Machine Learning based Optimization of Valve Timing and Intake Charge Boosting in a Hydrogen Port Fuel Injection Engine

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DECLARATION

I declare that this is my own work and this thesis/dissertation does not incorporate without acknowledgement any material previously submitted for a degree or diploma in any other University or Institute of higher learning and to the best of my knowledge and belief it does not contain any material previously published or written by another person except where the acknowledgement is made in the text. I retain the right to use this content in whole or part in future works (such as articles or books).

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The above candidate has carried out research for the Master's thesis under my supervision. I confirm that the declaration made above by the student is true and correct.

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Finally, I dedicate this thesis to all those who strive to advance cleaner energy and sustainable engine technologies. Your efforts continue to inspire my own journey.

ABSTRACT

Hydrogen-fuelled internal combustion engines (H_2ICEs) present a promising near-term pathway for decarbonizing transport; however, their widespread adoption is constrained by abnormal combustion phenomena such as backfire and by trade-offs between performance and emissions. To address the above issues, current study developed a computational framework that integrates high-fidelity Computational Fluid Dynamics (CFD) simulations with machine learning-based surrogate modeling to optimize valve timing and intake charge boosting in a hydrogen port fuel injection (PFI) engine. CFD simulations were performed in the commercial code CONVERGE v4.1. The CFD model captured ignition kernel formation, flame propagation, and backfire evolution accurately. A Design of Experiments (DOE) using Latin Hypercube Sampling (LHS) quantified the influence of valve overlap timing (VOT) and intake pressure on indicated power, NOx emissions, and backfire risk. General trends showed that boosting strongly increases power however, it exacerbates NOx and backfire risk, while extended overlap reduces backfire but increases NOx. To reduce computational cost, an ensemble of surrogate models—comprising Random Forest, Support Vector Regression, Ridge Regression, Extreme Gradient Boosting, and Neural Networks—was trained, achieving R^2 values exceeding 0.95 across all objectives. These models enabled efficient optimization via a merit function framework, where tunable weights (α, β) balance competing objectives. Instead of conventional fixed-weight optimization, continuous trade-off surfaces were constructed across the (α, β) space, providing global insight into how weightings affect outcomes. This approach revealed key sensitivities and feasible regions under emission and backfire constraints, allowing informed selection of operating strategies. The developed CFD–ML framework and trade-off surface methodology provide a computationally efficient and generalizable strategy for multi-objective optimization in hydrogen engine design.

Keywords: Hydrogen Port Fuel Injection Engine; Valve Timing Optimization; Intake Charge Boosting; CFD Simulation; Surrogate-Based Multi-Objective Optimization

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LIST OF ABBREVIATIONS

Abbreviation	Description
ABC	Artificial Bee Colony (optimization algorithm)
AMR	Adaptive Mesh Refinement
ANN	Artificial Neural Network
aTDC	After Top Dead Center
BFL	Backfire Limit (equivalence ratio threshold)
BMEP	Brake Mean Effective Pressure
BSFC	Brake-Specific Fuel Consumption
BTE	Brake Thermal Efficiency
CA	Crank Angle
CAD	Crank Angle Degrees
CFD	Computational Fluid Dynamics
COV_IMEP	Coefficient of Variation of IMEP
CVODE	Variable-coefficient ODE solver (in SUNDIALS)
DI	Direct Injection
DoE	Design of Experiments
ECN	Engine Combustion Network
EGR	Exhaust Gas Recirculation
EVC	Exhaust Valve Closing
EVO	Exhaust Valve Opening
FCEV	Fuel Cell Electric Vehicle
GA	Genetic Algorithm
GHG	Greenhouse Gas
GISFC	Gross Indicated Specific Fuel Consumption
GPR	Gaussian Process Regression
H_2ICE	Hydrogen Internal Combustion Engine
HPC	High-Performance Computing
ICE	Internal Combustion Engine

IEA	International Energy Agency
IMEP	Indicated Mean Effective Pressure
IP	Indicated Power
IPCC	Intergovernmental Panel on Climate Change
ITE	Indicated Thermal Efficiency
IVC	Intake Valve Closing
IVO	Intake Valve Opening
kNN	k-Nearest Neighbors
k–ε (RNG)	k–epsilon turbulence model (Renormalization Group form)
LHS	Latin Hypercube Sampling
MAP	Manifold Absolute Pressure
ML	Machine Learning
MOO	Multi-Objective Optimization
MPRR	Maximum Pressure Rise Rate
NN	Neural Network
NNLS	Non-Negative Least Squares
NSGA-II	Non-dominated Sorting Genetic Algorithm II
PFI	Port Fuel Injection
PMAX	Peak Cylinder Pressure
PSO	Particle Swarm Optimization
R^2	Coefficient of Determination
RANS	Reynolds-Averaged Navier–Stokes
RBFNN	Radial Basis Function Neural Network
RF	Random Forest
RR	Ridge Regression
RNG	Renormalization Group (Turbulence model variant)
RSM	Response Surface Model
SAGE	Detailed chemical-kinetics solver in CONVERGE
SCR	Selective Catalytic Reduction
SI	Spark Ignition
SOpHy	Sandia Optically accessible Hydrogen engine

SUNDIALS	Suite of Nonlinear and Differential/Algebraic equation Solvers
SVR	Support Vector Regression
TDC	Top Dead Center
VOT	Valve Overlap Time
WI	Water Injection
XGBoost	Extreme Gradient Boosting
α, β	Merit-function weight coefficients
ϕ (phi)	Equivalence ratio
λ (lambda)	Excess-air ratio
bTDC	Before Top Dead Center

LIST OF APPENDICES