotational speed ranges remains unverified. Another practical challenge lies in the complex, irregular contour of the optimized groove topologies, which pose difficulties in machinability and manufacturing precision under cryogenic seal processing requirements.

For future work, we plan to implement multi-objective topology optimization that simultaneously maximizes the liquid film opening force and minimizes the volumetric leakage rate, instead of using load-carrying capacity as the sole objective. Subsequent numerical models will incorporate viscous heat generation, thermoelastic deformation, and heterogeneous two-phase flow theories. Furthermore, targeted experimental measurements will be conducted to revise the empirical phase-change constants and to evaluate the manufacturability of the optimized groove profiles.

5. Conclusions

Conventional parametric optimization of mechanical face seal grooves is inherently constrained by fixed, predefined texture geometries and struggles to accommodate the complex gas–liquid two-phase lubrication environments of LOX. Targeting turbopump mechanical seals operating with LOX, this study establishes a topology optimization framework based on reaction-diffusion equations, tailored specifically for gas–liquid two-phase flow conditions. Finite element numerical simulations are systematically conducted to evaluate groove performance across a wide range of geometric and operating parameter combinations. The primary conclusions are summarized as follows:

1. A generative topology optimization method is proposed for gas–liquid two-phase mechanical seal grooves, with the liquid film opening force adopted as the objective function to be maximized. The framework evolves optimal groove layouts via reaction-diffusion partial differential equations, producing high-performance, non-intuitive groove topologies that are unattainable through conventional parametric optimization.
2. The final converged groove morphology, opening force, and grooved area fraction exhibit minimal dependence on the initial guess topologies. All distinct starting configurations converge to consistent macroscopic layouts characterized by three geometric segments: an inclined straight edge on the upstream side, a concentric arc along the inner seal radius, and an irregular curved contour at the outer radius. These results verify the excellent algorithmic robustness of the proposed approach.
3. Under gas–liquid two-phase lubrication with LOX, both geometric and operating parameters exert pronounced regulatory effects on the optimized groove configurations. The recommended design windows are a groove-to-dam ratio of 0.7–0.8 and a groove depth ratio of 3.0–3.5. Dual discrete grooves are formed under low rotational speeds and low groove-to-dam ratios, whereas a single continuous groove dominates all other parametric combinations. LOX vaporization is concentrated at low inlet sealing pressures, and the intensity of phase transition is closely correlated with the magnitude of the supply pressure.
4. Compared with classical spiral grooves having matched geometric dimensions, the reaction-diffusion topology-optimized grooves elevate the average liquid film opening force by 17.80–20.67%. These results comprehensively confirm the effectiveness and performance advantages of the proposed topology optimization strategy in enhancing the load-carrying capacity of mechanical seals.

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