Project: ACE179

2022 DOE Vehicle Technologies Office Annual Merit Review

Propane Longstroke Engine R&D

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Overview

Timeline

- **Program approved and awarded in November 2020**
- **Program duration of 39 months**
  - 9-month pandemic and supply chain delay during calendar year 2021
- **Program is 30% complete to date**

Budget

Total Project Funding $1,550K

Task	FY21	FY22	FY23
ORNL Simulation	$150K	$250K	$150K
ORNL Experiments	$150K	$300K	$325K
Partners	$175K	$50K	$0K

Barriers

- **Knock Mitigation** → *Developing a better understanding of the effectiveness of EGR to mitigate knock*
- **Dilution** → *Increase EGR dilution tolerance*

<u>21st Century Truck Roadmap</u>

- **Drive efficiency towards 60% for MD** & HD powertrains
- **Enhance** Natural gas and **Propane engine efficiency** while reducing cost premium

Partners

- **Formal partners**
  - Oakland University = Kinetics mechanism
    - University of Tennessee Space Institute = Diffusion
  - University of Wisconsin Madison = LCA, GREET
  - Katech = physical engine build
  - Wisconsin Engine Research Consultants = FRESCO
- **Informal partners**
  - Stellantis =CAD models and discussions support

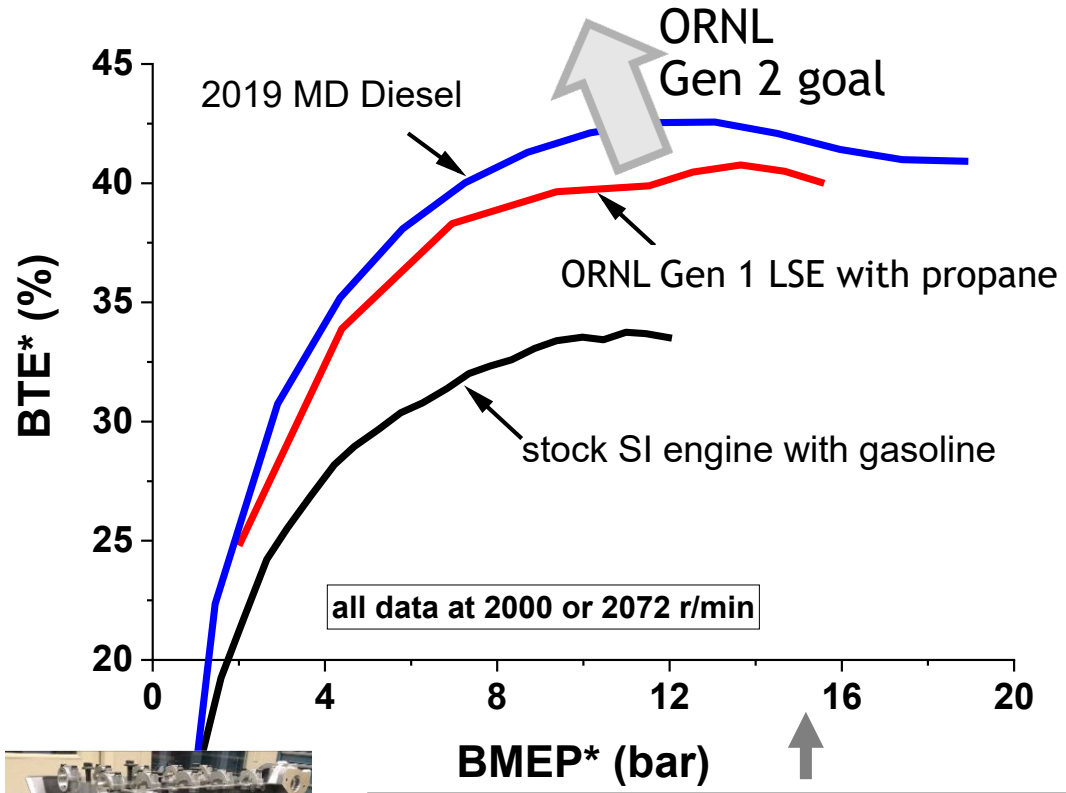
Relevance

This project will develop and demonstrate a propane-specific prototype single-cylinder advanced spark ignition MD relevant engine that achieves diesel engine efficiency parity and shows pathways for dramatic engine efficiency increases.

A propane engine with 41% SET-cycle efficiency (2019 MD Diesel) results in 6% below the 2027 GHG limits

Diesel requires 46.1% SET cycle efficiency to achieve CO_2 parity

- Increased propane utilization improves energy security through energy diversification and available known national resources
- CO_2 from conventional propane is lower than conventional fuels, but routes to zero net carbon propane are being developed
- Broad reaching simulation tools and understanding will be undertaken and are cross technology applicable



Gen 1 LSE engine demonstrated high efficiency potential of propane, but substantial opportunity for propane remains

Milestones for FY22

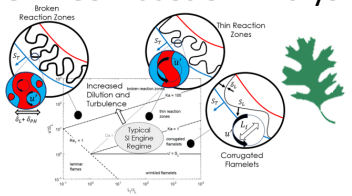
Milestone	Due Date	Status
Deliver validated model for selected experimental cases that can capture experimental CCV to + 1% absolute.	9/30/2022	On-Track
Advanced single cylinder engine installed at ORNL (ORNL)	9/30/2022	On-Track

Go/No-Go Decision Points	Due Date	Status
Installed advanced single cylinder engine at ORNL	09/30/2022	On-Track

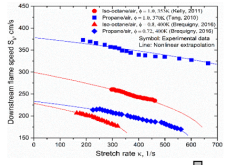
Comprehensive Program Involving Fundamental and Applied Modeling, Experiments and System Level Analysis.

Fundamental and Applied Computation

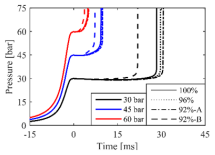
CFD Combustion Analysis



Flame Stretch Analysis



Chemical Kinetics Dev.



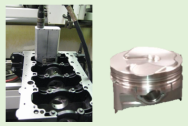
Experiments and Design

Gen 2 Design

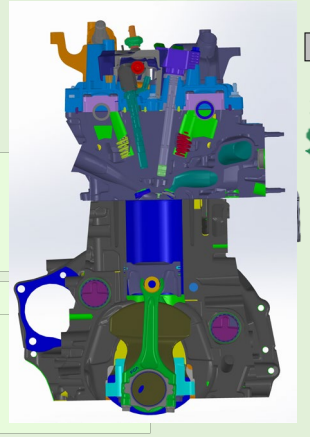
Validation

Gen 1 SCE

Gen 2 SCE Design Integration

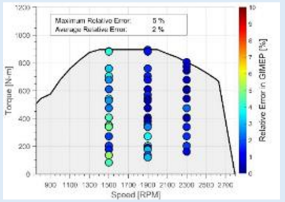


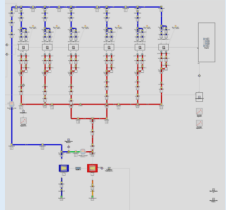
Gen 2 SCE with CFD Guided Design



System Level Simulation

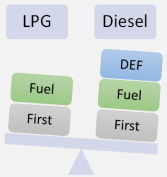
1-D System Level Analysis





TCO/LCA Analysis

Techno-economic and GHG analysis



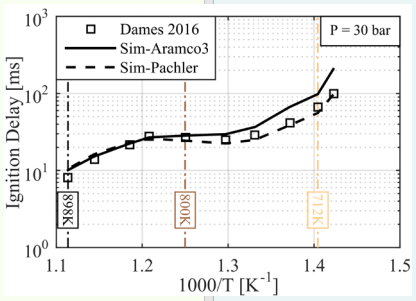
Approach Fundamental Simulations and Design for Updated Engine

Conceptual Understanding of dilution limit

Fundamental Modeling

Direct Numerical Simulation (DNS)

Chemical Kinetics Development



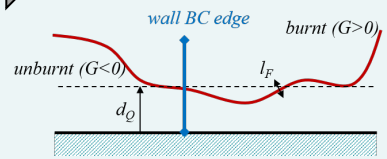
Fundamental Ignition Simulations

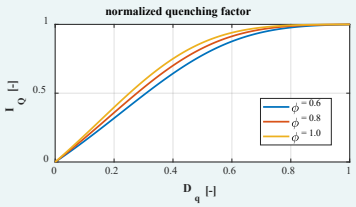
Conceptual Understanding of Dilution Effects on Flame and Ignition

