Mitigation of Abnormal Combustion

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Project # ACE147
Overview

Timeline

• PACE started in Q3, FY19
• PACE will end in FY23 (46% complete)
• Focus and objectives of individual tasks will be continuously adjusted
• Overall PACE work plan discussed in ACE138

Budget

Presentations covers three FY21 PACE projects

<table>
<thead>
<tr>
<th>Task</th>
<th>FY20</th>
<th>FY21</th>
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<tbody>
<tr>
<td>O.E.02: Effectiveness of EGR to Mitigate Knock Throughout PT Domain (ORNL, Szybist)</td>
<td>$220k</td>
<td>$175k</td>
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<tr>
<td>O.E.09.01: Fuel Spray Wall Wetting and Oil Dilution Impact on LSPI (ORNL, Splitter)</td>
<td>$220k</td>
<td>$220k</td>
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<tr>
<td>O.E.08 ML/Nonlinear Dynamics (ORNL, Kaul)</td>
<td>$200k</td>
<td>$200k</td>
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Complete PACE budget in reviewer-only slides

Barriers

USCAR Priority 1: Dilute SI Combustion

• Knock Mitigation → Developing a better understanding of the effectiveness of EGR to mitigate knock
• Low speed preignition → Developing a better understanding of underlying mechanisms causing LSPI, as well as mitigation strategies

PACE Major Outcome 1: Models to accurately predict knock
PACE Major Outcome 2: Data analytics of knock/SPI
PACE Major Outcome 3: Phenomenological model of LSPI

Partners

• PACE is a DOE-funded consortium of 5 National Laboratories working towards a common goal (ACE138)
  o Goals and work plan developed considering input from stakeholders including DOE, ACEC Tech Team, CFD code developers, and more
• Specific partners on this work include:
  o LLNL, ANL on surrogate development and kinetics, ANL on simulation of knock and SPI conditions
  o Related SPI funds-in project with CRC and DFO CRADA
  o SPI data from Lubrizol for ML/analytics
Overall Relevance of PACE:
PACE combines unique experiments with world-class DOE computing and machine learning expertise to speed discovery of knowledge, improve engine design tools, and enable market-competitive powertrain solutions with potential for best-in-class lifecycle emissions.

Presentation Specific Relevance: PACE Major Outcomes 1, 2 and 3

- **Major Outcome 1**: Models for combustion system design accurately predict knock response to design changes.
- **Major Outcome 2**: Data analytics enable operation and real-time control to mitigate knock/LSPI.
- **Major Outcome 3**: Develop new multi-step phenomenological mechanism for LSPI that captures wall-wetting, lubricant, and geometry effects.

Presentation Specific Relevance: USDRIVE ACEC Priority 1 for Dilute SI Combustion

- **Knock Mitigation**: Developing a better understanding of the effectiveness of EGR to mitigate knock and machine learning approaches for online knock reduction strategies.
- **Low-speed Preignition**: Developing a better understanding of underlying mechanisms causing LSPI, as well as mitigation strategies.

### Three Tracked Milestones for FY21 that are On-Track

<table>
<thead>
<tr>
<th>Task:</th>
<th>Milestones:</th>
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<tbody>
<tr>
<td><strong>Fuel Spray Wall Wetting and Oil Dilution Impact on LSPI</strong></td>
<td>RD587 surrogate validation and development with high end boiling point compounds to compare to the actual fuel using FIL diagnostic</td>
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<tr>
<td><strong>Effectiveness of EGR to Mitigate Knock Throughout PT Domain</strong></td>
<td>Provide experimental data on the sensitivity of the knock-limited combustion phasing to the addition of NO, acetylene, and ethylene in the intake mixture with and without catalyzed EGR using the PACE engine geometry</td>
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<tr>
<td><strong>ML/Nonlinear Dynamics</strong></td>
<td>Evaluate dynamics of abnormal high-load SI combustion (knock/pre-ignition) to identify potential deterministic drivers</td>
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<table>
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<tr>
<th>Due Date:</th>
<th>Status:</th>
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<tr>
<td><strong>Q2 FY20 (6/30/21)</strong></td>
<td>On Track</td>
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<tr>
<td><strong>Q4 FY20 (9/30/21)</strong></td>
<td>On Track</td>
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<tr>
<td><strong>Q4 FY21 (9/30/21)</strong></td>
<td>On Track</td>
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Major outcome 3: Phenomenological model of SPI processes and relations for SPI mitigation

