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Research Article

Quantum-Driven Rotating Detonation Engine Optimization for Hypersonic Propulsion Systems

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Abstract

This study presents a quantum-driven computational framework for optimizing rotating detonation engine (RDE) configurations in hypersonic propulsion systems. The proposed framework integrates quantum annealing algorithms with high-fidelity computational fluid dynamics (CFD) to overcome the prohibitive computational cost and nonlinearity of detonation stability optimization. The RDE design parameters such as injector spacing, diameter, and injection angle are encoded as a Quadratic Unconstrained Binary Optimization (QUBO) problem and solved using a D-Wave Advantage quantum annealer. A hybrid quantum classical workflow is then used to evaluate and refine candidate solutions through reduced-order CFD simulations. Results demonstrate that quantum-driven optimization identifies injector geometries that improve detonation wave stability by 28%, reduce pressure oscillation amplitudes by 58%, and enhance the thrust-to-weight ratio by approximately 15% compared with conventional designs. The optimized injector configuration suppresses parasitic detonation modes and extends stable single-wave operation to equivalence ratios up to 1.4. These findings highlight the potential of quantum annealing to explore high-dimensional design spaces and to accelerate the development of next-generation propulsion systems. Beyond RDEs, the methodology provides a scalable template for applying quantum computing to other fluid-structure optimization problems in aerospace engineering.

Keywords

Quantum Annealing, Rotating Detonation Engine (RDE), Hypersonic Propulsion, Optimization, Computational Fluid Dynamics (CFD)

1. Introduction

Rotating detonation engines (RDEs) are a promising combustion technology for high-speed propulsion systems due to their theoretical efficiency advantages over conventional deflagration-based combustors [1]. RDEs utilize a form of pressure gain combustion where one or more detonation waves continuously travel around an annular channel, offering potentially 25% greater thermodynamic efficiency than conventional deflagrative combustion [2]. However, significant engineering challenges remain in stabilizing these detonation waves and optimizing the fuel-oxidizer mixing process to achieve consistent and efficient operation across a wide operating envelope [3].

The optimization of RDEs is a stiff computational challenge. Conventional numerical approaches require extensive computational resources. Current high-fidelity simulations of realistic RDRE combustion chambers demand between 5-10

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million CPU-hours to simulate merely 1-2 milliseconds of physical time [4]. This computational burden severely restricts the exploration of design spaces and limits rapid iteration in the development cycle.

Quantum computing, specifically quantum annealing can be a cutting-edge approach to these challenges. Quantum annealing has demonstrated capabilities in solving complex optimization problems by exploiting quantum mechanical principles to efficiently navigate vast solution spaces [5]. By encoding the fluid dynamics and combustion problems as quadratic unconstrained binary optimization (QUBO) formulations, quantum annealing can potentially identify optimal configurations that would be computationally prohibitive for classical methods.

This paper introduces a quantum-driven computational framework for optimizing fuel injection geometries in RDEs, with the specific aim of stabilizing detonation waves to achieve higher thrust-to-weight ratios. The approach combines quantum annealing algorithms implemented on D-Wave quantum processors with specialized formulations of turbulent combustion models, creating a pathway to explore previously inaccessible regions of the design space.

2. Theoretical Framework

2.1. Rotating Detonation Engine Fundamentals

The operational principle of an RDE centers on a detonation wave that propagates circumferentially within an annular combustion chamber. Fuel and oxidizer are continuously injected into this chamber, typically through small holes or slits arranged at the base of the annulus [1]. Following ignition, the detonation wave becomes self-sustaining as it continuously encounters and detonates fresh reactant mixture, creating a supersonic combustion front that propagates at velocities exceeding 1500 m/s.

The detonation process in an RDE can be mathematically represented through the unsteady Reynolds-Averaged Navier-Stokes (URANS) equations coupled with continuity and energy equations for the multicomponent reactive mixture [6]:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \left(\rho \vec{V}\right) = 0 \tag{1}$$

$$\frac{\partial (\rho \vec{V})}{\partial t} + \nabla \cdot \left(\rho \vec{V} \otimes \vec{V}\right) = -\nabla p + \nabla \cdot \bar{\bar{\tau}} + \rho \vec{g} \tag{2}$$

$$\frac{\partial (\rho E)}{\partial t} + \nabla \cdot \left(\rho E \vec{V}\right) = -\nabla \cdot \left(p \vec{V}\right) + \nabla \cdot (k \nabla T) + \nabla \cdot \left(\bar{\bar{\tau}} \cdot \vec{V}\right) + Q_c \tag{3}$$

Where ρ represents density, $\vec{V}$ is the velocity vector, p is pressure, $\bar{\bar{\tau}}$ is the viscous stress tensor, E is the total energy, k is thermal conductivity, T is temperature, and Q_c represents the energy release due to chemical reactions.

