Discharge Chamber Primary Electron Modeling Activities in Three-Dimension

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Summary

Designing discharge chambers for ion thrusters involve many geometric configuration decisions. Various decisions will impact discharge chamber performance with respect to propellant utilization efficiency, ion production costs, and grid lifetime. These hardware design decisions can benefit from the assistance of computational modeling. Computational modeling for discharge chambers has been limited to two-dimensional (2–D) codes that leveraged symmetry for interpretation into three-dimensional (3–D) analysis. This paper presents model development activities towards a 3–D discharge chamber simulation to aid discharge chamber design decisions. Specifically, of the many geometric configuration decisions towards attainment of a worthy discharge chamber, this paper focuses on addressing magnetic circuit considerations with a 3–D discharge chamber simulation as a tool. With this tool, candidate discharge chamber magnetic circuit designs can be analyzed computationally to gain insight into factors that may influence discharge chamber performance such as: primary electron loss width in magnetic cusps, cathode tip position with respect to the low magnetic field volume, definition of a low magnetic field region, and maintenance of a low magnetic field region across the grid span. Corroborating experimental data will be obtained from mockup hardware tests. Initially, simulated candidate magnetic circuit designs will resemble previous successful thruster designs. To provide opportunity to improve beyond previous performance benchmarks, off-design modifications will be simulated and experimentally tested.

Introduction

The electron-bombardment ion thruster was introduced in 1960 using mercury as the propellant.1,2 Ever since, much research has been conducted on these thrusters to improve stability, efficiency, and operability to meet experimental and mission requirements. To aid thruster development, computational models have been designed to leverage plasma physics theory towards practical thruster design through simulation. The reference list is not an exhaustive list of modeling activity but captures some of the undertakings over the past 20 years. Research endeavors have led to parametric modeling of plasma in an ion discharge chamber. Other modeling research initiatives employed 2–D computational fluid dynamics code for magnetic field analysis and particle tracking. These particle tracking codes are 2–D and leverage axial cylindrical symmetry for 2–D to 3–D interpretations.

Of interest to the NASA Glenn Research Center (GRC) and the NASA community is a computational tool, transferable to academia and industry partners, capable of supporting design considerations for optimization of electron-bombardment ion thrusters to meet future mission requirements. Historically, computational hardware limitations warranted simplification of the discharge chamber modeling task to 2–D. Technological advances in computer speed, memory access, and clustering for massive parallelization make way for design and development of 3–D models. This research is towards designing a 3–D discharge chamber simulation that employs magnetic field modeling and particle tracking code using a widely accepted programming environment to ease interactions with research partners.
Current state of the 3–D modeling code is limited to 3–D simulations of magnetic circuits and an unobstructed primary electron particle tracker. The 3–D magnetic field simulation capability enables consideration of many candidate magnetic circuit designs prior to hardware buildup. This capability provides quick feedback regarding the low magnetic field volume, low magnetic field area at the ion optics, and verification of a closed continuous magnetic field boundary for all candidate magnetic circuit. The 3–D magnetic field modeler is also the front end to the primary electron particle tracking simulation. The unobstructed primary electron particle tracker simulation, although not realistic because of its lack of particle collision consideration, can lend insight to performance metrics by measuring containment length, primary electron cusp leakage width, and primary electron distribution density. These three factors, coupled with experimental data, will aid definition of a desired low magnetic field region boundary condition and an ideal location of the cathode tip with respect to the magnetic circuit.

This paper is organized to first present the overall perspective of the model development, and then discuss some initial modeling results. Finally, the next model enhancement activities are presented.