Prototype Hardware Demonstration

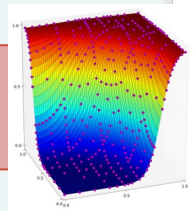
Applied Modeling

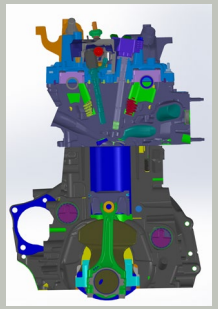
Sub-Model Development





Combustion System and Engine Design Optimization





Gen 2 Long-Stroke Engine

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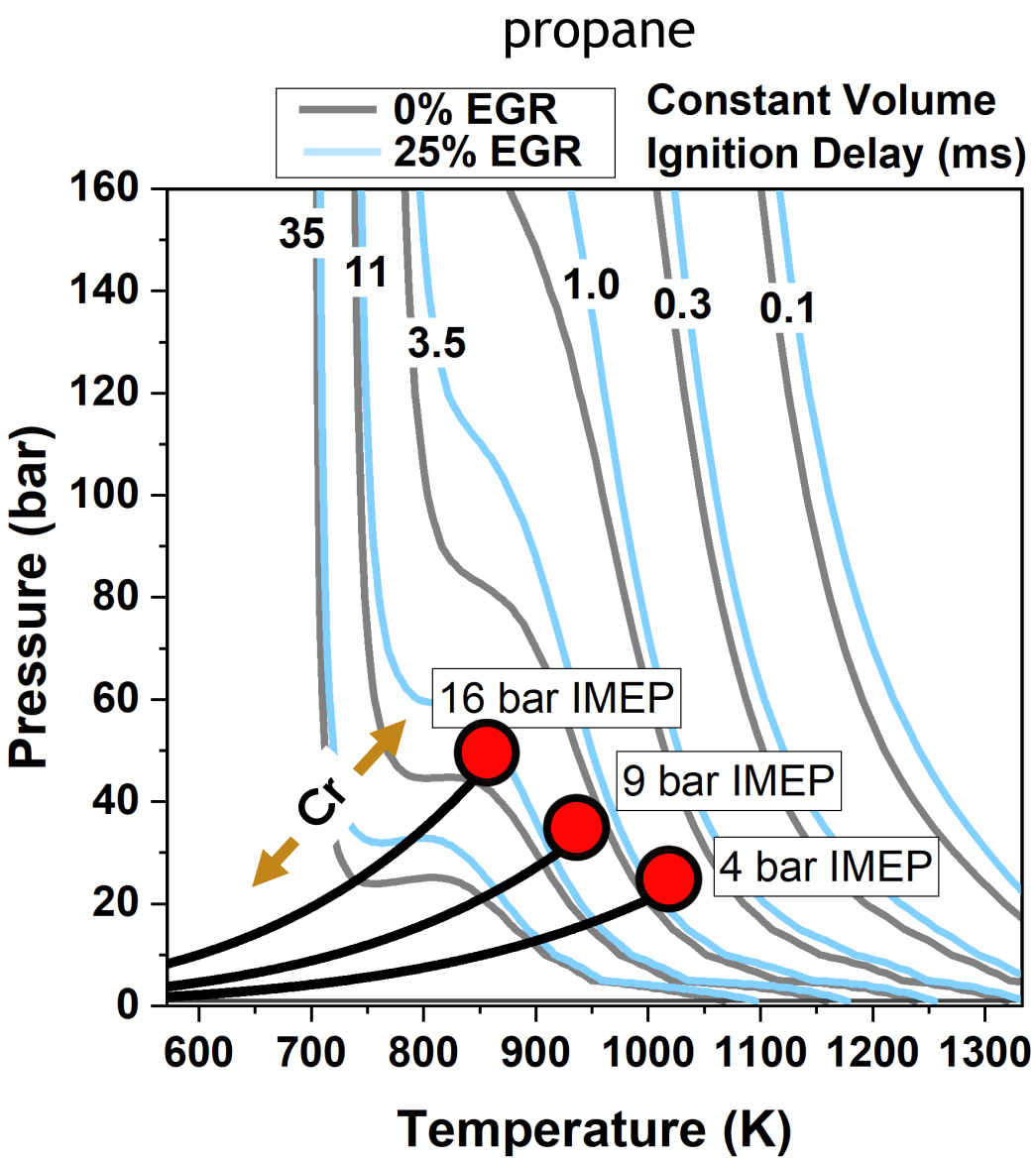
Fuel Ignition Delay Properties Determine Cr and EGR Effect

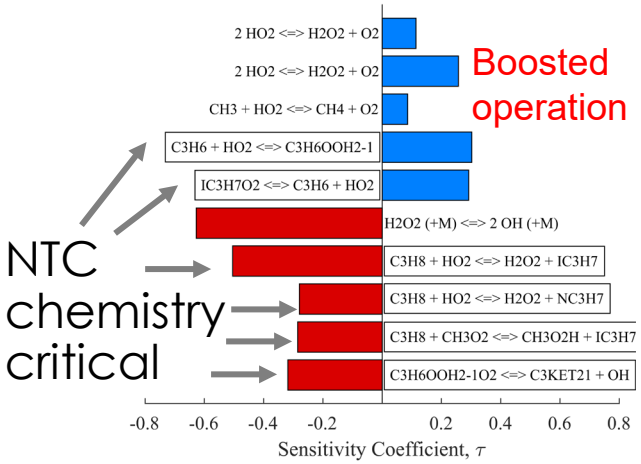
- Starting with 0-D framework ignition delay analysis, propane specific opportunities and challenges with EGR and compression ratio were examined
- Clearly EGR only affects the NTC region
  - Similar effect in "conventional" fuels where this region is entered under throttled operation (between the RON and MON trajectories)
- Compared to "conventional" fuels, propane "pushes up" the NTC region in the pressure space, resulting in NTC effects to become present during boosted operation

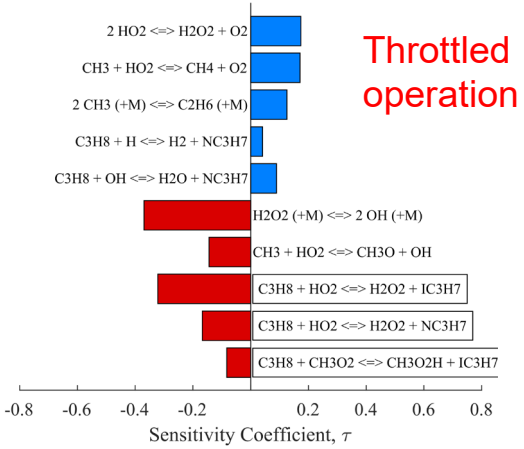
Clear and accurate understanding of NTC reactions become critical for setting the compression ratio for boosted engines with propane fueling

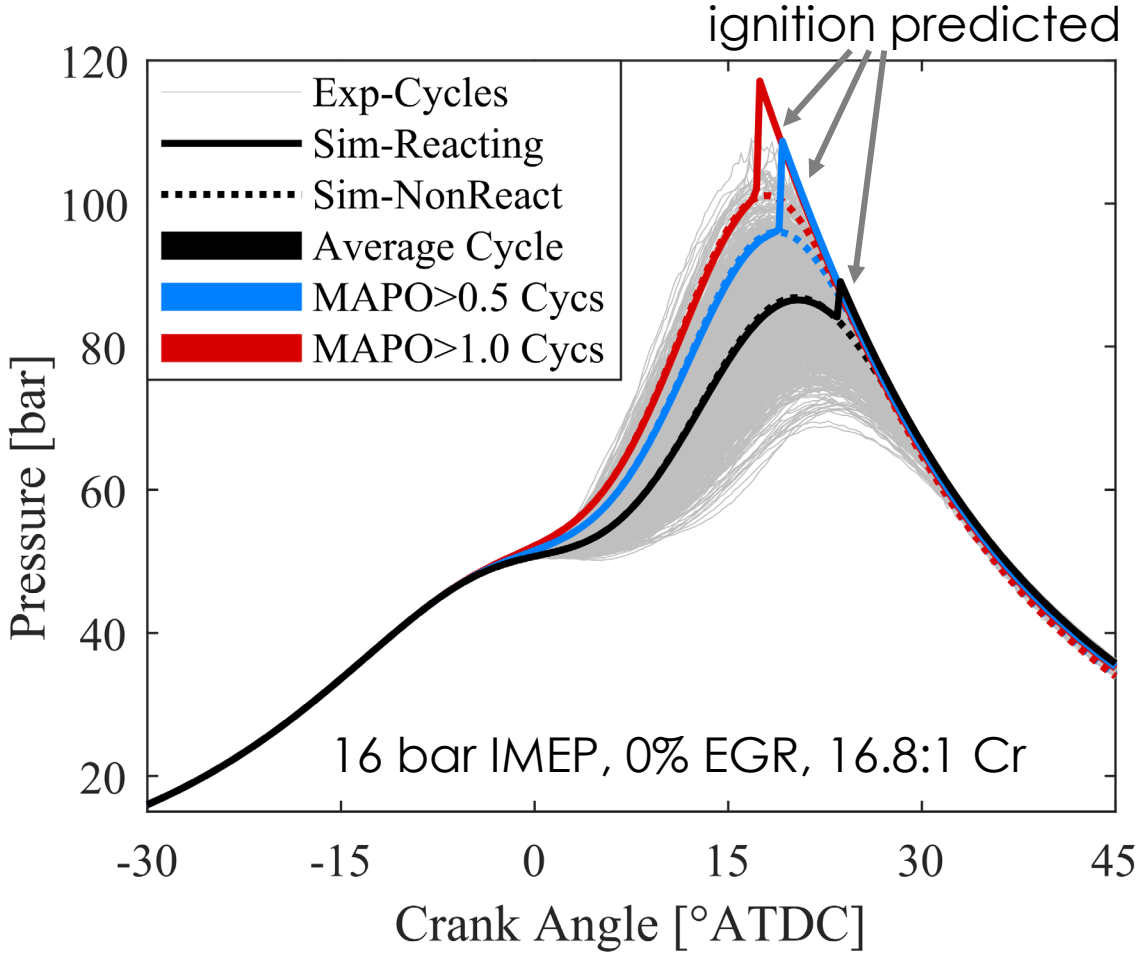


Literature Mechanisms Overpredict Knock Under Boost

- 0-D engine simulations highlight literature propane mechanisms (Pachler et al.) over predict knock for boosted conditions in Gen 1 engine
  - Multiple knocking paths simulated for each operating condition
  - Mechanism ignition/NTC mismatch are qualitatively consistent with literature RCM data
- Genetic algorithm deployed to optimize reaction rates
  - Sensitivity analysis for Boosted, and throttled conditions differ highlighting HO_2 reaction tuning
  - Secondary objective: reduce mechanism stiffness







engineering level CFD mechanism with 70 species, 352 reactions

- tuning 6 reactions in the optimization

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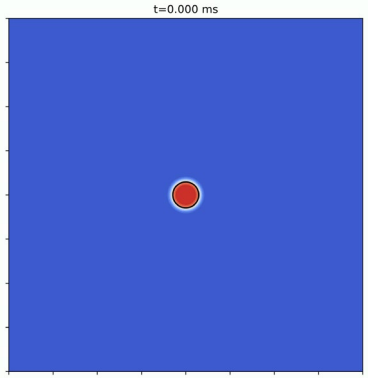
2-D DNS Results Show Fundamental Fuel Properties of Propane Enable Improved EGR Tolerance

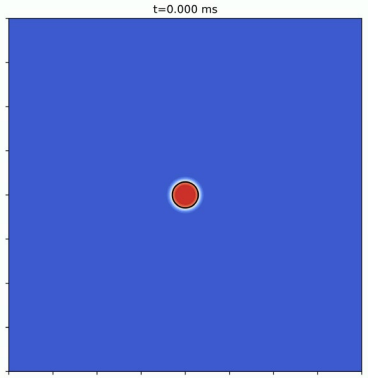
DNS study targeting fundamental understanding of propane's dilution advantage.