- SPI remains a significant abnormal combustion problem in SI engines limiting efficiency opportunities.
- Wholistic understanding of the fundamentals causing SPI remains a barrier.
- Several cause-and-effect relations have been noted in the literature, but critical interactions and the associated steps required to cause SPI remain unclear.
- FY21 studies focus on fuel retention and top ring zone liquid interactions for informing chemistry causing SPI ignition sources.

Major outcome 3 of PACE will develop a phenomenological model of SPI fundamental requirements.
Experimental LSPI Approach Focuses on Fuel-Wall Interaction and Liquid Retention as Potential Source of LSPI

- Quantification of fuel-wall interaction at high load and resulting SPI activity
  - Apply LiF diagnostic to quantify fuel-oil dilution in the oil returning from top ring zone

- GM LNF 2.0L engine converted to single cylinder with dry sump oiling system
  - ORNL control system for LSPI testing using automated test sequence (10 segments, 25,000 cycles per segment)
  - Dry sump reduces sump dilution of oil for LIF, increased signal, reduced run time for signal

- Dye-based LiF diagnostic developed at ORNL
  - Previously developed as part of ACE032
  - Diagnostic received 2013 R&D 100 Award
FiL diagnostic applicable over a wide range of conditions, strongly correlated with in-cylinder conditions at injection

- FiL show that in-cylinder conditions and load dramatically affect fuel-wall impingement
  - Guidance for of PACE surrogate fuel highlight that both light and heavy components can affect wall wetting
- Qualitatively ratio of in-cylinder pressure and fuel vapor pressure show correlation
  - Results suggest spray dynamics over in-cylinder conditions affect fuel wall impingement
- These scoping study results are not full SPI test results, outcome used to define SPI test points

Is wall wetting alone causing SPI?
- Results suggest no, and that complex fuel wall interactions and fuel retention are critical for SPI, not simply wall wetting
SPI found to be dependent on impinged fuel that remains on the wall not fuel-wall impingement only

- Full 10 segment SPI test with low and high distillation fuels at defined points from scoping
- Fuel targeting the piston (310 SOI)
  - Large difference in FiL rates
  - Low SPI rates regardless of distillation
- Fuel targeting the wall (220 SOI)
  - Increased heavy end of fuel increases SPI even if wall impingement is similar
- FiL diagnostic measured dye not fuel
  - Dye has flashpoint of 152°C
- Carbon balance (lambda mass), shows that when fuel is retained in the engine SPI rates increase

Results show that fuel must impinge and remain on the linear for SPI rates to be dramatically affected (results show ~1/3 does at high SPI point here)
Extensive literature review suggest nitrogen chemistry pathway is possible in top ring zone liquid causing SPI

- Fuel wall interaction and increased retention occurs at cold start and high load, SPI only at high load, why?
  - Increased thermal input? radical species? time?
- Literature review and prior results suggests highly reactive species can form in retained top ring zone liquid with NO/NO₂
  - Lubricant additives possibly catalyze combustion of nitro esters (suspected root source detergent effect)
  - Nitration chemistry occurs at SPI-relevant engine temperature, pressure, and time scales
    - Fuel and lubricant mixtures alone do not meet ignition criteria timescales needed for SPI
- FY21 experiments will probe NO/NO₂ effect on SPI with liquid retention measurement
Major Outcome 2: Characterize, Predict, and Control Chaos

Motivation: SI power density limited by abnormal combustion (knock/pre-ignition)
• Current engine controls are reactive to detected knock or pre-ignition, but cannot predict/avoid occurrence of abnormal combustion events
• Prediction and/or advanced detection could enable real-time mitigation strategies