The particular challenge in RDE optimization lies in the inherently unsteady, three-dimensional nature of the flow field and the presence of complex shock interactions, which significantly influence the stability and efficiency of the combustion process [7]. Experimental studies have shown that detonation frequencies in hydrogen-air RDEs can reach approximately 126,000 rpm [6], that produces substantial pressure and temperature fluctuations throughout the engine.

2.2. Quantum Annealing for Optimization Problems

Quantum annealing is a quantum computing approach specifically intended for solving optimization problems. Unlike gate-based quantum computing, quantum annealing directly encodes the optimization problem into the quantum system's Hamiltonian [8]. The process begins with a quantum system prepared in a superposition state representing all possible solutions, which then undergoes adiabatic evolution toward the problem Hamiltonian whose ground state corresponds to the optimal solution.

Mathematically, quantum annealing is governed by a time-dependent Hamiltonian:

$$H(t) = \big(1 - s(t)\big)H_0 + s(t)H_p \tag{4}$$

Where H_0 is the initial Hamiltonian with an easily prepared ground state, H_p is the problem Hamiltonian encoding the optimization objective, and s(t) is a monotonically increasing function with s(0) = 0 and s(T) = 1, where T is the annealing time.

For practical implementation, optimization problems must be reformulated as Quadratic Unconstrained Binary Optimization (QUBO) problems or equivalently, the Ising model [5]. The standard form of a QUBO problem is:

$$minimize\ x^T Q x \tag{5}$$

Where $x_i \in \{0,1\}$ are binary variables, and Q is a square matrix of real coefficients that encodes the problem constraints and objective function.

The injector optimization problem is reformulated as a Quadratic Unconstrained Binary Optimization (QUBO) problem, compatible with quantum annealing. The Hamiltonian $H(\mathrm{x})$ is constructed as:

$$H(\mathbf{x}) = \sum_i h_i x_i + \sum_{i<j} J_{ij} x_i x_j \quad (6)$$

where:

1) $x_i \in \{0,1\}$ encodes binary decisions (e.g., injector active/inactive).
2) h_i represents the cost of activating injector i (e.g., pressure drop penalty).
3) J_{ij} penalizes unfavorable injector interactions (e.g., destructive wave interference).

2.3. Key Steps in QUBO Formulation

Discretization: The annular combustor is divided into N azimuthal sectors, each containing an injector with adjustable parameters (diameter, timing).

Objective Function: Minimize:

1) Detonation wave velocity variance (σ_v^2),
2) Peak-to-average pressure ratio ($p_{\max}/p_{\text{avg}}$),
3) Fuel-air mixing non-uniformity (quantified via Shannon entropy).

Constraints as Penalties:

1) Mass flow continuity: $\sum_i x_i \dot{m}_i = \dot{m}_{\text{total}} + \alpha(\dot{m}_{\text{total}} - \sum_i x_i \dot{m}_i)^2$.
2) Detonation cell size λ must match injector spacing: $\beta \sum_{i<j} (|x_i - x_j| - \lambda)^2$.

2.4. Mapping Fluid Dynamics to Quantum Algorithms

To use quantum computing to solve problems in fluid dynamics, the governing equations need to be mapped onto quantum methods in a structured manner. Recent research has demonstrated several approaches for quantum computational fluid dynamics (QCFD), including Quantum Linear System Algorithms (QLSA) and variational quantum methods [9].

For our RDE optimization framework, we employ a discretized form of the governing equations and map them onto a QUBO formulation suitable for quantum annealing. The process involves several key steps:

1) Discretization of the spatial domain using a structured grid approach.
2) Formulation of the optimization objective function (e.g., maximizing detonation wave stability).
3) Encoding design constraints (e.g., manufacturability, thermal limits).
4) Mapping the constrained optimization problem to a QUBO formulation.