2-D DNS results using a **non-unity Lewis number** approach for the flame complement measurements from engine experiments:

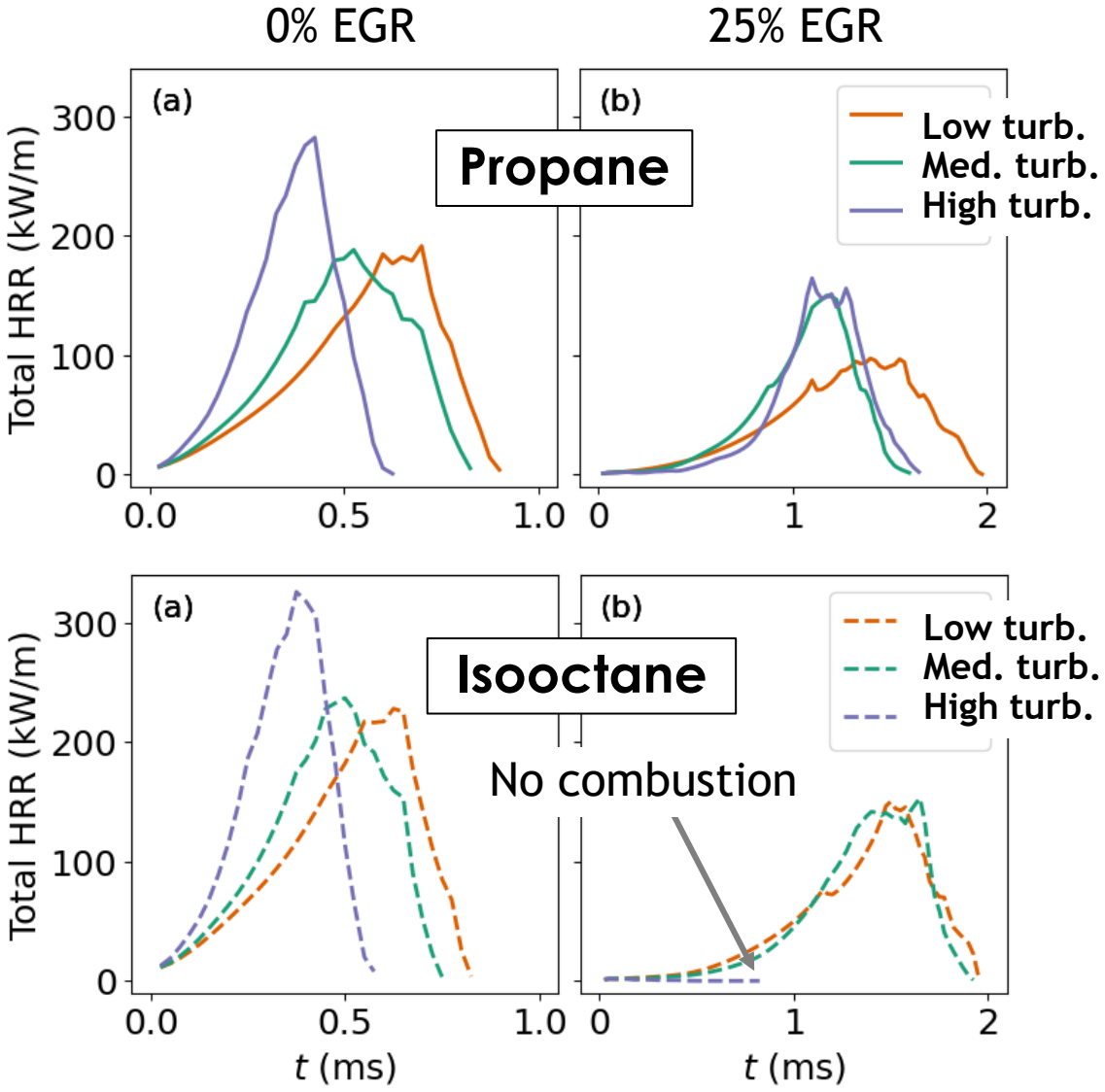
- With EGR, Propane is more resilient than iso-octane to turbulence.



Isooctane, 25% EGR, high turbulence



Propane, 25% EGR, high turbulence



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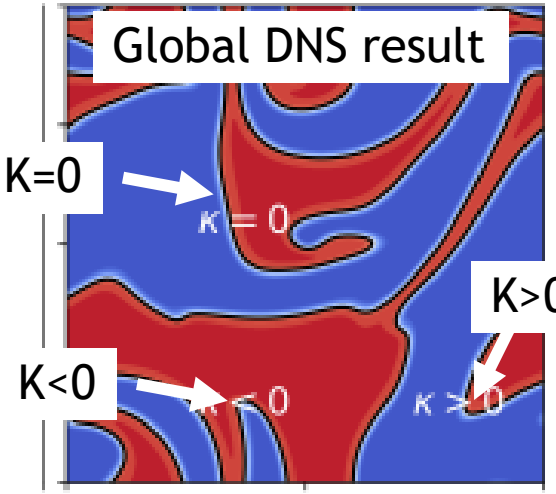
2-D DNS Results Show Diffusion Effects Dominate Displacement Speed with EGR, but Propane is Less Affected

- **Contribution to displacement speed is split into reaction and diffusion (normal + tangential)**

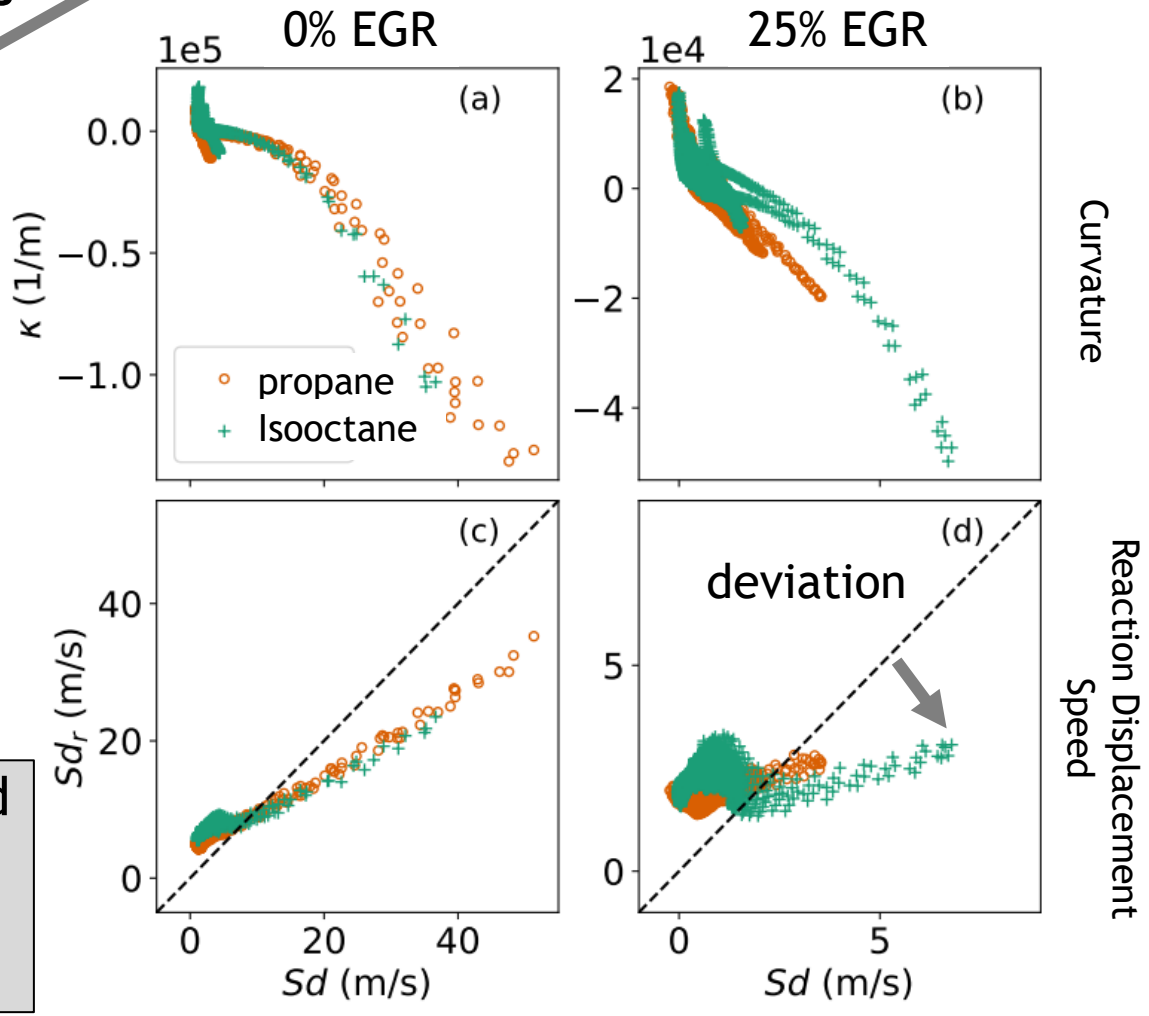
- 0% EGR results
  - No fuel specific effect observed

- 25% EGR
  - Diffusion becomes increasingly important as curvatures get more negative and S_d increases
    - **Diffusion is dominant with EGR**

Insights into diffusion and critical turbulence effects



Flame structure and diffusion for medium turbulence level at 30% MFB



With EGR, Isooctane becomes diffusional rate limited sooner and experiences increased negative curvature, causing a fundamental source of flame instability, reduced flame speeds and EGR tolerance.