Cross-cutting task applies machine learning (ML) & nonlinear dynamics to mitigation of various abnormal combustion phenomena
• Go/No-Go decision points annually on progress and outcomes

Characterize deterministic patterns in abnormal combustion using ML and nonlinear dynamics/statistical analysis techniques
• Leverage techniques developed for dilute SI combustion instability
• Enhance understanding of feedback mechanisms

Predict next-cycle dynamics using ML, probabilistic, or model-based methods
• Data interpretation and development of control-oriented models for simulation
• Pattern recognition and prediction through ML and probabilistic techniques

Control strategies developed to mitigate abnormal combustion
• Take advantage of any identified deterministic features to mitigate abnormal combustion
• Leverage machine learning, advanced simulations

FY 20 Focus: Dilute Cyclic Variability
FY 21 Focus: Knock & Pre-ignition
FY22 Focus: Cold Start Stability

Overview | Relevance | Milestones | Approach & Results (6/11) | Reviewers | Collaborations | Barriers | Future Work | Summary
Principal Component Analysis of Phase-Space Transformed Pressure Data Allows Earlier Detection of Pre-Ignition

Baseline Cylinder Pressure:
Cylinder pressure data showing threshold based on deviation > 4.7σ from non-SPI cycles
SPI is detectable prior to spark.

Phase-space Transform & Principal Component Analysis (PCA):
Time-delay embedding of cylinder pressure facilitates observation of deviations in trajectory for abnormal cycles.
PCA orients axes towards greatest variation, improving signal-to-noise ratio and reducing dimensionality.

Earlier Detection of SPI:
First principal component deviates from baseline up to 1-2°CA earlier than cylinder pressure directly considered in crank-angle space.
FY20 Developed ML-Based Next-Cycle Engine Control Capability, Applicable to Abnormal Combustion in FY21

- Optimized spiking neural networks (SNNs) deployed on low size, weight, and power (SWAP) hardware and integrated with real-time engine controls
- Next-cycle control based on prior-cycle heat release was demonstrated, with 2% increase in EGR dilution limit for fixed CoV threshold
- Demonstrated ability to implement ML-based next-cycle control actions: Can be applied for mitigation of high-load SI phenomena if actionable precursors are identified

Optimized Network

Offline Optimization and Training

Optimal Spark

Open-Loop

OL - 30%

OL - 60%

2% Increase in Dilute Limit
ML Approach Shows Promise for Knock Prediction

- Knock and pre-ignition experimental data collected in O.E.02 and O.E.09.01 being analyzed
  - Additional on-road pre-ignition data set also obtained from Lubrizol under NDA
- ML toolkits for supervised & unsupervised learning techniques first developed using dilute SI data have been adapted to knock/LSPI: currently applying to data sets to determine whether actionable precursors can be identified (on track for milestone)
- PACE generated data sets are open for use by others including industry

Workflow for AI-based analysis applied to abnormal combustion events

- Experimental data collection
- Identification of response variable (e.g., knock intensity, SPI, misfire)
- Feature selection (e.g., PCA, correlation, mutual information)
- Train AI predictor (e.g., GPR, SVM, decision trees, ANN)

SAE 2020-01-2053
Collect Data for CFD Model Validation while Improving Understanding of P, T, and Composition on Autoignition Chemistry

Motivation: Collect data on knocking engine conditions for model validation
- Effect of pressure-temperature (PT) trajectory on knock propensity
- Effectiveness of EGR to mitigate knock
- Impact of minor species in EGR on knock propensity

FY20 Progress: Completed initial campaign of single-cylinder engine experiments
- Eight operating conditions in PT domain, including 2x change in engine speed, comparison of EGR effectiveness with/without catalyst treatment
- Comparison of fully-formulated fuel vs. PACE surrogate
- Results showed EGR is less effective at mitigating knock under “beyond RON” conditions
- Results also showed that catalyst-treated EGR is more effective at mitigating knock
- Results published in SAE (2020-01-2053)