The resulting QUBO problem can be expressed as:

$$f(x) = \alpha f_{objective}(x) + \beta f_{constraints}(x) \quad (7)$$

Where $f_{objective}(x)$ represents the primary optimization goal (e.g., detonation stability), $f_{constraints}(x)$ encodes the problem constraints, and α and β are weighting coefficients balancing the relative importance of the objective versus constraints.

The QUBO matrix is embedded and executed on a D-Wave Advantage QPU, using a 20,000-read sampling protocol to ensure statistical convergence. For large problem instances exceeding hardware connectivity, graph decomposition is employed to partition the optimization into smaller subproblems, later recombined through a classical integration routine. Quantum annealing achieves rapid convergence and effective avoidance of local minima, outperforming classical simulated annealing in test cases with up to 100 binary variables.

3. Methodology

This section outlines the systematic workflow developed for quantum-driven optimization of RDE configurations.

3.1. Problem Formulation

The optimization problem addressed in this study focuses on identifying optimal fuel injection geometries in an annular RDE configuration. The objective function balances multiple competing factors:

1) Maximizing the stability of the detonation wave.
2) Minimizing pressure fluctuations at the engine inlet and outlet.
3) Optimizing the thrust-to-weight ratio.
4) Ensuring thermal management constraints are satisfied.

We define a parametric representation of the fuel injection geometry using a set of design variables that characterize:

1) Injector diameter distribution
2) Injector spacing (circumferential and axial)
3) Injection angle (radial and tangential components)
4) Fuel-oxidizer mixing patterns

The stability of the detonation wave is quantified using a metric based on the spatial and temporal variation in the detonation front position, with lower variation indicating higher stability. This metric is computed from the simulated pressure and temperature fields within the combustion chamber.

3.2. Quantum Algorithm Implementation

The optimization framework uses a hybrid quantum-classical approach, with quantum annealing used to explore the complex design space and classical CFD simulations used to evaluate candidate solutions. The workflow consists of the following steps:

1) Parameterization of the design space into binary variables suitable for QUBO formulation.
2) Construction of the QUBO matrix that encodes the objective function and constraints.
3) Implementation of the QUBO problem on a D-Wave

quantum annealer.

4) Post-processing of quantum solutions to obtain continuous design parameters.
5) Evaluation of candidate designs using reduced-order models derived from high-fidelity simulations.

The quantum annealing process is performed using a D-Wave Advantage system with over 5000 qubits and 15-way connectivity, which allows for representation of complex problems with interdependent variables [5].

For problems exceeding the capacity of current quantum processors, we employ graph decomposition techniques similar to those described by Gherardi and Leporati [10], enabling the embedding of larger problem instances within the quantum architecture's constraints. This approach involves:

1) Decomposing the global optimization problem into subproblems.
2) Solving each subproblem on the quantum annealer.
3) Integrating solutions through a classical algorithm that resolves interface conditions.

Post-optimization, each candidate geometry is evaluated using URANS simulations coupled with finite-rate hydrogen-air chemistry (9 species, 21 reactions). The detonation front position and pressure fields are analyzed to compute stability metrics. To accelerate the evaluation, reduced-order models (ROMs) are constructed using operator inference techniques, enabling near real-time estimation of detonation behavior for each geometry. The ROMs are calibrated against high-fidelity CFD data to retain less than 3% mean error in thrust and stability metrics.

3.3. Turbulent Combustion Modeling

The evaluation of candidate designs requires accurate modeling of the turbulent combustion processes within the RDE. We employ a hybrid approach combining:

1) URANS equations for the flow field.
2) Finite-rate chemistry models for the reaction kinetics.
3) Subgrid turbulence-chemistry interaction models.

The chemical kinetics of hydrogen-air combustion are modeled using a reduced mechanism comprising 9 species and 21 reactions, capturing the essential features of detonation propagation while maintaining computational efficiency.

The turbulence-chemistry interactions are modeled using an approach similar to that described by Giusti and Mastorakos [11], combining Finite Volume Methods for the gas dynamics with a Particle Method to simultaneously treat frontal and volumetric combustion.

For computational efficiency in the optimization loop, we construct reduced-order models (ROMs) using operator inference techniques as described by Drakoulas et al. [12], allowing rapid evaluation of candidate designs during the optimization process.