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Independent of Curvature, with EGR Chemistry Specific H_2O_2 Effects Observed Between Fuels

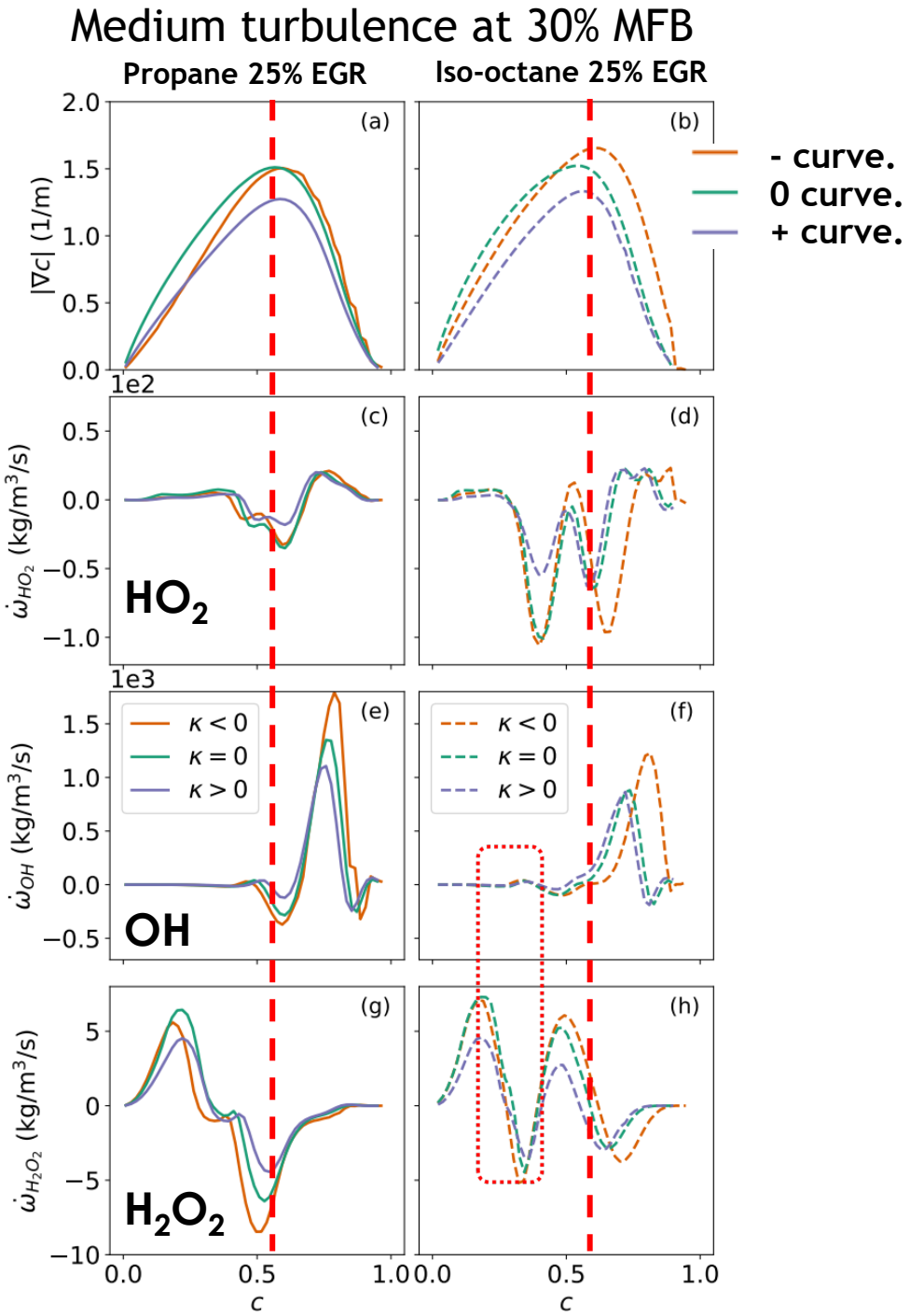
Isooctane

- Independent of curvature, H_2O_2 is formed twice, with reduced OH production overall compared to propane.
- Larger participation of HO_2 radicals, where HO_2 consumption doesn't seem to translate to increased OH production, highlighting competing reaction pathways of HO_2 and H_2O_2

Propane

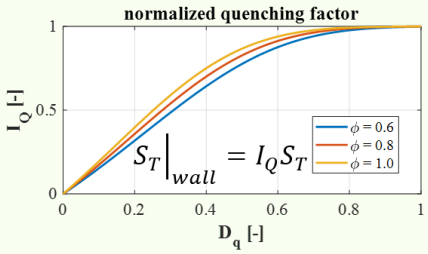
- Formation of H_2O_2 is followed by its consumption and rapid formation of OH at c≈0.5, with smaller participation of HO_2 (i.e., H_2O_2 chain branching reaction pathway)

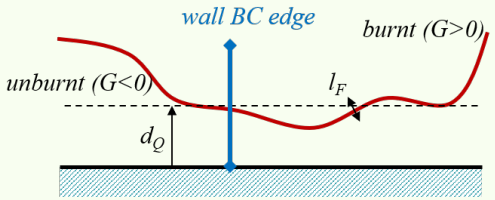
Fuel chemistry with EGR is a significant effect independent of flame structure



Measurements Suggested Wall Quenching was Critical for HC Emissions with Propane, Wall Model Approach Improved, Necessary for Piston Design Optimization

Wall Quenching Model

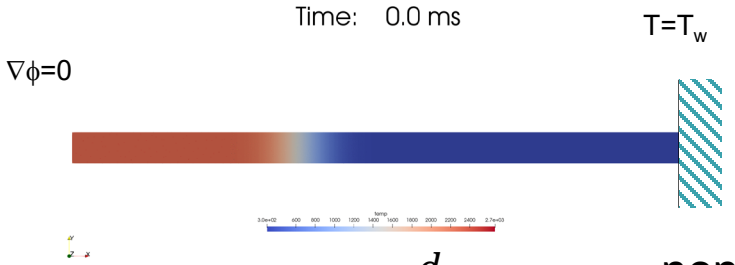




Enables prediction of squish-driven quenching

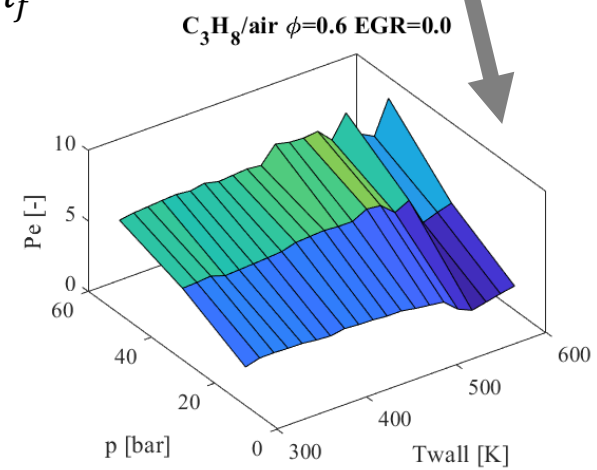
- Improved hydrocarbon and efficiency predictions

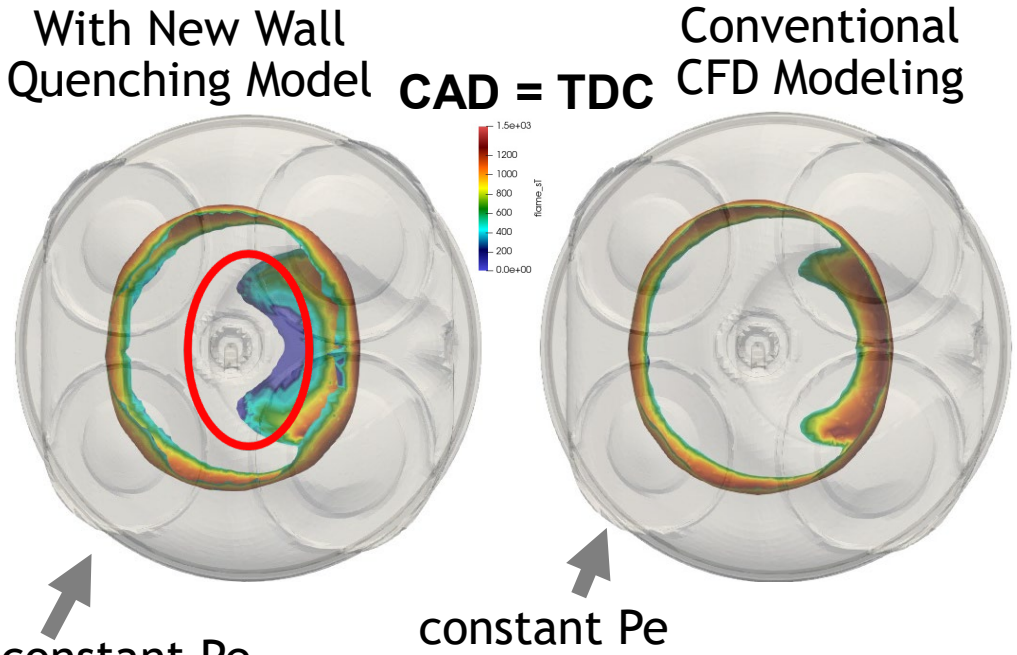
- Using direct chemistry integration to calculate true wall quenching Peclet number
  - Realistic flame burn rates near boundaries.



$$Pe_Q = \frac{d_Q}{l_f}$$

- Studying role of ϕ / Le to define a quenching Peclet for propane





- Wall quenching model was successfully implemented in the combustion simulation.
- Usage of the wall quenching model "smears" flame near the wall due to low burning velocities
- Changes have implications that improve the predictions of UHC emissions.