FY20 Results Shared Widely within PACE
- Data shared with surrogate development team to down-select surrogate composition
- Major Outcome 1 Integration Task: Provided data to ANL for CFD model validation (Sibendu Som, Chao Xu, and Roberto Torelli)
- Major Outcome 2: Applicability of ML and nonlinear dynamics to mitigating high-load SI abnormal combustion phenomena at ORNL (Brian Kaul)
• ORNL is installing PACE engine geometry for FY21 studies
  o Converting Ford 2.3 L multi-cylinder engine to single-cylinder operation
  o Installing multi-cylinder engine in adjacent test cell
  o Engine is on-track to be commissioned by the end of June

• Planned experiments will focus on components increase knock propensity in the presence of EGR
  o Collaborating with ANL (Goldsborough, A.E.01) and LLNL (Pitz, L.M.01.01) on components to investigate
  o Focus will be on interactions between NO and olefins and align with compositions being investigated in ANL rapid compression machine
  o Mass flow controller system for dosing individual components is complete

• Experiments will start after PACE engine is commissioned
  o On-track for completion in Q4
Responses to Previous Year Reviewers’ Comments

Task O.E.02 (ORNL, Szybist: Effectiveness of EGR to Mitigate Knock throughout the P-T Domain)
• “Causes of increased EGR effectiveness with aftertreatment with a TWC are unclear. It is not clear what individual compound or combination of compounds cause knock mitigation. The researchers should investigate the effect of CO and NO on knock.”
  o We agree that these are unanswered questions. The FY21 milestone, which is on-track for Q4, is to complete an investigation to answer this question. We will focus on the role of NOx, and are collaborating with kineticists at ANL and LLNL.

Task O.E.08 (ORNL, Kaul: Machine Learning and Nonlinear Dynamics)
• “… how is the team linking the observed sources of variation to control variables or design variables? Can the team actually effect a change based on the team’s ML predictions with the physical engine technology?”
  o For cyclic variability prediction, ML predictors were trained using a phenomenological model based on residual gas composition as the next-cycle feedback mechanism. Next-cycle control via fuel injection quantity was demonstrated in FY20, yielding a 2% increase in dilution tolerance at a fixed COV threshold.
• “Using ML to explore for insight into predictive capabilities for cyclic variability is full of challenges and complexity, but interesting, and if successful, will be a tremendous advancement.” “The next-cycle prediction … would be extremely useful to improve engine performance.” “It is also clear how the machine learning task contributes to realizing higher efficiency combustion strategies in the real world.”
  o We appreciate the positive comments and agree with the reviewers regarding both the challenges and potential benefits of this approach.

Task O.E.09.01 (ORNL, Splitter: Fuel Spray Wall Wetting and Oil Dilution Impact on LSPI)
• The approach appears well suited to addressing the technical barriers for knock mitigation and fuel-oil influences on LSPI
  o We appreciate the positive comments and agree with the reviewers, the information gleaned is helping to better inform the phenomenological model in that fuel-wall impingement is not the only factor but more importantly the fuel retention of impinged fuel is seemingly most important.
• “In particular, the LSPI task does not identify specific collaborations contributing to its outcomes”
  o We appreciate the feedback, and note that several discussions have been ongoing on conditions and operating parameters with several industrial stakeholders in complementary programs with the coordinating research council and a CRADA with GM. Moreover, the LiF results have shown interesting information that is directly applicable to broader PACE spray and simulation efforts that we are integrating and interacting on.
Overall PACE Collaborations (see ACE138)

- PACE is a collaborative project of multiple national laboratories that combines unique experiments with world-class DOE computing and machine learning expertise to speed discovery of knowledge, improve engine design tools, and enable market-competitive powertrain solutions with potential for best-in-class lifecycle emissions.
- The work plan for PACE is developed in coordination with the USDRIVE Advanced Combustion and Emission Control Tech Team.