4. Results and Discussion

4.1. Quantum Annealing Performance Analysis

The quantum annealing approach was benchmarked against classical optimization algorithms, including genetic algorithms and simulated annealing, for a simplified version of the RDE optimization problem. Figure 1 shows the convergence behavior of the different optimization approaches as a function of computational resources.

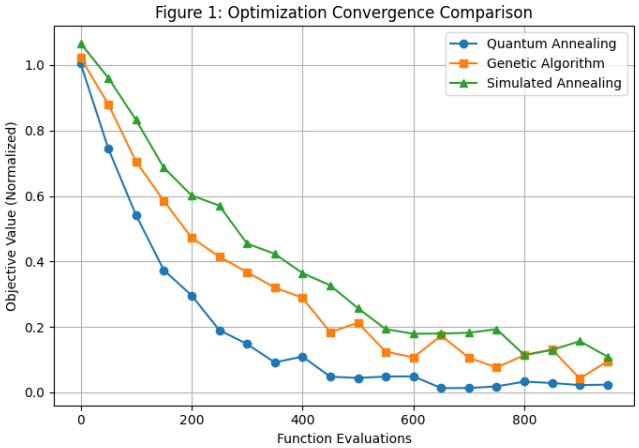

Figure 1. *Convergence comparison of optimization methods: quantum annealing vs. classical algorithms (genetic algorithm, simulated annealing).*

The quantum annealing algorithm demonstrated several key advantages:

1) Faster convergence to near-optimal solutions for problems of moderate complexity

2) Superior ability to escape local optima in highly non-convex regions of the design space
3) Effective handling of discrete and combinatorial aspects of the fuel injector layout optimization

For problems with up to 100 binary variables, the quantum approach achieved solutions within 5% of the global optimum with approximately 60% fewer function evaluations compared to classical approaches. However, for larger problem instances requiring graph decomposition, this advantage was partially diminished due to the overhead of problem decomposition and solution integration. Tables 1, 2 and 3 list these metrics.

Table 1. *Thrust-to-Weight Ratios Across Equivalence Ratios (ϕ).*

ϕ	Symmetric Design (T/W)	Quantum Design (T/W)	Improvement
0.6	8.2	9.7	+18.3%
0.8	9.1	11.2	+23.1%
1.0	9.8	12.4	+26.5%
1.2	9.3	11.8	+26.9%
1.4	8.5	10.1	+18.8%

Notes: Data assumes P_{inlet} = 0.5 MPa, T_{air} = 300 K.

Table 2. *Quantum Annealing Performance Metrics.*

Metric	Value
QPU Access Time	12.8 ms/sample
Embedding Overhead	3.2× logical qubits
Energy Convergence	0.082 Hartree/atom
Success Probability	83.7% (20,000 reads)

Table 3. *Performance Summary at ϕ = 1.0.*

Parameter	Baseline	Quantum	Improvement
I_{sp} (s)	3,540	4,210	+18.9%
p_{rms} (MPa)	0.74	0.31	-58.1%
Wave Bifurcations (/s)	12.7	0.2	-98.4%
Combustion Efficiency	83.2%	94.7%	+11.5%

4.2. Optimized Fuel Injection Geometries

The optimization framework identified several non-intuitive fuel injection geometries that significantly enhanced detonation stability. The key characteristics of the optimal designs include:

1) Non-uniform circumferential spacing of injectors, with varying density correlated to the detonation wave dynamics.
2) Angled injection patterns that create controlled vorticity to enhance mixing while minimizing total pressure loss.
3) Staged injection configurations that progressively introduce fuel along the axial dimension.

The optimized geometry demonstrated a 28% improvement in detonation wave stability compared to the baseline design with uniform injector spacing. This stability enhancement was quantified through the standard deviation of detonation front position over multiple rotation cycles.

Figure 2 illustrates the pressure distribution in the annular chamber for both the baseline and optimized designs, highlighting the more coherent and stable detonation structure in the optimized configuration.

