Project: ft099

2021 DOE Vehicle Technologies Office Annual Merit Review

Propane Long-Stroke Engine

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6/24/2021

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Overview

Timeline

- **Program approved and awarded in November 2020**
- **Program duration of 39 months**
- **Program is 15% complete to date**

Budget

Total Project Funding $1,549,915

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

Barriers

21st Century Truck Roadmap

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

USCAR Priority 1: Dilute SI Combustion

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

Partners

- **Formal partners**
  - Oakland University
    - University of Tennessee Knoxville
  - University of Wisconsin Madison
  - Katech
  - Wisconsin Engine Research Consultants
- **Informal partners**
  - Stellantis (formerly FCA)

Relevance

The objective of this project is to develop and demonstrate an LPG-specific prototype single-cylinder advanced spark ignition MD engine that achieves diesel engine efficiency parity and shows pathways for dramatic engine efficiency increases.

- **Emission control compatibility with 3-way catalysts, mature technology pathways for meeting future regulations**
- Increased LPG utilization in this sector improves energy security through energy diversification and available known national resources
- **Reduced GHG emissions through fuel properties and efficiency improvements**
- CO_2 reductions from fuel and engine efficiency improvements

Achieving an LPG 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

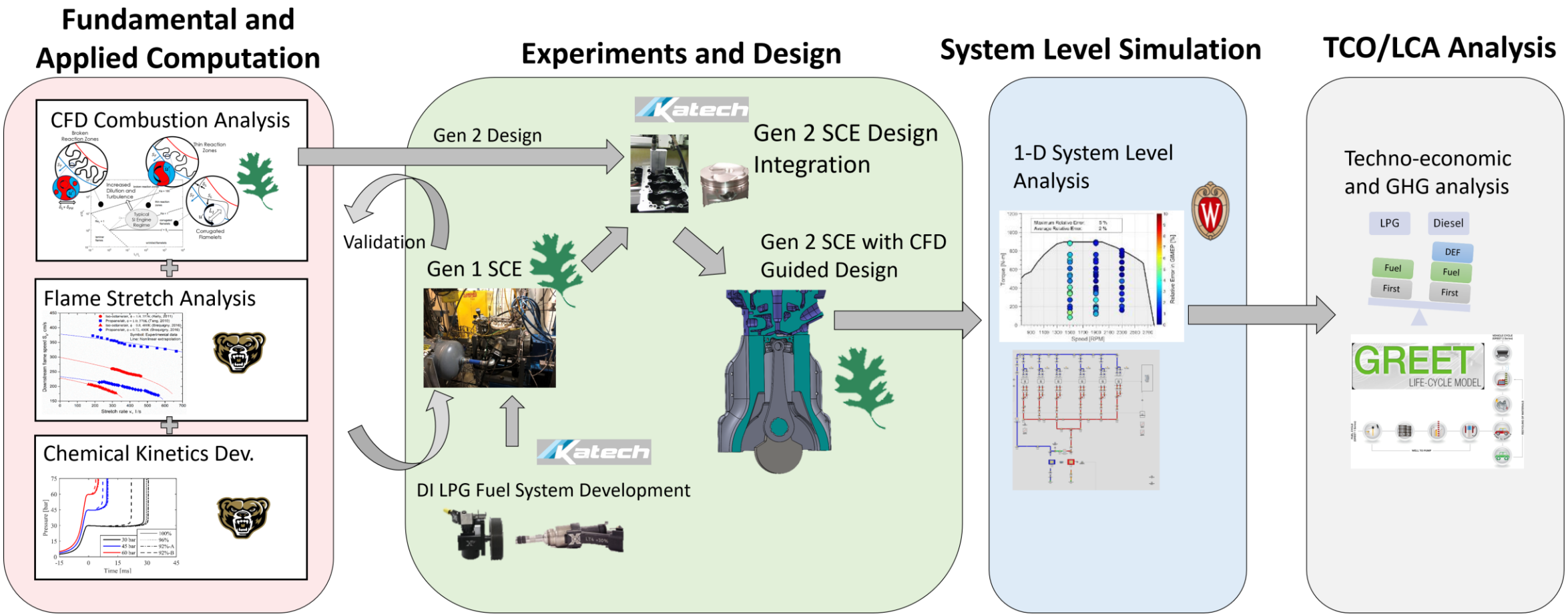
Objectives learned in this program are developed specific to LPG fueling but serve a much broader DOE mission goals of **USDRIVE ACEC Roadmap** and **21st Century Truck Research Blueprint** while developing broad reaching simulation tools and understanding.