**Nomenclature**

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>$A(k)$</td>
<td>3-dimensional Cartesian acceleration vector of simulated primary electron (mm/sec$^2$)</td>
</tr>
<tr>
<td>$Ax$</td>
<td>X Cartesian coordinate component of 3-dimension particle acceleration vector</td>
</tr>
<tr>
<td>$Ay$</td>
<td>Y Cartesian coordinate component of 3-dimension particle acceleration vector</td>
</tr>
<tr>
<td>$Az$</td>
<td>Z Cartesian coordinate component of 3-dimension particle acceleration vector</td>
</tr>
<tr>
<td>$B(p)$</td>
<td>3-dimensional magnetic field vector at primary electron location $p(k)$ (Tesla)</td>
</tr>
<tr>
<td>$Bx$</td>
<td>X Cartesian coordinate component of 3-dimension magnetic field vector</td>
</tr>
<tr>
<td>$By$</td>
<td>Y Cartesian coordinate component of 3-dimension magnetic field vector</td>
</tr>
<tr>
<td>$Bz$</td>
<td>Z Cartesian coordinate component of 3-dimension magnetic field vector</td>
</tr>
<tr>
<td>$k$</td>
<td>discrete indexer where $k$ is the current time and $k + 1$ is the next time step</td>
</tr>
<tr>
<td>$p(k)$</td>
<td>Current 3-dimensional Cartesian coordinate location of simulated primary electron (mm)</td>
</tr>
<tr>
<td>$m_e$</td>
<td>Electron mass (kg)</td>
</tr>
<tr>
<td>$q$</td>
<td>Elementary charge ($1.602 \times 10^{-19}$ C)</td>
</tr>
<tr>
<td>$v(k)$</td>
<td>3-dimensional Cartesian velocity vector of simulated primary electron (mm/sec)</td>
</tr>
<tr>
<td>$X$</td>
<td>X Cartesian coordinate component of 3-dimension particle location</td>
</tr>
<tr>
<td>$Y$</td>
<td>Y Cartesian coordinate component of 3-dimension particle location</td>
</tr>
<tr>
<td>$Z$</td>
<td>Z Cartesian coordinate component of 3-dimension particle location</td>
</tr>
<tr>
<td>$Xvel$</td>
<td>X Cartesian coordinate component of 3-dimension particle velocity vector</td>
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<tr>
<td>$Yvel$</td>
<td>Y Cartesian coordinate component of 3-dimension particle velocity vector</td>
</tr>
<tr>
<td>$Zvel$</td>
<td>Z Cartesian coordinate component of 3-dimension particle velocity vector</td>
</tr>
<tr>
<td>$\delta t$</td>
<td>Time step used in discrete integration (sec)</td>
</tr>
</tbody>
</table>

**General Model**

The 3–D discharge chamber computational model consists of software for modeling static magnetic field circuits and employs a programming environment with architecture to exploit current state-of-the-art high performance computer clusters (HPCC). The following sections describe the hardware and software employed for the GRC 3–D discharge chamber modeling activities.
Discharge Chamber Modeling Hardware

The NASA GRC HPCC employed for discharge chamber modeling consists of multiple rack mounted Intel\textsuperscript{®} based dual Xeon\textsuperscript{®} processor computational servers. One server is designated as the front-end to the cluster and the other servers are the computational-nodes (nodes). This HPCC is designed such that all servers are isolated from the internet, the HPCC can be remotely controlled from a laptop computer via Ethernet cable, and all servers are networked together to facilitate communication. Isolating the HPCC from the internet frees up computational resources from internet concerns; therefore, computational resources can be focused on modeling activities. Laptop computer control of the HPCC enables easy access to the facility. Multiple nodes connected together through a communication link enable the nodes to work in concert towards completion of a simulation. Two methods are being considered to capitalize on the HPCC multiple nodes: The first method, current practice, enables simultaneous particle tracking. For this method, each node will track particles from launch to conclusion. Therefore, each node will define the complete discharge chamber environment. Since the discharge chamber is enormous compared to the particles, tremendous memory capacity (RAM) is necessary for a simulation. RAM requirements for a complete description of the discharge chamber are completely beyond what is available to each node. The resolution is to maintain RAM information via frequent reads from the local hard disk. The local hard disk files describing discharge chamber environmental conditions on each node are updated from the front-end via Ethernet cable. For this method, efficient memory management techniques along with ample, fast hardware are essential for useful simulation time. The second method involves virtual sectioning the discharge chamber into multiple zones. For this method, a node would be responsible for one zone, each node will be capable of holding all information pertinent to a particular discharge chamber zone, and the front-end is tasked to transfer particles from one node to another via Ethernet communication link. The hardware bottleneck for this second method is the communication link between the front-end and the nodes.

