Executive Summary

Adding non-dispatchable solar and wind resources to power grids requires ~120% dispatchable, fast-ramping backup to prevent blackouts. Declining annual capacity factors and rapidly increasing cyclic fatigue are increasing combined cycle power costs. Peaker gas turbines are being increasingly used to cover rapid load transitions and essential backup in today's power grids, but they are inefficient. Rising concerns over pollutant emissions are driving increasingly stringent federal and state regulations and constraints.

"Wet" combustion using water and steam is a promising technology to strongly reduce harmful emissions while boosting Brayton cycle efficiency by ~ 24%. Controlling combustion with water and/or steam lowers peak combustion temperature and oxygen concentration, thereby reducing NOx. Managing excess oxygen and residence time reduce CO emissions. In this work, the design of a breakthrough scalable wet combustor burning natural gas by VAST Power Systems is optimized. This uses reactive computational fluid dynamics (CFD) simulations and machine learning (ML)-based reduced-order models. A Reynolds-Averaged Navier-Stokes (RANS) CFD model with finite-rate chemistry is first developed for the baseline combustor design.

Model performance is initially benchmarked against one-dimensional datasets. The CFD results provide insights into key flow and combustion features in this combustor. The combustor design is then parameterized by selecting 23 geometric and design variables (out of >100 that VAST uses.) An automated framework is developed to generate the combustor geometries and boundary conditions needed for CFD based on a given set of 23 design variable values. To reduce the dimension of the design space, a sensitivity analysis is performed that identifies the top 10 design variables most influential on CO and NOx emission levels, and pressure drop across the combustor. Then, using advanced sampling techniques, 321 parameter combinations are selected to form a large sample of designs to be simulated via CFD modeling.

Based on the results from the simulation campaign, best-performing designs are identified with CO and NOx emissions below the US Environmental Protection Agency (EPA)'s 25 ppmvd (diluted to 15% O_2 on a dry basis) regulated limits for VAST's 15 MW to 100 MW gas turbine market focus. This was further reduced below California stringent 2.3 ppmvd limits and to < 1 ppmvd for many configurations. This was achieved for turbine inlet temperatures ranging from <1200°C to >1500°C. LLNL then prepared a reduced-order model for the combustor based on these CFD campaign results to provide rapid design turnaround and optimization.

Introduction

California has legislated 100% carbon-neutral electricity by 2045. By 2030, solar power is creating already a "Duck Curve", with a >30,000 MW 3-hour late afternoon backup power ramp projected by 2030. Renewables are generating higher demand and greater value for rapid-ramp gas turbines to stabilize grids. Solar and wind growth require a corresponding increase in fast-ramping peakers and/or energy storage. Rapid solar and wind expansion without more backup is already causing California's rolling blackouts. Similarly, South Australia has experienced rolling blackouts, with a transmission line failure causing a statewide blackout. In 2019, Texas' power grid (ERCOT) paid $9,000/MWh to prevent several blackouts. US grid operators are now warning of likely blackouts for Washington DC etc. from rapid coal power shutdowns. Germany's electricity imports increased 43% in 2020 with increasing renewables and retiring coal-fired dispatchable power.

VAST has a portfolio of 28 current US and international patents on its hybrid turbine and related applications. Others have cited VAST's US patent portfolio 1,829 times. VAST’s active US patents have been cited 1,317 times, particularly to our combustion patents. VAST received TechConnect's Innovation award. Two of VAST’s patents earned Ocean Tomo's highest A+ rating. VAST's technology promises sub-ppm emissions without catalysts or ammonia. That breakthrough meets both US EPA requirements, and stringent California emission standards. VAST's FastRamp gas turbines with Trifluid Combustors offer ultra-clean peaking power for 10 MW to 500 MW. FastRamp turbines create a new niche between Brayton Cycle peakers and Combined Cycle baseload turbines. VAST-powered microgrids would enhance grid stability.

To accelerate technology commercialization, further design optimization of the combustor and turbine is imperative. However, practical gas turbine combustors involve over one hundred design parameters, rendering it infeasible to explore the full design using experimental tests. Computational Fluid Dynamics (CFD) simulations provide a viable pathway to investigating the high-dimensional design space, combined with advanced sampling algorithms at an affordable cost. CFD can provide new physical insights into combustor designs. It can also generate a large dataset that can be further exploited to build fast-turnaround reduced-order models for use by design engineers.