Milestones for FY21 and FY22

Milestone	Due Date	Status
Provide high compression ratio data set to CFD tools for compression ratio and piston optimization (ORNL)	6/30/2021	**Complete**
Provide reduced stroke-to-bore ratio (~1.25:1) data set to CFD optimization tools for stroke-to-bore ratio optimization on turbulence effects for advanced single cylinder engine design and piston optimization (ORNL)	12/31/2021	On-Track
Advanced single cylinder engine installed at ORNL (ORNL)	6/30/2022	On-Track

Go/No-Go Decision Points	Due Date	Status
EGR data provided at various loads and speeds such that EGR tolerance effects and boundary conditions can be accurately used for fundamental and applied assessments of combustion and efficiency in simulation tools	09/30/2021	On-Track
Installed advanced single cylinder engine at ORNL	09/30/2022	On-Track

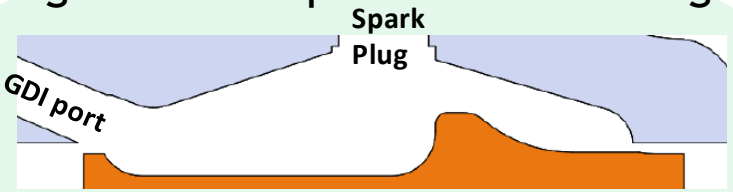
Comprehensive program involving fundamental and applied modeling, experiments and system level analysis.



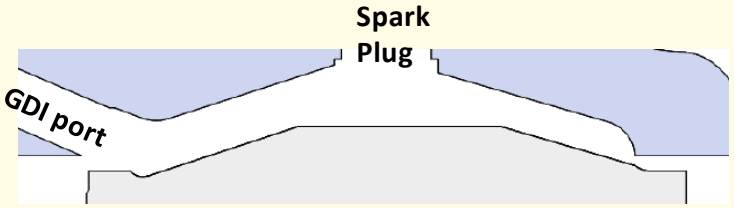
Approach (Generation 1 engine from prior work) physical experiments informing next generation design

- **<u>Prior work is informing pathways for this program</u>**
- Production GM LNF cylinder head with Sturman HVA used on custom block with 50% more stroke, a research tool
  - 50% increase in displacement per cylinder
  - 50% increase in compression ratio with same piston as LNF
  - Direct injection fuel (DI LPG)
- Dramatically increased in-cylinder turbulence and Cr
- Remaining questions on tradeoffs in efficiency and

High Cr with open chamber design

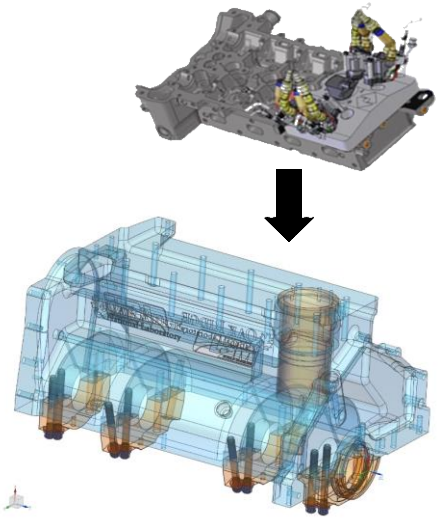


LNF r_c = 9.2:1
LSE r_c = 13.3:1



LNF r_c = 13.8:1

	Stock GM LNF	ORNL LSE
Bore (mm)	86	86
Stroke (mm)	86	129
Connecting rod (mm)	145	182.9
Compression ratio(-)	9.2 (stock) up to 13.8	13.3 (“stock”) up to 20.7
Displacement per cylinder (l)	0.495	0.749