Discharge Chamber Modeling Software

All previous discharge chamber modeling has used 2–D custom codes or particle-in-cell (PIC) codes.\textsuperscript{3,7-15} This paper describes the first attempt to simulate particle tracking in a 3–D discharge chamber model. Current state of the GRC modeling activities includes static magnetic circuit modeling and primary electron tracking in a simulated discharge chamber. This section is further reduced to two sections. One section will describe the magnetic field and the second section will describe the particle tracking modeling activities.

Magnetic field modeling.—There are two primary purposes for the magnetic circuit simulation tool: It is a front end to the particle tracking simulation and it is a tool to aid analysis of candidate discharge chamber magnetic circuits. The 3–D discharge chamber simulation involving particle tracking described in this paper has the following 3 requirements from a magnetic field model. First, particle tracking within the discharge chamber is significantly dependent on a model of the static magnet circuit employed to contain the discharge chamber plasma; therefore, a reliable magnetic field model is required. Since this research pertains to a 3–D discharge chamber simulation, another requirement is the capability to generate 3–D maps of the static magnetic field as opposed to extrapolation from a 2–D simulation. A third requirement is to make the complete 3–D discharge chamber simulation package transferable to academia and industry. Hence, the magnetic field modeling software must be well documented and available for NASA research partners. To this end, this 3–D discharge chamber simulation employs a static magnetic circuit modeling code capable of generating and saving on file a complete 3–D magnetic field vector map. These files of magnetic field maps are employed by the 3–D particle tracking code and can also be used for report generation.

\textsuperscript{®} Intel is a registered trademark of Intel Corporation and Xeon is a trademark of Intel Corporation.
Establishment of an effective magnetic circuit is one of the first steps when designing a discharge chamber for an electron-bombardment ion thruster. A worthy discharge chamber magnetic circuit design ensures a closed low magnetic field contour line, maximizes the low magnetic field volume, and considers cathode tip placement issues.\textsuperscript{16,17} The illustration in figure 1 is a 2–D magnetic circuit graphic simulation of a hypothetical cylindrical discharge chamber with a partial conic closed end. The end opposite the partial conic end is where the thruster ion optics reside. The contour trace within the discharge chamber volume is the closed magnetic field contour that defines the low field volume. The cathode tip, is typically located outside the low field volume, near the partial conic end of the discharge chamber, and points axial towards the ion optics. The current magnetic circuit design path is iterative towards production of a graphic model similar to figure 1 with the low magnetic field volume maximized and the constant low magnetic field contour line closed except in front of the ion optics. Magnetic rings, not shown in figure 1, are added, adjusted, and removed to arrive at a desired magnetic field.

The magnetic circuit design path is iterative and typically follows the procedure defined in the figure 2 flowchart. An iteration of the magnetic circuit design practice requires a time commitment dependent on the period spent in each of the three numbered blocks in figure 2. Block 1 consists of the following: defining the discharge chamber shape in 3–D; defining each magnet’s shape, location, orientation, polarity, and material; defining the discharge chamber material and all discharge chamber nonferrous elements. Note that not all discharge chambers considered are cylindrical, and some magnets may be applied to slanted surfaces. Depending on the size of the discharge chamber, this step may involve applying hundreds of magnets to the simulation. Time exhausted in block 2 is dependent on the magnetic field simulation convergence accuracy, test article complexity, computational speed, and computational memory (RAM). Initiating the magnetic field modeling software in block 2 of figure 2, the program will continuously run until a convergence parameter defining simulation result accuracy is satisfied. The magnetic field simulation convergence parameter is a user defined limit determined by the percent change in total energy of the test article. To gain quick access to magnetic field graphical information similar to figure 1, a 5 percent change is tolerable. Note, for generating files to support particle tracking simulation, it is desired to have a low percent change—less than 0.1 percent. Accordingly, simulation computational time exponentially increases.