In this project, we use High Performance Computing (HPC) with neural net optimization of Computer Aided Design (CAD) and CFD to model VAST's new paradigm. We leverage ANL's reactive CFD modeling expertise to simulate VAST's ultra-clean wet combustion, generating terabytes (TB) of data on ANL's supercomputers. This was combined with LLNL's reduced-order modeling expertise to develop neural network models based on the massive CFD datasets for laptop optimization. In Phase I, initial modeling and optimization explored 6 DoE parameters with 729 CFD runs. In Phase 2, we extend that to progressively model and optimize VAST's priority combustor and turbine design parameters.

Results

Following the Phase I study, the team in Phase 2 first determined where in the design space new simulations should be run to maximize the predictiveness of the surrogate model. A series of parametric simulations were performed to confirm a few minor adjustments needed from the Phase I simulations.

Major improvements to the CAD model compared to the previous phase were then implemented to include additional adjustability to the gas turbine geometry. A significant number of iterations on the VAST spreadsheet and the CAD model were performed by ANL to integrate these new changes into the new CAD model pipeline, enabling simulations to be more easily run for the wide set of parameters to be investigated. Compared to Phase I, two new geometrical features were added to the CAD model: 1) cylindrical versus curved orifice geometries for each flow inlet to understand the effect of the presence of nozzle geometry, and 2) elongation of the computational domain in the streamwise direction to investigate the effect of length on mixture composition at the combustor exit. To accommodate these two geometrical changes, ANL updated the CFD setup in CONVERGE and further improved the accuracy and speed of the CFD model. Using ANL’s latest CFD setup, each simulation takes two days to finish using 64 CPU cores on ANL's LCRC cluster.

To systematically reduce the dimension of the design space, a sensitivity analysis for 20 important parameters identified in previous studies was performed. The top-ten design variables were identified based on a merit function that accounts for exit CO emissions, exit NOx emission, and pressure drop across the combustor.

Based on the results of the sensitivity run, LLNL identified 321 combinations of design parameters for the next-step Design of Experiments using advanced sampling. CAD geometries and CFD boundary conditions were generated corresponding to these parameter combinations. ANL and VAST worked towards refining the combustor model spreadsheet and CAD model to accommodate the new batch of 321 combustor designs. Scripts to automate the process of generating the geometries and corresponding boundary conditions were developed by ANL.

The 321 CFD simulations were carried out and key CFD results, including mass fractions of CO and NOx emissions and temperature at the combustor exit, the pressure-drop across the combustor, as well as the axial profiles of these quantities (CO and NOx emissions and temperature) were tabulated, compiled, and provided to the VAST team for further analysis. Based on the results from the simulation campaign, best performing designs were identified with CO and NOx emissions below 2.5 ppmvd (diluted to 15% O_2 on a dry basis) for turbine inlet temperatures ranging from 1,200°C to 1,500°C. The best performing designs were further analyzed using an additional CFD campaign consisting of 97 simulations to investigate potential flame quenching. The result provided additional insights to the mixing process of fuel/oxidizer/diluent fluids in the upstream portion of the combustor and reassured that combustion is healthy for the best performing designs.

LLNL then used these updated design inputs and CFD outputs to build a reduced-order model of the VAST combustor. This runs on a professional laptop computer.

Discussion

During the course of the Phase 2 project, VAST has identified and ranked the sensitivities of 23 combustor design parameters, compared to the 6 parameters modeled in Phase 1, out of VAST’s over 100 independent combustor design variables. However, substantial delays were caused by the geometric complexities of VAST's combustor, and discovering bugs in the new CAESES 5.0 parametric CAD/optimization program. These bugs were very difficult for the German development team at Friendship Systems, Inc. to identify and correct. The bugs delayed VAST's runs, causing apparently random CFD meshing failures that required ANL's manual intervention and restarts. These problems first appeared in November 2021 and continued until they were apparently resolved by the German programmers in May 2022.

The main lesson from this experience is that when dealing with complex geometries for design optimization with HPC, it would be beneficial to initially use simple geometries while retaining reasonable complexity to minimize human errors. Then develop a modern code review/debug platform to systematically and efficiently detect software errors.

Implementation

The project is implemented with the following project tasks with associated deliverables.

Task 1: Prioritize Parameters for New Study

The team first reviewed the data collected from the Phase 1 study to better determine what parameters should be studied in more detail in Phase 2. Based on this data review, LLNL and VAST prioritized a few additional parameters for further sensitivity studies. This helped determine what expanded parameter set would be most relevant to reducing pollutant formation and improving combustor performance. ANL then ran this reduced parameter set study. This was extended to include another major combustor parameter sensitivity study. ANL relayed that data to the rest of the team to prioritize further studies.

Deliverables: (3 months after project start): ANL: Results from the expanded parameter set sensitivity study. VAST: Prioritized list of new parameters for subsequent CFD runs.