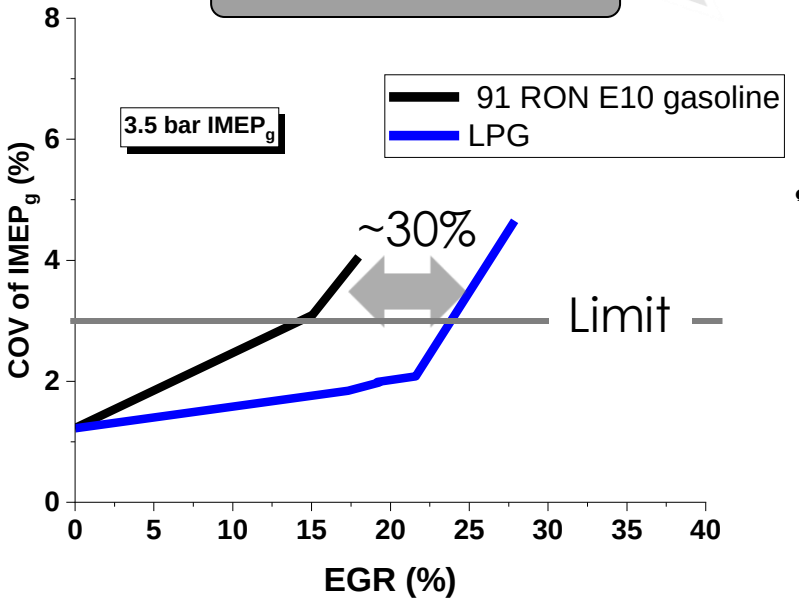


Three factors from experiments identified as key to achieving diesel-like efficiency: dilution tolerance, knock resistance and fast burn duration

Standing on the shoulders of prior work towards informing current work on EGR fundamentals and efficiency sources

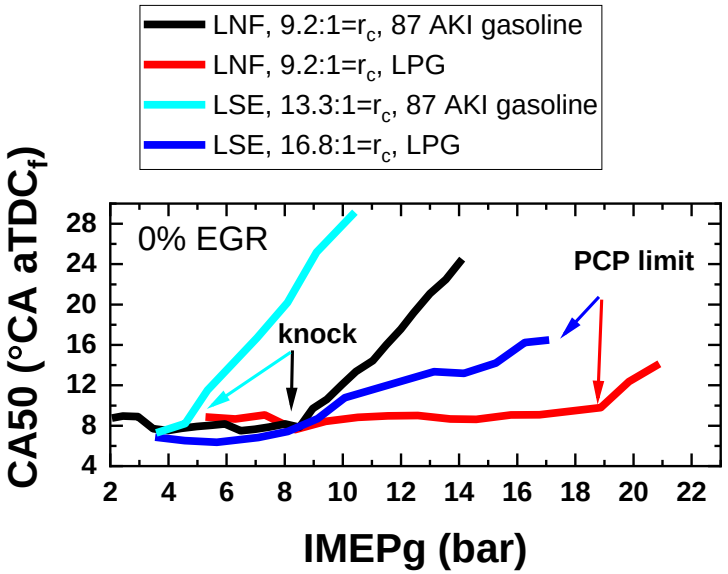
High Efficiency Stoichiometric Spark Ignition

EGR Dilution



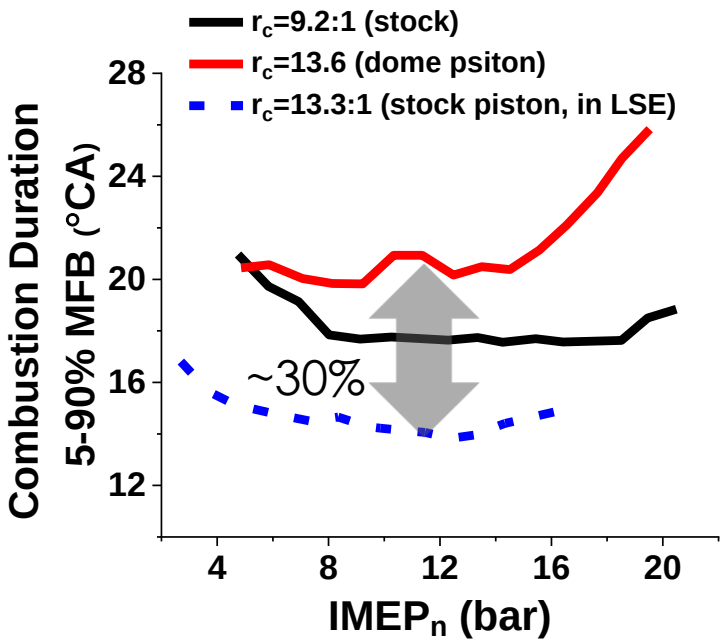
- Program will investigate factors affecting dilution tolerance
  - comprehensively understand physical-chemical processes and opportunities

Fuel Knock Resistance



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

Fast Burn (turbulence)