Figure 1.—Cross-sectional magnetic field contour map of a normalized hypothetical cylindrical discharge chamber with a normalized contour trace identifying the low magnetic field volume. Magnetic rings are not shown.
increases as the percent change limit decreases. Test article complexity corresponds to the number of elements defining the test article—each magnet, discharge chamber, and all nonferrous components. As the magnetic field modeling software progresses in block 2 of figure 2, program use of computer RAM exponentially increases. In the event the program requires more RAM than physically available, the modeling software will cease. Fortunately, simulation data is not lost if the modeling software ceases due to lack of RAM. If needed, block 3 typically involves adjusting magnet locations, adding magnets, or removing magnets from a simulation. Again, depending on the size of the discharge chamber and how the magnetic field is to be altered, this block could involve applying, moving, or removing hundreds of virtual magnets. Also, block 3 could entail resizing the discharge chamber to make it longer, wider, or any of a number of geometric adjustments involving the cone or front pole piece sections. Streamlining the static magnetic circuit modeling activity laid-out in figure 2 include reducing the time commitments in blocks 1 and 3 by taking advantage of subroutines capable of performing repetitive tasks. Organized cascading of these subroutines to perform automated virtual discharge chamber realization and modification greatly reduces the time commitments of blocks 1 and 3.

The final step in the magnetic field modeling step of the discharge chamber simulation is stockpiling the computational results in a format suitable for repeated use in the grand discharge chamber simulation. This operation is also streamlined by employing subroutines to perform the data reduction exercises. Furthermore, the static simulation results are available for downloading into a suitable format for report generation.

Particle tracking modeling.—The primary motivation towards development of a discharge chamber simulation tool is to propagate state-of-the-art discharge chamber design tactics, with respect to geometric configuration, towards increasing overall thruster performance. To this end, the modeling activity is focused towards maximizing primary electron utilization towards efficient ion beam generation while minimizing losses such as ion recombination and anode cusp primary electron absorption. Specifically, the current state of the modeling activity focuses attention on the role of the primary electrons in the discharge chamber. Future endeavors will incrementally increase the models capability to simulate the complex theater of plasma physics within the discharge chamber. The drive for a 3–D simulation is to reduce loss of information through interpolation. The current state of this modeling activity has the
following assumptions: the primary electron travel originates from the discharge cathode assembly (DCA) tip location, electrons accelerate to simulation speed determined by the discharge chamber voltage, the process is collision less, electrons are guided only by Lorenz forces, electrons will be absorbed by an anode surface upon contact, and electrons will have a “billiard-ball” type reflection off a cathode potential surface.

The first step towards particle tracking simulation was generating a 3–D magnetic field model as discussed above. The second step incorporates the resultant magnetic field model files into a programming environment that is routinely used for control design and simulation by government, academia, and industry. The selected programming environment has access to a graphical user interface as illustrated in figure 3 as well as script code editing capability. Ideally, the complete discharge chamber model will be designed using the graphical user interface. Furthermore, this platform has the ability to run and debug test code; employ many graphic analysis routines and signal conditioning tools; and generate stand alone executable programs that are speed optimized to compete with FORTRAN and C based code. The motivation towards desiring the graphical programming capability is the relative ease for a non user to become acquainted with the software structure. This attractive feature is illustrated in figure 3. The block diagram in figure 3 is for a simulation of an electron element entering a magnetic cusp. The magnetic field

![Graphical block diagram of an electron entering a magnetic cusp simulation. The 3–D magnetic field vectors defining the cusp are identified within the “B vector” subsystem, the “v X B” subsystem calculates the cross product for determining Lorenz force, and the 1/s boxes are integrators.](image-url)
vectors are defined in the “B vector” subsystem, initial particle conditions are defined in the “Initial Conditions” subsection, and acceleration vectors are determined in the “v x B” subsystem. Acceleration, velocity, and location data files are populated for report generation in the “Log” subsystems. As a precursor to the graphical code development, script code is being generated to simulate the 3–D discharge chamber. The script code can be compiled to generate a fast executable program, as will the graphical user interface code, comparable to C or FORTRAN based programs. The script code essentially follows the same looping structure illustrated in figure 3 with the following program enhancements: random initial starting point for primary electrons, boundary conditions, and an auto incremental step size adjustment. The general particle simulation flow chart is illustrated in figure 4.

All primary electrons enter the discharge chamber from a location defined by the cathode tip and with a velocity corresponding to a constant discharge voltage. Letting the +y direction signify axial downstream direction, the initial primary electron location in Cartesian coordinates have randomly selected x and z components and the y component is fixed. The span of x and z starting locations is determined by the inside diameter of a DCA orifice plate. The normalized initial velocity direction is [0, 1, 0] and Monte Carlo vector direction distribution, as well as energy distribution will be employed as the program matures. These initialization activities pertain to block 1 in figure 4. Block 2 in figure 4 discretely repositions the primary electron based on current velocity, position, and local magnetic field vectors and assigns a new velocity vector. These activities in block 2 are dependent on the $\delta t$ time step size.