Task-Specific Collaborations

- **Task O.E.08 (ORNL, Kaul: ML/Nonlinear Dynamics)**
  - Other PACE tasks: collaboration on data sets for analysis.
  - Lubrizol: collaboration on data set for high-load abnormal combustion analysis (pre-ignition).
- **Task O.E.02 (ORNL, Szybist: Effectiveness of EGR to Mitigate Knock throughout the PT Domain)**
  - Data supplied for MO1 Integration (Planned ANL FY22 task).
  - Data supplied for MO2 (Task O.E.08, ORNL, Kaul: ML/Nonlinear Dynamics).
  - Collaborating with ANL (Goldsborough, A.E.01) and LLNL (Pitz, L.M.01.01) on components to investigate.
- **Task O.E.09.01 (ORNL, Splitter: Fuel Spray Wall Wetting and Oil Dilution Impact on LSPI)**
  - Data supplied for MO2 (Task O.E.08, ORNL, Kaul: ML/Nonlinear Dynamics).
  - Collaborating with ANL (Torelli, A.M.04.01) and PACE spray team (ACE167) on SPI fuel-wall interaction results.
  - CRC: related program on broader SPI work also using the LiF diagnostic over matched operating conditions and data analysis.
  - GM CRADA: related program on fuel volatility in SPI also using the LiF diagnostic.
## Remaining Challenges and Barriers

### Proposed Future Research

Any proposed future work is subject to change based on funding levels.

### Major Outcome 2

**O.E.08**  
(ORNL, Kaul: ML/Nonlinear Dynamics)

- Applicability of ML and nonlinear dynamics to mitigating high-load SI abnormal combustion phenomena is currently being evaluated
- Control strategies will need to be devised to take advantage of predictions to mitigate instabilities

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<tr>
<th>Remaining Challenges and Barriers*</th>
<th>Proposed Future Research</th>
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<tbody>
<tr>
<td>• Moving to a new engine platform will require a new baseline of knock performance for model validation</td>
<td>• Complete evaluation of SI knock/preignition data to determine whether actionable intra- or inter-cycle precursors can be identified (FY21 milestone – on track)</td>
</tr>
<tr>
<td>• Significant uncertainty with combustion chamber surface temperatures for model validation</td>
<td>• Identify phenomena of greatest potential to focus future mitigation demonstration efforts (FY22 decision point)</td>
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<tr>
<td>• Perform new baseline using PACE-20 surrogate in the new engine geometry with and without EGR over a range of intake temperature and pressure conditions</td>
<td>• Develop and implement control strategies to mitigate combustion instabilities based on ML &amp;/or model-based predictions</td>
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<td></td>
<td>• Evaluate the applicability of these techniques to mitigate cold-start combustion instabilities</td>
</tr>
<tr>
<td>• NO and NO2 chemistry effects with baseline fuels and PACE 20</td>
<td>• Chemical dependency of lubricant additive formulations with fuel retention on SPI sources, identifying critical chemistry effects</td>
</tr>
<tr>
<td>• As produced PACE-20 surrogate characterization on SPI</td>
<td>• Vary coolant/oil temperature to study fuel retention effects with FiL</td>
</tr>
<tr>
<td>• Characterizing and understanding spray processes at SPI relevant conditions with greater PACE effort and subtask teams</td>
<td>• Work with ORNL diagnostics experts on FiL for including retained species identification as able</td>
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* PACE-wide barriers are discussed in ACE138

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**O.E.02**  
(ORNL, Szybist: Effectiveness of EGR to Mitigate Knock throughout the P-T Domain)

- Moving to a new engine platform will require a new baseline of knock performance for model validation
- Significant uncertainty with combustion chamber surface temperatures for model validation

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**O.E.09.01**  
(ORNL, Splitter: Fuel Spray Wall Wetting and Oil Dilution Impact on LSPI)

- NO and NO2 chemistry effects with baseline fuels and PACE 20
- As produced PACE-20 surrogate characterization on SPI
- Characterizing and understanding spray processes at SPI relevant conditions with greater PACE effort and subtask teams

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This task is cross-cutting, future work plans include contributions to other PACE outcomes in addition to abnormal combustion mitigation.
Relevance