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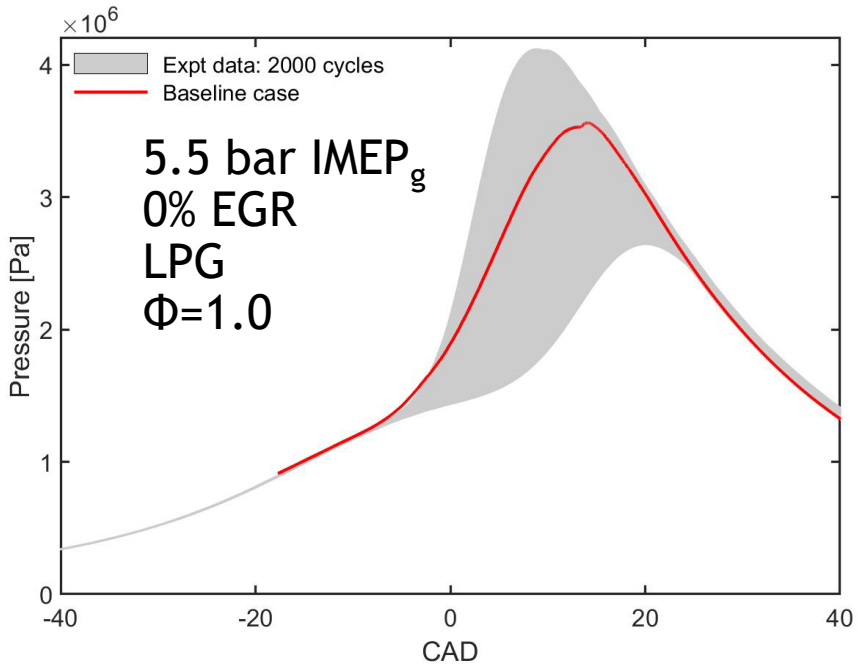
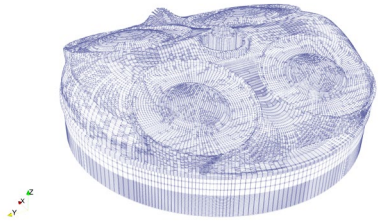
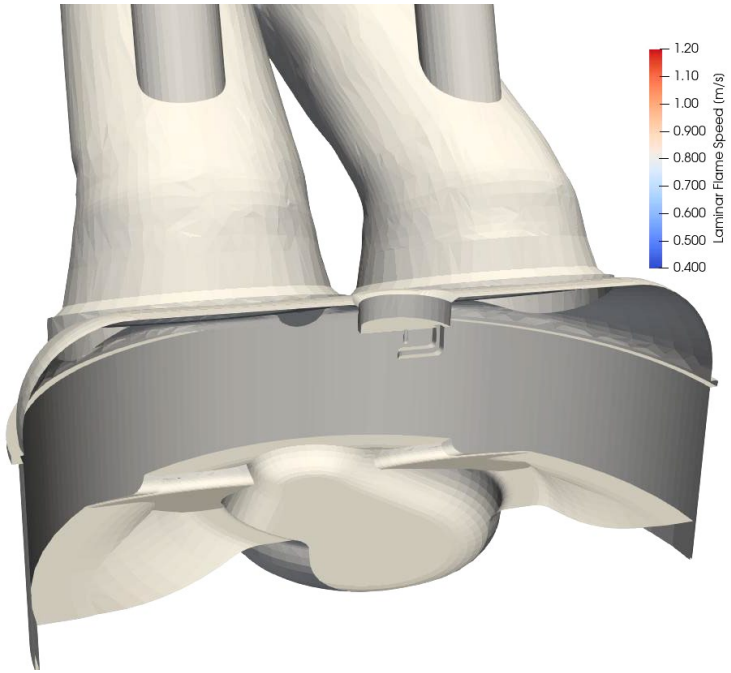
FRESCO Simulation Validated Against Experiments

- Measurements replicated in FRESCO with newly implemented sub-models
- Results are comparing very well to measurements
- Parametric study on stroke, compression ratio, and piston shape for Gen 2 engine is ongoing
  - Knock prediction with updated kinetic and wall models at high-load and Cr running currently



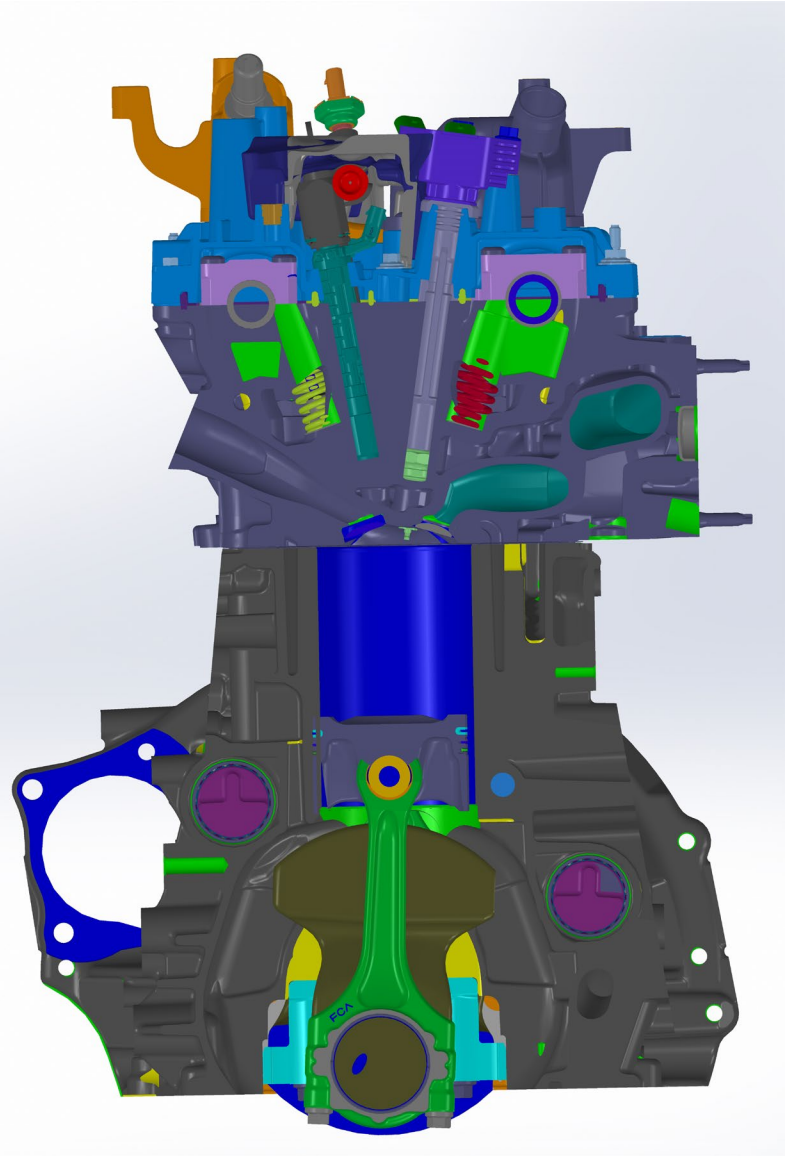
Body fitted mesh





Second Generation Long Stroke Engine in Development

- Modeling informed design approach for Compression ratio and EGR in second generation Engine
  - Second generation engine utilizing cylinder head and initial combustion chamber shape designed for EGR
    - Gen 1 engine used hardware originally designed for 0% EGR operation
  - Increased stroke and corresponding compression ratio being engine finalized informed by model results and fundamental propane results.
    - Design will be capable of a stroke to bore ratio up to 1.5:1 (stock GME4T engine is ~1.07:1)
    - Stock piston to be used initially (up to 14:1 Cr with stock combustion chamber
      - Model informed design for Cr increase to follow
- Current status is in design review process, physical metal cutting to follow



Responses to previous Years Reviewer's Comments

- …a comprehensive and well-designed project involving fundamental and applied CFD modeling, experiments, and system-level analysis, along with total cost of ownership (TCO) and life-cycle assessment (LCA) analysis.
  - **Thank you, in this program we will highlight opportunities and identify potential barriers as best as possible in this technology space**
- …DI, exhaust gas recirculation (EGR)-diluted LPG engines do not exist; hence, learning that LPG is more tolerant to EGR is really useful.
  - **Thank you, the intent of this program is to lay groundwork for this understanding**
- …the role of direct numerical simulation (DNS) is critical to understanding the fundamental reasons for EGR tolerance.
  - **Thank you, our 2022 results hopefully highlight this area and the LPG specific opportunities we are observing**
- …it is not clear how much of this project differs from recent Cummins development programs on their small displacement engine
  - **Thank you, as of the time of this project, public disclosing of EGR and compression ratio greater than 13 has not been demonstrated**
- …it could have been even better if the aftertreatment system was also studied along with the existing integrated approach, perhaps via collaboration with other teams if possible
  - **Previous programs funded by DOE have shown TWC promise with LPG, that portion of this program not selected to be included at this time**

Collaboration and Coordination with Other Institutions

- This program is a collaborative project of multiple universities, industry and ORNL combining a unique experimental platform and world-class DOE computing expertise to achieve substantial efficiency gains in spark ignition engines relevant medium duty.
- The work plan for this program was developed following roadmaps for 21st Century Truck partnership and Priority 1 topics from USCAR.
- Leveraging stakeholder feedback at the AEC MOU partner member companies
- Individual collaborations for this project:
  - **Oakland University** – Sub recipient: Chemical kinetic development for propane and LPG blends.
  - **University of Tennessee Space Institute** (Formerly of Oakland University) – Sub recipient: 1-D spherical flames and stretch effects.
  - **Katech** – Sub recipient: Engine design integration for Gen 2 prototype
  - **University of Wisconsin - Madison** – Sub recipient: System level simulations and LCA
  - **Wisconsin Engine Research Consultants** – Contractor: Sub-model development for Gen 2
  - **Stellantis** – Informal Collaborator: Provided engine design specs as base for Gen 2 and advising technical progress and targeting industry needs