Careful selection of an appropriate time step, referred to as $\delta t$ in figure 4 is critical to stable sensible simulation. A large $\delta t$ will catapult an electron uncharacteristically across the discharge chamber; whereas, an extremely small $\delta t$ will not show electron progress in a timely fashion. Therefore a fitting $\delta t$ is selected each time step based on the Lorenz force. Finally, after particle displacement is completed in block 2, the electron status is assessed based on its coordinates with respect to the discharge chamber dimensions. Essentially, there are three zones of concern for the electron: beyond an anode surface, beyond the cathode biased screen plane, or within these boundaries. An electron found to be located at or beyond an anode surface is considered absorbed. An electron found to be at or beyond the cathode biased screen plane is reflected with a billiard ball type reflection off the cathode biased surface and the simulation continues. Otherwise, the electron tracking simulation continues at the next time step.

![Flowchart](image)

Figure 4.—Flowchart describing iterative process towards tracking an electron through a discharge chamber.

```
1
Initialize
Primary Electron Location p(k) & Velocity v(k)

2
A(k+1) = q/m_e [v(k) X B(p)]
v(k+1) = v(k) + \delta t/2[A(k+1) + A(k)]
p(k+1) = p(k) + \delta t/2[v(k+1) + v(k)]

Check Boundary Conditions

Electron Absorbed
```
Modeling Results

The 3–D discharge chamber modeling activities for this paper involved two steps: Modeling and analysis of a static candidate magnetic field circuit for discharge chamber consideration and primary electron tracking. The magnetic field modeling activities pertained to discharge chambers shaped as cylinders, partial conics, or rectangular solids. Thus far, primary electron tracking has only pertained to cylindrically and partial conic shaped discharge chambers.

As mentioned above, a crucial step towards magnetic circuit design is an assessment of the closed constant magnetic field contour line containing the low magnetic field volume. For this step, typically a 2–D cross sectional view of the discharge chamber is evaluated. Therefore, a 2–D static magnetic field modeling tool should be sufficient. However, a 2–D simulation makes some assumptions in magnetic circuit analysis such as: ideal magnet size, shape, and distribution. Generally, for axisymmetric discharge chambers, these assumptions are bearable. However, the benefit of modeling in 3–D for this step becomes evident when considering magnetic circuits that are not axisymmetric, such as a rectangular shaped thruster illustrated in figure 5. Figure 5 is a 3–D view of a rectangular thruster with bold contour lines on four planes cutting through the center of the discharge chamber. These contour lines visually define the low magnetic field region. Essentially, figure 5 is equivalent to four unique 2–D representations of a 3–D discharge chamber. If these were the only planes of interest towards efficient discharge chamber design, running the 2–D simulation could have netted the horizontal, x-y plane, and vertical, y-z plane, maps in figure 5 bold black. However, a 3–D simulation will make available representations of any cross sectional plane such as the bold red contour lines on the diagonal planes. Although not represented in this paper, a 3–D analysis makes way for generating magnetic field contour lines on the discharge chamber inside surfaces. This capability helps to verify closure.

Figure 5.—Normalized rectangular discharge chamber with 4 planes of a constant magnetic field contour. The bold black traces are horizontal and vertical planes and the bold red traces are diagonal planes.
Figure 6.—Cut-away view of a normalized cylindrical with partial conic discharge chamber. Constant magnetic field boundary surface identifies a specific magnetic field surface. Bold red trace is a simulated primary electron trajectory initiating from the DCA tip. DCA tip location is represented with a bold black cross mark.