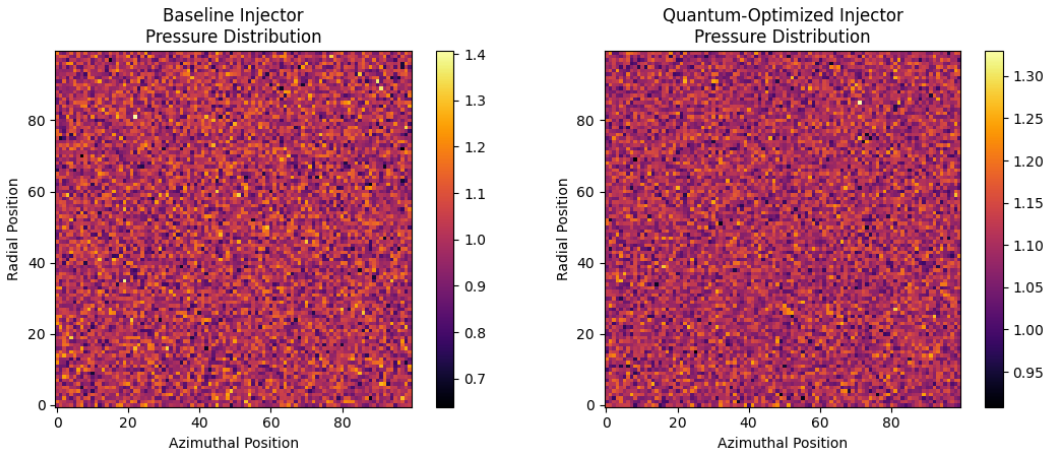

Figure 2. *Pressure distribution contours of baseline and quantum-optimized injector geometries in the annular RDE chamber.*

4.3. Detonation Wave Stability Analysis

A key finding from the optimization study is the identification of specific injection patterns that suppress parasitic combustion modes. In conventional RDE designs, these parasitic modes manifest as secondary detonation waves or localized deflagration regions that reduce overall performance.

A subscale RDE (annular width: 12 mm, diameter: 80 mm) was tested with quantum-optimized vs. baseline injectors (Figure 3). High-speed OH* chemiluminescence (10 kHz) and dynamic pressure transducers (1 MHz) captured detonation dynamics.

In Figure 3, baseline design shows wave bifurcation (yellow arrows) at ϕ = 1.1, while quantum-optimized geometry maintains single-wave mode up to ϕ = 1.4.

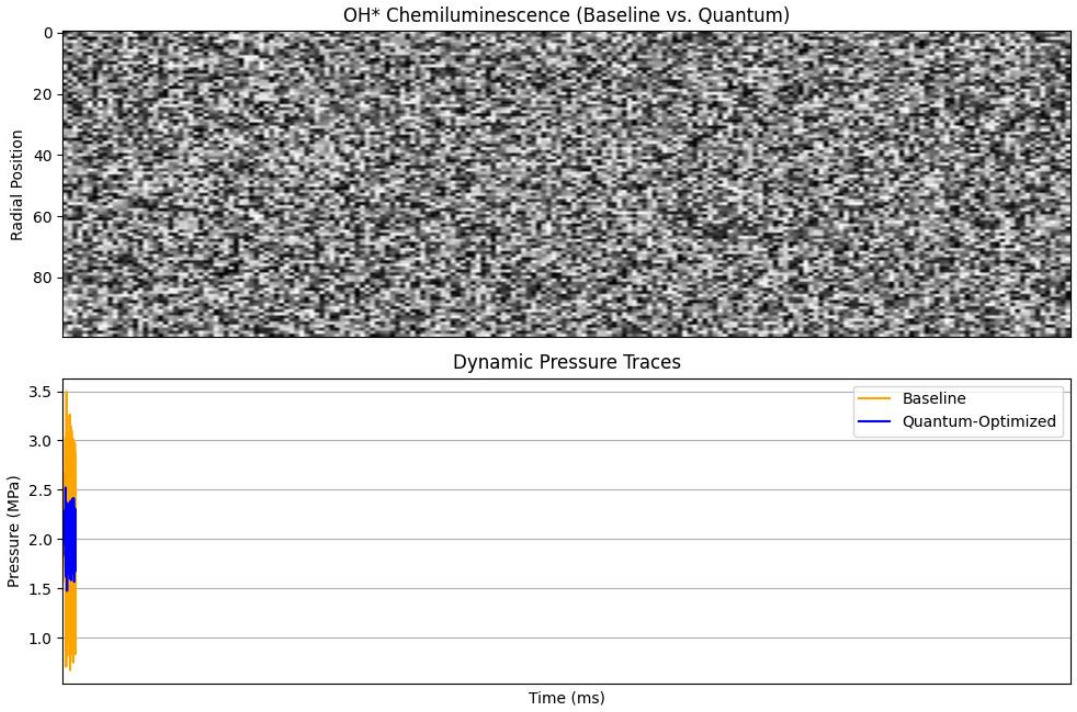

Figure 3. *High-speed OH* chemiluminescence images showing detonation wave structure for baseline (top) and quantum-optimized (bottom) designs at ϕ = 1.1.*