Remaining Challenges and Barriers

- Production of Gen 2 prototype engine
  - Integration of Stellantis stock head on custom build billet block
- Understand the chemical effect of impurities in the LPG composition such as butane/butane isomers and ethane
  - Up to 9% of fuel based on national sampling studies, can have strong impact on knock performance
  - Renewable propane provides low/no carbon pathway for chemical symmetry, tighter composition control
- Fundamental understanding of the effects of LPG on dilution tolerance and how to expand its benefit through engine design
  - Deterministic and stochastic effects that contribute to its improved performance
- Conduct comprehensive system level analysis and life cycle analysis to demonstrate overall impact of an LPG engine with diesel efficiency parity
  - Understand the trade-off between friction and stroke-to-bore ratio requires an understanding of the effect of stroke-to-bore ratio on engine indicated efficiency

Proposed Future Research

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

FY22

I. **Computably guided Gen 2 prototype development:**
   I. Decision on Stroke-to-bore ratio, compression ratio and piston shape

II. **1-D flame stretch simulations**
   I. Finalize analysis and publish results

III. **Direct Numerical Simulations**
   I. Publish results in CNF

IV. **Production and installation of Stellantis GME4T GEN 2 engine with custom built block and crankshaft.**

FY23

I. **Piston and stroke-to-bore final assessment in Gen 2 platform**

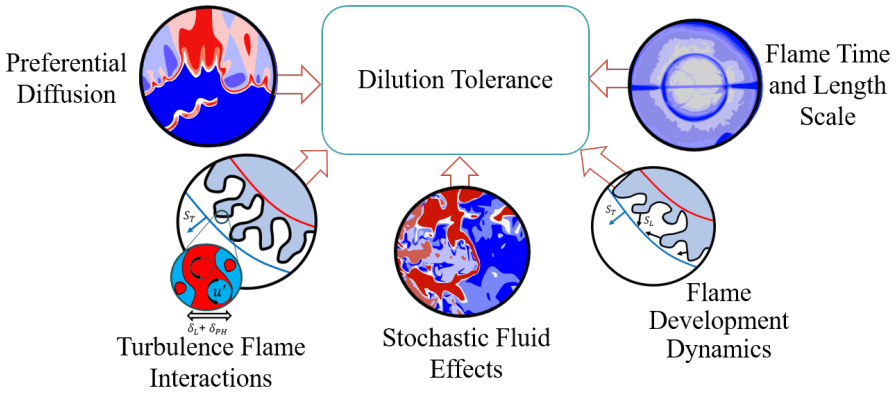
II. **Demonstration of Gen 2 prototype efficiency**

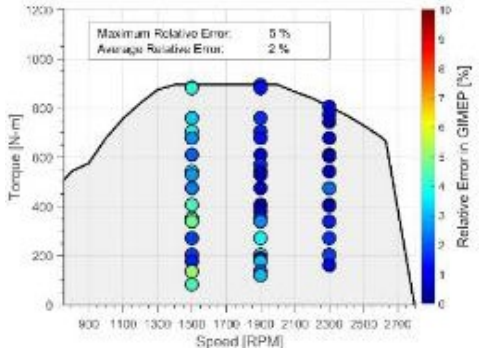
III. **Assessment of stochastic and deterministic effects using Large Eddy Simulations and detailed chemistry**

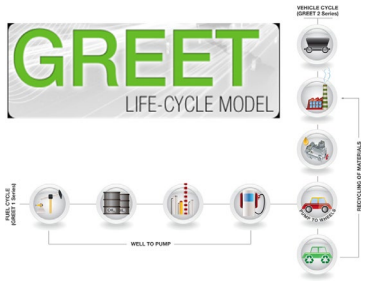
IV. **System GHG, TCO, and life-cycle analysis**

FY24

I. **Publication of results**







Summary

Relevance

- Program is in line with 21st Century Truck partnership research roadmap of increasing propane engine efficiency with no cost premium.

Approach

- Combination of single cylinder experiments and modeling tools used to optimize engine performance in Gen. 2 prototype.
- Modeling activities divided into “conceptual understanding” tasks and “prototype development” tasks dividing fundamental and applied modeling.

Accomplishments

- Identified critical NTC reaction pathways that are active in boosted propane engine operation, and current kinetic mechanism updated needed to accurately account for these, deploying and integrating optimization schemes to update.
- 2-D DNS results highlight fundamental flame dynamics and opportunities for propane relative to conventional fuels.
- Wall quenching model updated with non-constant Peclet number approach, greatly improving near wall flame effects and corresponding EGR dilution tolerance and hydrocarbon emissions/quenching prediction capabilities.
- Integrated findings on EGR and knock into engineering level codes for engine design optimization, deploying approach validated against GEN 1 engine experiments
- Gen 2 engine development being guided by simulation results and in physical hardware pre-production stages

Collaborations

- Collaboration of 4 universities, industry, and a national laboratory to develop high efficiency LPG engines.

Future Work

- Gen 2 engine installation and experiments across a wide range of conditions demonstrating efficiency achievements
- Closing the loop on simulation results with Gen-2 engine validation, prediction, and optimization simulation
- Life cycle and efficiency analysis against diesel baseline engine

Technical Back-Up Slides

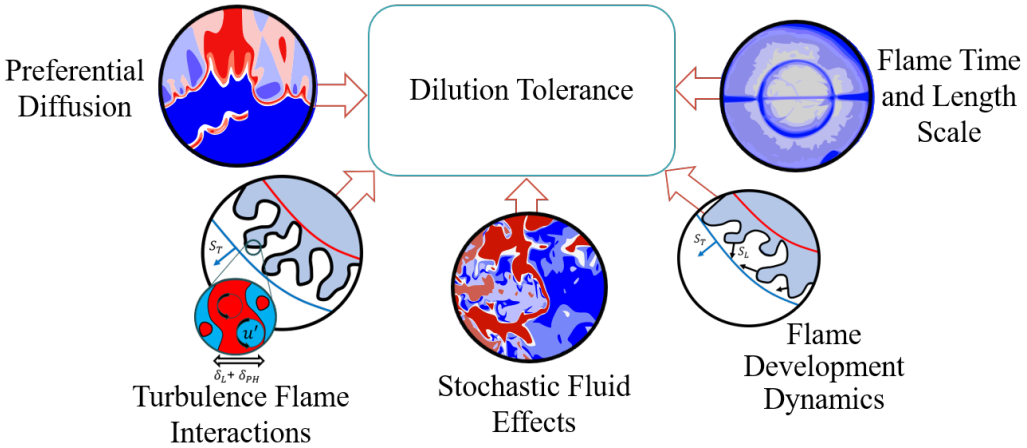
Three factors from experiments identified as key to achieving diesel-like efficiency: dilution tolerance, knock resistance and fast burn duration

Validated simulation effort exploring fundamentals governing fuel and chemical-physical relations enabling high efficiency operation

High Efficiency Stoichiometric Spark Ignition

FY21/22/23 work

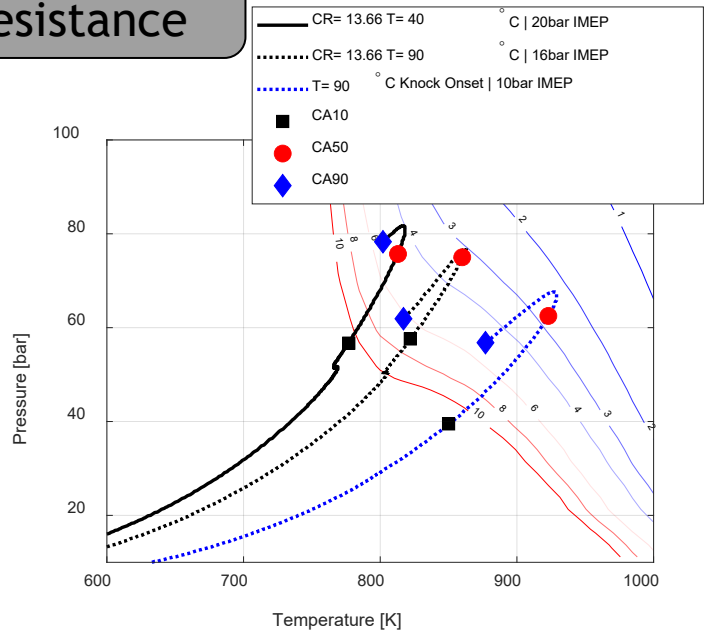
EGR Dilution



- Program will investigate factors affecting dilution tolerance
  - Comprehensively understand physical-chemical processes and opportunities
  - Includes ignition through late-cycle quenching phenomena

FY21/22 work

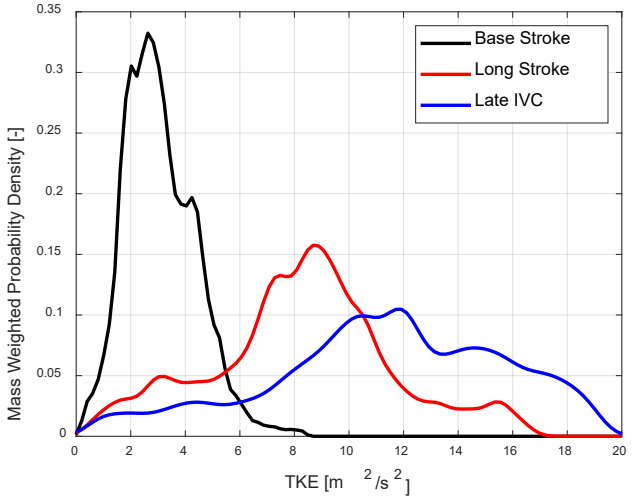
Fuel Knock Resistance



- Fuel's chemical kinetic properties and engine P-T trajectory
  - Propane properties are far different form gasoline.