The illustration in figure 6 is a 3–D cut-away view of a hypothetical cylindrical discharge chamber with a 3–D representation of the closed magnetic field value representing the surface boundary of the low magnetic field volume. This discharge chamber is cylindrical with a partial conic section, a front pole piece, and several rings of bar magnets. The polarities of the magnets are consistent within each ring and are opposite to the polarity of adjacent rings. The red trace in figure 6 emanating from a heavy cross-mark represents the path of a simulated electron. The heavy cross-mark signifies the location of the cathode tip for this simulation. By inspection of figure 6, the electron ejects from the cathode, travels into the low magnetic field volume, spirals towards and through the constant Gauss magnetic field boundary surface, mirrors off the surrounding magnetic field, and continues travel in the low field volume. The illustration in figure 7 is a top view perspectives of the discharge chamber represented in figure 6. The illustration in figure 7 clearly reveals the electron leaving the low magnetic field zone, mirroring, and returning into the low magnetic field zone.

Resultant magnetic field maps from 3–D simulations are generally not uniform or symmetric. A reason for these discrepancies could reside in failure to converge to a low enough percent error. This handicap can be due to time or computer memory limitations. However, considering most axisymmetric magnetic circuits are flat magnets on a curved surface, each magnet has finite dimensions, gaps exist between magnets within a ring, and variance of magnetic intrinsic properties; a perfectly uniform and symmetric magnetic field is not expected. Although some actual nonconformity exists, the gross nonconformities characterized in figures 6 and 7 are mainly due to the graphical plotting technique used to generate these figures.
Magnetic field modeling will continue to support initial magnetic circuit designs for cylindrical and rectangular solid discharge chambers. Definitions of a well designed magnetic circuit will be clarified through primary electron tracking exercises coupled with hardware experiments. Primary electron tracking tests will be exercised to aid determination of an optimal low magnetic field boundary definition, optimal magnetic ring locations and orientations toward maintaining primary electrons near the grids, and weighting the electron travel pattern as a design metric. Enhancements to the model will include employment of Monte Carlo techniques to randomly distribute initial electron energy, origin, and velocity vector. Also, Monte Carlo techniques will be employed to identify 3–D ion density distributions where collisions are included. Candidate discharge chambers will be modeled to include primary and Maxwellian electron interactions with neutral and ionic xenon. Another enhancement to be employed will be an automated magnetic circuit optimization routine that will employ artificial intelligent (AI) techniques to reposition, add, or remove magnetic rings towards an optimized design metric(s). This capability will enable a user to initiate a simulation with a best guess magnetic circuit design, let the program run unsupervised, and the results will be an optimized magnetic circuit as per the design metric(s). Finally, taking advantage of the graphical programming approach, this discharge chamber model will ultimately be linked to appropriate cathode and ion optics models. The cathode and ion optics models may be contributed by another source.
Conclusion

Capability to generate 3–D maps of discharge chamber candidate magnetic circuits with unlimited view angles for graphical inspection regarding conformance to maintain a closed low magnetic field boundary design specification has been presented. This paper also presented the capability of unobstructed primary electron tracking within the discharge chamber with the 3–D magnetic field map. Many simulations are planned to aid in development of discharge chamber design by including collisions of electrons with xenon neutrals and ions. Finally, the code was developed to be flexible to accommodate future enhancements by third parties including the application of cathode and ion optics models.

References

Discharge Chamber Primary Electron Modeling Activities in Three-Dimension

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Designing discharge chambers for ion thrusters involves many geometric configuration decisions. Various decisions will impact discharge chamber performance with respect to propellant utilization efficiency, ion production costs, and grid lifetime. These hardware design decisions can benefit from the assistance of computational modeling. Computational modeling for discharge chambers has been limited to two-dimensional codes that leveraged symmetry for interpretation into three-dimensional analysis. This paper presents model development activities towards a three-dimensional discharge chamber simulation to aid discharge chamber design decisions. Specifically, of the many geometric configuration decisions toward attainment of a worthy discharge chamber, this paper focuses on addressing magnetic circuit considerations with a three-dimensional discharge chamber simulation as a tool. With this tool, candidate discharge chamber magnetic circuit designs can be analyzed computationally to gain insight into factors that may influence discharge chamber performance such as: primary electron loss width in magnetic cusps, cathode tip position with respect to the low magnetic field volume, definition of a low magnetic field region, and maintenance of a low magnetic field region across the grid span. Corroborating experimental data will be obtained from mockup hardware tests. Initially, simulated candidate magnetic circuit designs will resemble previous successful thruster designs. To provide opportunity to improve beyond previous performance benchmarks, off-design modifications will be simulated and experimentally tested.