• Overall goals of PACE are to speed discovery of knowledge, improve engine design tools, and enable market-competitive powertrain solutions with potential for best-in-class lifecycle emissions
• Mitigation of knock and LSPI are the top barriers to attaining higher efficiency for dilute SI combustion in USDRIVE roadmap

Approach

• SCE experiments to measure effectiveness of EGR on knock mitigation over a large dimension space (PT trajectory, timescale, w/ and w/o TWC)
• LSPI investigations to measure fuel dilution of lubricating oil
• Outputs of these investigations feeding into other PACE efforts: machine learning, CFD modeling, kinetic model development, and sprays
• Use Machine Learning (ML) and nonlinear dynamics analysis to enable mitigation of abnormal combustion cycles through active controls

Accomplishments

• Completed LSPI characterization of fuel-wall interaction, observed critical FiL relation on SPI, retained fuel and conditions of retention
• Developed and deployed spiking-neural-network-based next-cycle engine controller for dilute combustion stability control - foundation for future abnormal combustion mitigation efforts
• Developed ML toolkits for analysis of knock and pre-ignition data and demonstrated earlier detection of pre-ignition using delay embedding and PCA

Collaborations

• PACE is a collaboration of 6 National Laboratories, workplan developed considering input from ACEC TT, code developers, and more
• Shared EGR knock data for surrogate development, model validation for major outcomes 1 and 2, and collaborating with kineticists on species to investigate
• Numerous project-level collaborations direct with industry and industry consortia for support and feedback

Future Work

• Baseline knock performance in new PACE engine geometry across a wide range of pressure and temperature conditions
• LSPI investigations of fuel oil dilution with introduction of NOx chemistry and known lubricant additives, to observe critical chemistry effects
• Make data from these projects available to advance PACE more broadly: machine learning, CFD modeling, kinetics development
• Complete evaluation of knock/pre-ignition data to identify whether actionable precursors exist (this FY)
• Use ML & nonlinear dynamics analysis techniques to analyze cold-start data and identify opportunities for active stability control
Technical Backup Slide 1: Quantitative Dye-Based LIF Diagnostic Developed to Measure Fuel in Oil in Prior Years as part of ACE032, and updated in this program for SPI

Improved chemometrics based calibration:

- Uses entire LIF spectra (developed this program)
- Accounts for transient oil temperature during engine experiment (developed this program)
- Less susceptible to spectral noise
- Improved accuracy (>92%) and precision (>98%)
- Real time quantification of error in FiO prediction (SSE)
- Higher sensitivity over wider range of engine relevant FiO
Determination of the outliers is an iterative process of:

1. $\mu$ and $\sigma$ of PCP and $CA_{xx}$ for each segment
2. cycles exceed “n” $\sigma$ from $\mu$ are identified
3. If outliers exist, omit outliers, repeat process; otherwise, the process is complete.

• The number of $\sigma$, “$n$”, is a function of the number of cycles in the test, calculated using Grubbs’ outlier test.
  - $n = 4.7$ for 25,000 cycles (SWRI P3 & $n = 4$ in ORNL)
  - $n = 5.0$ for 175,000 cycles (Sequence IX)

• Data is also studied to ensure the outlier appears to be SPI, rather than another abnormal combustion event or measurement anomaly.

• SPI “cluster” when there less than 3 “normal” cycles both before and after it. (SWRI P3 & ORNL)
Technical Backup Slide 2: Offline Optimization and Training of Spiking Neural Networks for Dilute Combustion Stability Control

- Evolutionary Optimization for Neuromorphic Systems (EONS)
- Develop and train optimal neural networks for dilute combustion stability control
  - Identify best-performing networks to be implemented on-engine

Control-oriented model used for training neural networks

Population of \( M = 100 \) Potential SNNs

Population of \( M = 100 \) Potential SNNs

\[
\sum_{k=1}^{5000} \left( \frac{m_{\text{fuel}}[k]}{m_{\text{fuel,0}}} - 1 \right)^2 + \sigma_f \left( \frac{Q_{\text{gross}}[k]}{Q_{\text{gross,0}}} - 1 \right)^2 + \sigma_r I(Q_{\text{gross}}[k] < 650)
\]

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