FY21 and previous work

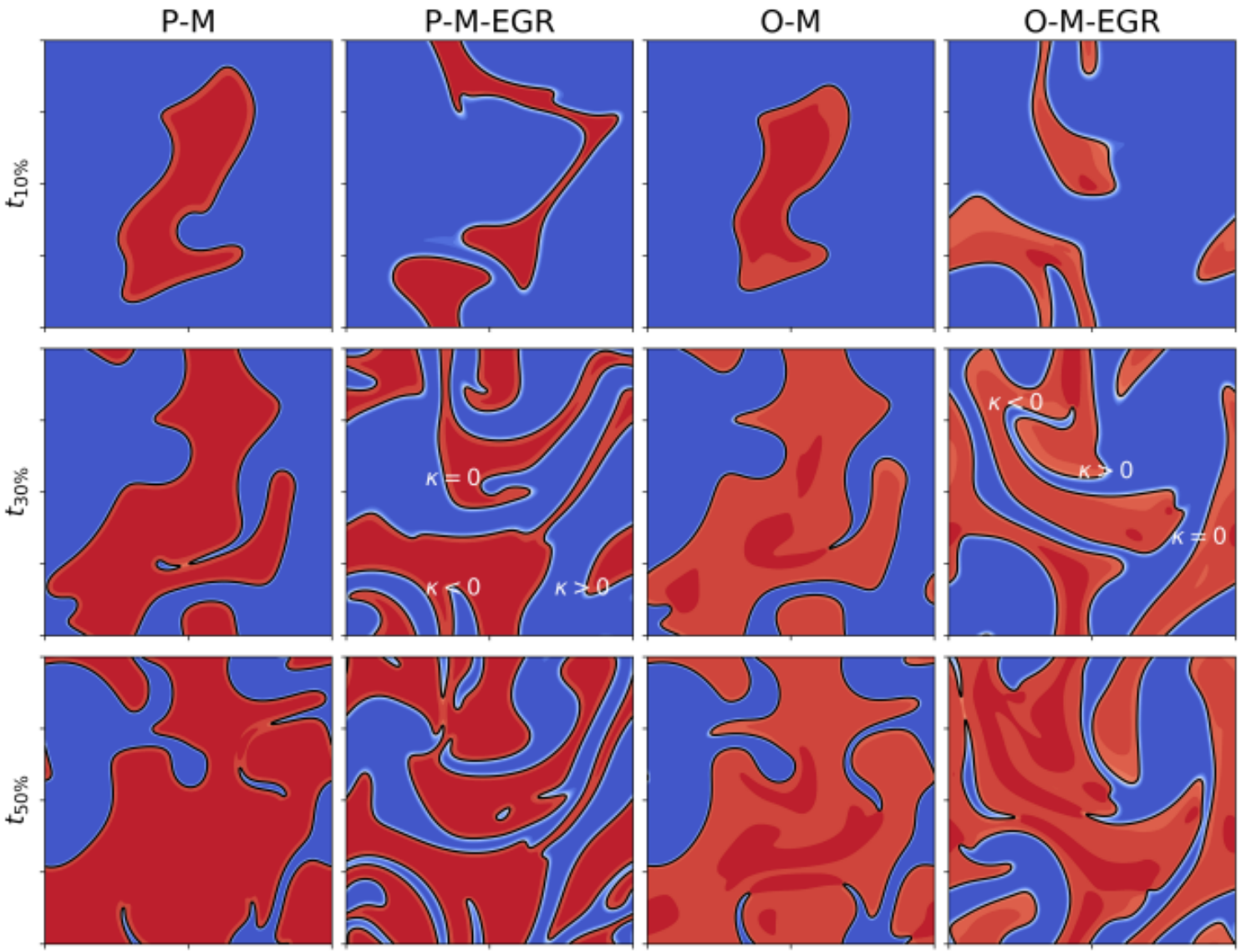
Fast Burn (turbulence)



- Increased stroke effects on combustion
  - Increased TKE at spark
  - Increased Cr and minimizes squish driven quenching.

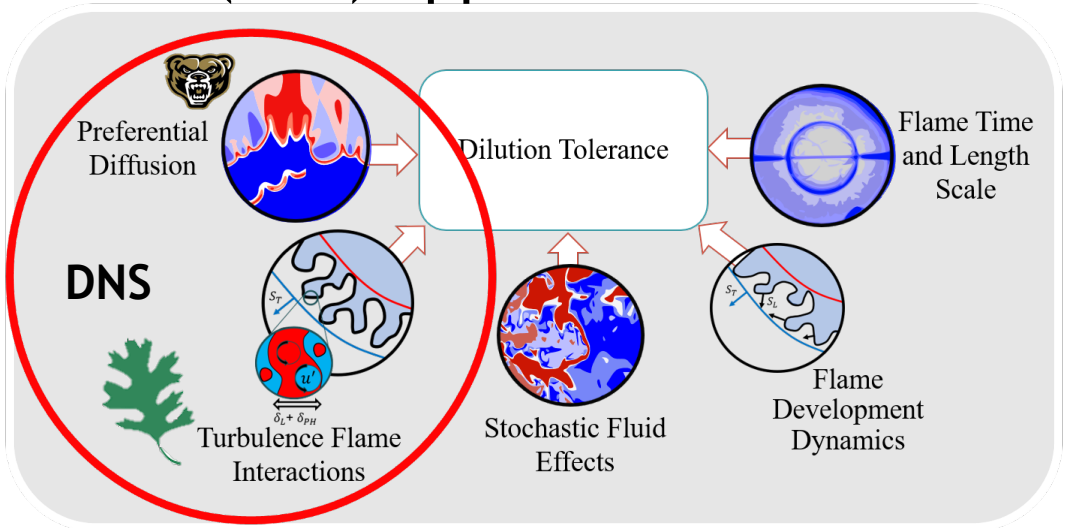
2-D DNS Results Highlight LPG Specific Opportunities

- Instantaneous progress variable for Isooctane (O) and LPG (P) with medium levels of turbulence (M) at 3 time stamps (10, 30, and 50% mass fraction burned)
  - Color scale shows progress variable
    - Blue =0 (no reaction yet)
    - Red/Orange=reacting region
    - Red=1 (complete)
- Results show that the progress variable for propane has a high gradient, meaning a thin reaction zone, improving dilution tolerance

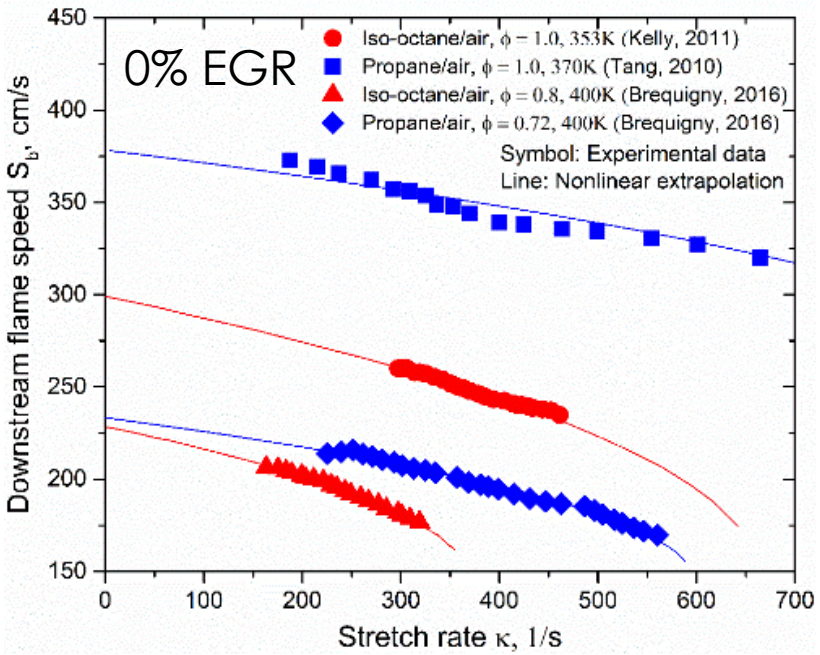


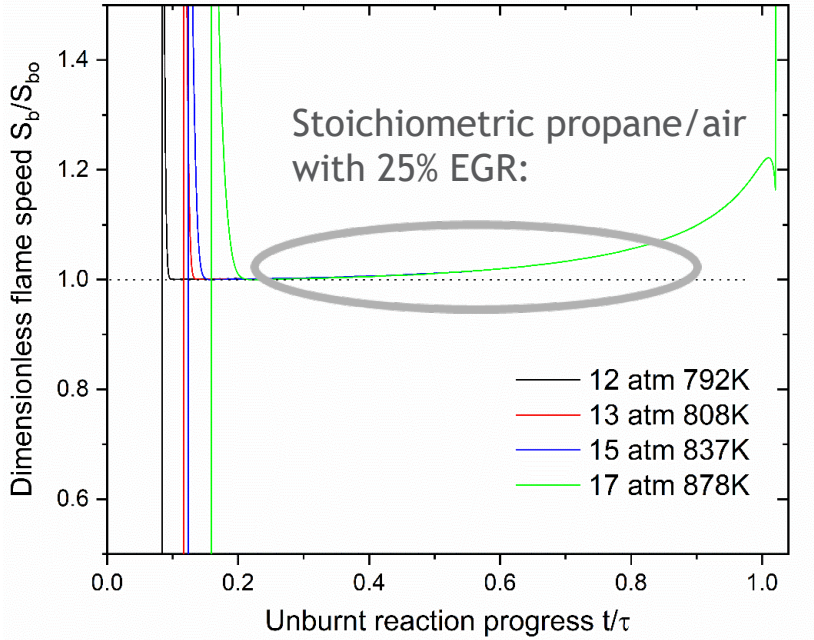
Fundamentals of Preferential Diffusion and Auto-Ignition EGR Dilution Tolerance of Propane Using a Direct Numerical Simulations (DNS) Approach