Task 2: Perform Detailed Pilot and Upstream Simulation

With VAST's key upstream parameters, ANL concurrently ran detailed simulations of VAST's assumed pilot and the upstream 5% Trifluid combustor region. This Design Of Experiment (DoE) study quantified combustor operating range limits with reduced order chemistry. It then clarified combustion blow off bounds of oxygen, temperature, primary zone loading, and relative delivery rate. These results will ensure designs that will safely and reliably operate within quantified limits.

Deliverables: (3 months after project start): ANL: Data from the pilot and upstream CFD study.

Task 3: Model Heat Transfer for Combustor Wall

With Phase I & 2 CFD runs, VAST formed a Heat Transfer model of combustion to an insulated cooled combustor wall, in CAESES for use with ANSYS Finite Element Analysis with PVAMU's help. PVAMU conducted preliminary combustor stresses for several flow rates. This effort was intended to explore rapid ramp rates versus conventional dispatch using quantitative FEA modeling for future modeling and cyclic stress fatigue analysis.

Deliverables: (3 & 10 months after project start): ANL: Enhanced CFD model for VAST combustor with cooled insulated wall heat transfer sensitivities. Then VAST combustor fatigue results.

Task 4: Perform Refined CFD Study with Expanded Parameters

VAST and LLNL reviewed results of Tasks 1 and 2 relative to Phase 1. They refined parameters for further runs. ANL ran further CFD studies based on refined parameters from Tasks 1, 2 and 4 and Phase 1. These enhanced the database for LLNL to use to elevate the surrogate model to make predictions.

Deliverables: (11 months from start or Task 1 end): ANL: Pilot & upstream region CFD study data.

Task 5: Elevate Reduced Order Model (ROM) from Phase I

ANL's CFD runs were post-processed to average outlet and axial properties (and optionally peripheral properties). LLNL processed those CFD results by using machine Neural Network Analysis to update its fast-running Reduced Order Model. LLNL combined these sensitivities with VAST's quadratic scaling models of cycle components fluid parameters obtained from VAST's Thermoflex model optimizations. LLNL provided a desktop computer capable inference optimization model to quickly simulate output from key operation and design parameters.

Deliverables: (11 months from start) LLNL's Reduced Order VAST Cycle Model

Task 6: Model VAST Cycle in pyCycle on OpenMDAO

VAST was to develop methods to configure a 1D streamline model of VAST's Cycle and combustor in NASA's pyCycle on OpenMDAO, adapting NASA's electric aircraft model. This was to model steam and hot water heat recovery and deliver it back upstream into a VAST combustor. This was to leverage, complement, and extend the complexity reduction of LLNL's Reduced Order Model. It was to use OpenMDAO equilibrium and reactive chemistry (equivalent to RefProp and Cantera). It would enable extending VAST's combustor and cycle optimization to more parameters. The much larger effort required in the earlier tasks combined with the COVID19 hindrances caused this task to be cancelled.

Deliverables: (11 months from start): VAST Cycle 1D pyCycle methodology.

Task 7: Prepare Final Report.

ANL, LLNL and VAST will prepare and submit the final report to DOE.

Issues or Challenges

The main issues were related to the complexity of the VAST CAD geometry and spreadsheet and its integration with the parametric CAESES software. Efforts dedicated to resolving the software integration challenge caused unexpected long delays to the project. To address this issue, a six-month extension was requested. This extension enabled ANL to conduct the major CFD runs that were previously limited by scheduling constraints, not the 16 million allocated core hours of computer time. The extension also enabled LLNL to perform major nonlinear neural network analysis and optimization of the complex data. The extension enabled some work to be done by three professors at Prairie View A&M University (PVAMU) who worked on the combustor cooling models towards the Task 3 deliverable.

The negative effects of COVID-19 access hindered PVAMU's functioning. It prevented PVAMU from mobilizing student researchers because the campus was closed for many months. COVID-19 also stopped contract negotiations for several months until February 2022.

Impact

Company Impact: The project established the breakthrough Platform Technology that combined the capabilities of the two national laboratories. It created an innovative, highly efficient, and much faster design paradigm combining supercomputer intensive reactive CFD modeling with neural net data reduction. It developed reduced-order equation models to facilitate design on VAST's professional laptop computers without requiring the ongoing support of supercomputers. This is providing much greater credibility to VAST in marketing its technology. Industry experts have recognized that this Platform Technology promises major reductions in time and cost for project design across a wide range of US industries.

National Impact: VAST® provides a new more cost-effective backup power generation system essential to enable increasing penetration of intermittent renewable solar and wind power. It offers new technology for the rapidly growing market of renewable power backup - beyond peaker turbines. VAST FastRamp™ Turbines offer economically superior IRR, competitive from peaking to baseload power. This enables growth of renewable energy with much lower blackout risk.