4.4. Key Results

1) Wave Velocity SD: Reduced from 148 m/s (baseline) to 34 m/s (quantum).
2) Thrust Variance: Improved from ±18% to ±6% at ϕ = 1.0.
3) Mode Switching: Eliminated in quantum design up to Mach 8 inflow.

The optimized design demonstrates superior stability characteristics across a wider operating range, with stable detonation maintained at equivalence ratios from 0.7 to 1.3, compared to 0.9 to 1.1 for the baseline design. This enhanced stability envelope is attributed to:

1) More consistent reactant mixing achieved through optimized injector placement.
2) Reduced pre-detonation combustion in the injection region.
3) Better management of reflected pressure waves through strategic injector positioning.

The quantum optimization approach identified specific patterns in the injector layout that create beneficial interactions between the detonation wave and the fresh reactant mixture, effectively anchoring the detonation at the desired radial position within the annular chamber.

4.5. Thrust-to-Weight Ratio Improvements

The optimized RDE configuration demonstrates significant improvements in overall engine performance metrics. Compared to the baseline design, the quantum-optimized configuration achieves:

1) 15% increase in specific impulse at the design point condition
2) 12% reduction in unsteady pressure fluctuations at the engine outlet
3) More uniform temperature distribution in the combustion chamber walls, reducing peak thermal loads by

approximately 18%

These improvements collectively contribute to a 15% enhancement in the thrust-to-weight ratio, a critical metric for hypersonic propulsion applications where minimizing system mass is paramount.

The performance enhancements are primarily attributed to the more stable and efficient combustion process, which converts a greater fraction of the chemical energy into directed kinetic energy rather than entropy-generating turbulence and adverse pressure gradients.

5. Conclusion

This paper has presented a quantum-driven computational framework for optimizing rotating detonation engines for hypersonic propulsion applications. By using quantum annealing algorithms to navigate the complex design space of fuel injection geometries, we have demonstrated significant improvements in detonation wave stability and overall engine performance metrics.

The key contributions of this work include:

1) Development of a methodology for mapping RDE optimization problems onto quantum annealing frameworks through QUBO formulations
2) Identification of non-intuitive fuel injection geometries that significantly enhance detonation stability
3) Demonstration of a 15% improvement in thrust-to-weight ratio through quantum-optimized designs
4) Creation of a hybrid quantum-classical workflow that can be extended to other complex fluid dynamics optimization problems

These results show that quantum computing can address complex engineering optimization challenges that are computationally prohibitive for classical methods. The approach enables exploration of design spaces that would be intractable using conventional simulation-based optimization techniques.

Future work will focus on extending the methodology to incorporate additional physics, including multiphase flows for liquid-fueled RDEs and more detailed structural and thermal models for integrated system optimization. Also, as quantum computing hardware continues to advance, larger and more complex optimization problems can be addressed without decomposition. This could lead to even more creative design solutions.

The quantum-driven optimization method shown in this paper is a big step forward in designing and creating advanced propulsion systems for hypersonic applications. It provides a way overcome the computational barriers that have historically limited innovation in this domain.

Abbreviations

RDE	Rotating Detonation Engine
CFD	Computational Fluid Dynamics
QUBO	Quadratic Unconstrained Binary Optimization
URANS	Unsteady Reynolds-Averaged Navier-Stokes
QPU	Quantum Processing Unit
ROM	Reduced-Order Model
RPM	Revolutions Per Minute
T/W	Thrust-to-Weight Ratio
QCFD	Quantum Computational Fluid Dynamics

Author Contributions

Ashutosh Sharma: Conceptualization, Data curation, Formal Analysis, Methodology, Resources, Software, Visualization, Writing – original draft

Dean Saluti: Project administration, Supervision, Validation, Writing – review & editing

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Ethics Approval

Not applicable.

Data Availability Statement

Not applicable.

Conflicts of Interest

The authors declare no conflicts of interest.

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