- Fundamental reason for improved EGR with Propane is not directly known
  - Is this laminar flame speed alone?
- Two-step approach to understand preferential diffusion and turbulence chemistry effects in EGR tolerance



- Initial 1-D simulations and literature review show that propane with 0% EGR is less susceptible and dependent on flame stretch
- With 25% EGR 1-D simulation results show that unburnt zone reactions in LPG increase flame speed
  - Radicals from propane are critical with EGR





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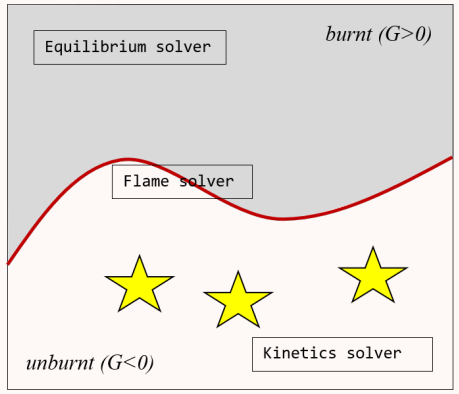
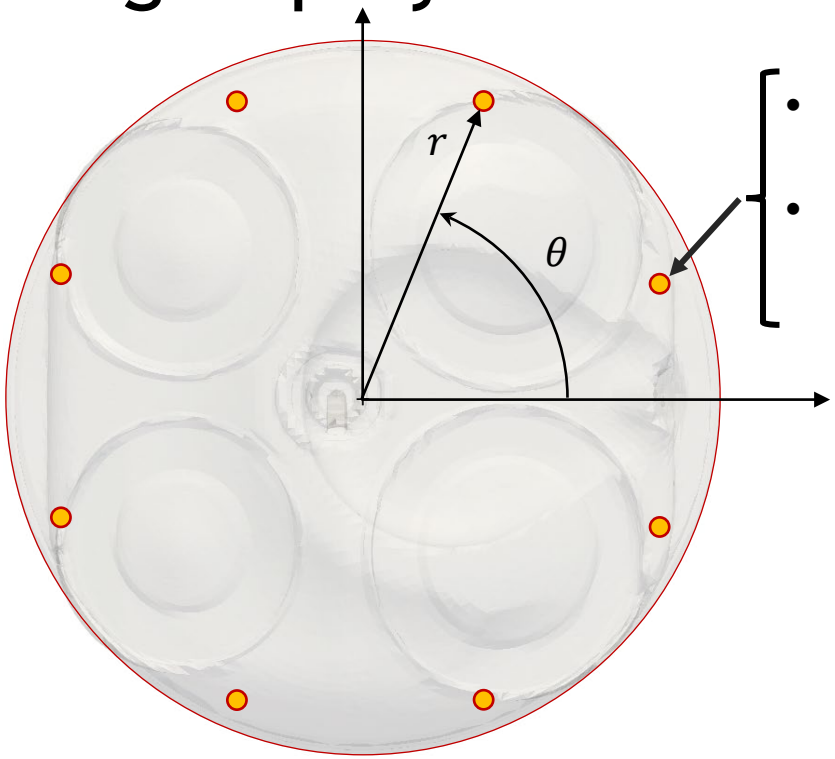
Fast Knock Predictor Being Deployed Cr Determination

Fast End-gas auto-ignition model



- Fast predictions of knock
- Allows improved prediction of optimal CR

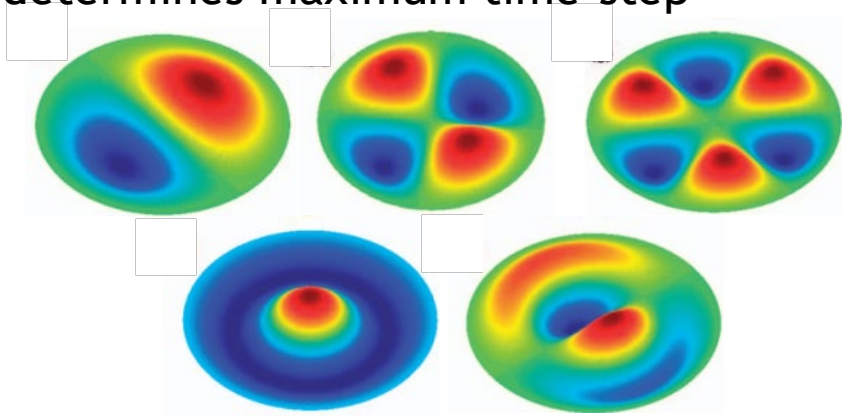


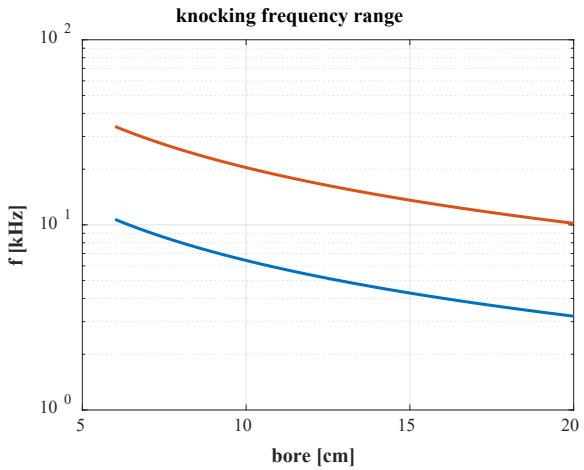
- 8 pressure probes located in simulation
- Information from probes is input to calculate knock intensity as a post processing step.

Knock Intensity

$$KI = \frac{1}{N_{probe}} \sum_{i=1}^{N_{probe}} PP_{max,i}$$

- Frequency range of six most relevant modes determines maximum time-step





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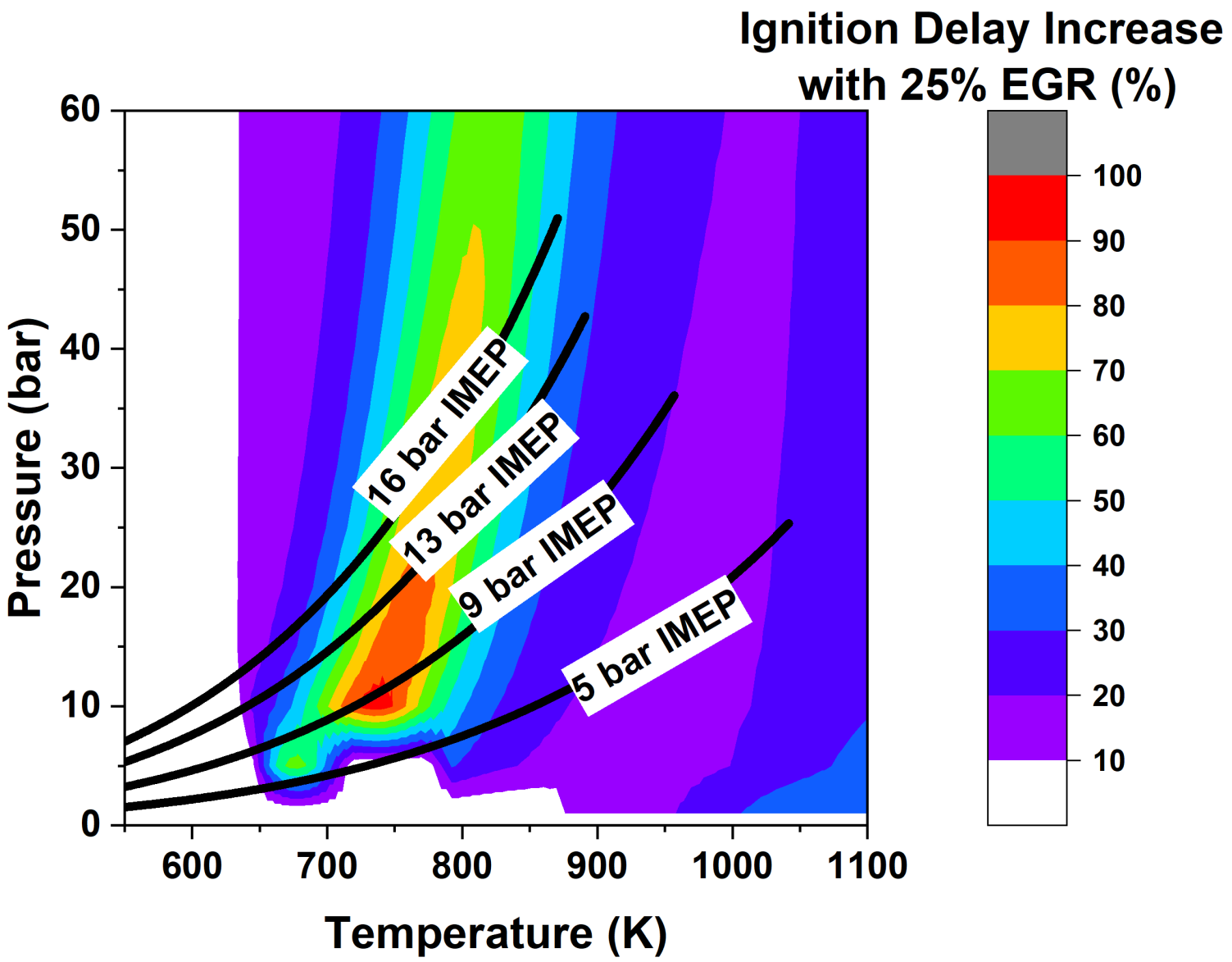
EGR Offers Ignition Delay Advantages at Higher Loads

- Largest knock benefit opportunity from EGR is under boosted operation with propane
  - Opportunity is more challenging to access practically
  - Still benefits at lower loads just a reduced effect
- EGR still offers throttled pumping and gamma benefits for low load efficiency improvements
- Heavier boosting is needed for “beyond RON” like behavior in propane