The Energy Information Administration (EIA) Annual Energy Outlook (2023) projects 179 GW growth of Peaker (simple cycle) turbines and generators by 2050. VAST offers 24% higher efficiency than current peaker gas turbines. VAST's ultraclean combustion eliminates 6% to 9% emission cleanup capital costs plus ongoing ammonia operating costs. These provide a basis for increasing exports with consequent US job creation.

Future Work

During this CRADA Phase 2 work, VAST modeled numerous variations on its ultra-clean combustor apparatus and methods technology and quantified the resulting performances. VAST has filed two provisional patent applications on its breakthrough scalable clean combustors entitled:

SYSTEMS AND METHODS FOR SCALABLE COMBUSTORS, Docket No. 6377.001PRV.
SYSTEMS AND METHODS FOR SCALABLE COMBUSTION, Docket No.: 6377.002PRV.

These applications will likely result in the filing of multiple Divisional, Continuation and Continuation-in-Part patents. VAST expects that it will obtain multiple US and international patents from these HPC4Mfg DoE CRADA grants, with multiple Divisional, Continuation and Continuation-in-Part patents.

VAST is working to extend this exploratory modeling to design, testing and commercializing of its ultra-clean combustors and breakthrough power cycles. It further plans to extend this work to renewable fuels.

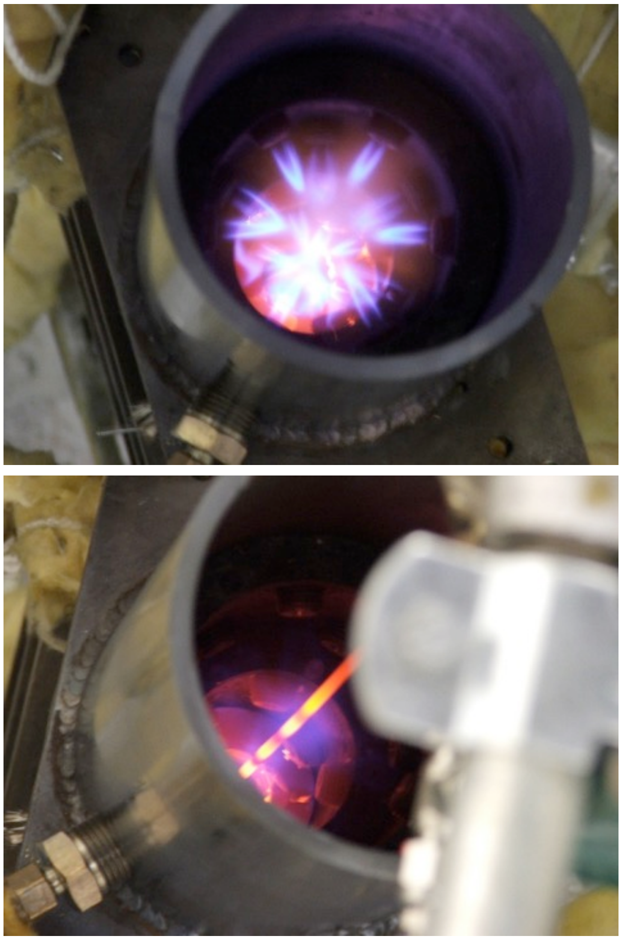

Figure 1. Flame images from traditional combustion technology (top) and VAST ultra-clean combustion technology (bottom).

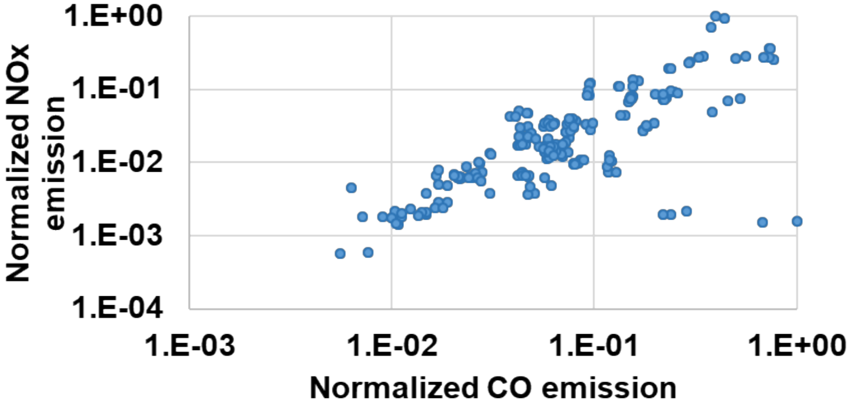

Figure 2. Correlation between normalized NOx and CO emissions for the Design of Experiment campaign that consists of 321 simulations.