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

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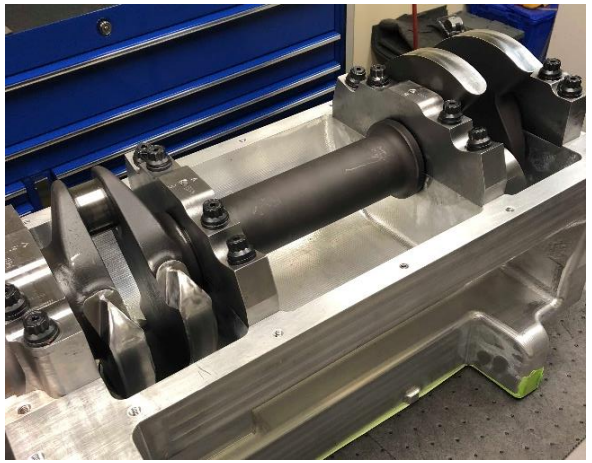
Fuel system development and reduced stroke data for simulation optimization efforts towards Gen 2 engine

- Laboratory piston accumulator fuel system used in initial research
  - Removes pump flash boiling effects
- Known fuel delivery volume issues with OEM design (Higher engine displacement and Lower fuel energy density).
  - 50% increase in fuel flow needed to match injection durations of gasoline

Off-engine belt driven pump being developed with increased flowrate injectors

- Generation 1 engine experimental campaign with 1.25:1 stroke-to-bore ratio.
  - Informing turbulence friction tradeoff for Gen 2 engine
- Development of validation data for CFD models and bounding of efficiency results compared to existing 1.5:1 stroke-to-bore data.



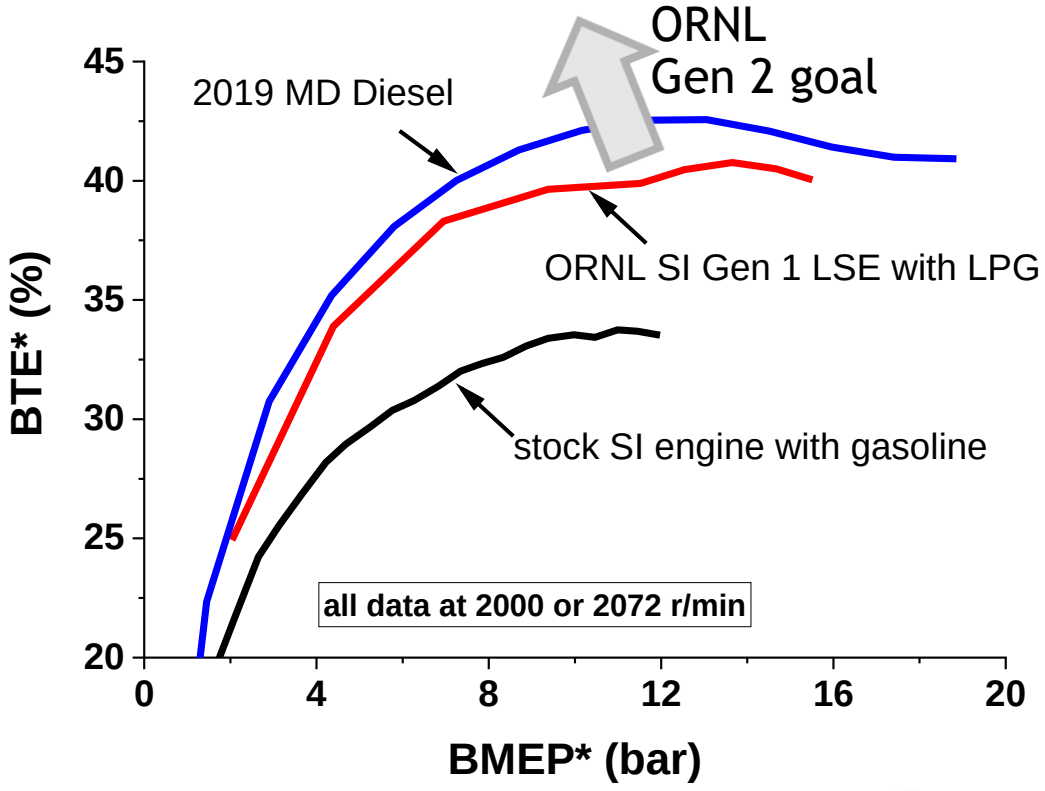
Physical engine and measurements, Gen 2 development

Why updated engine is needed (Gen 2)?

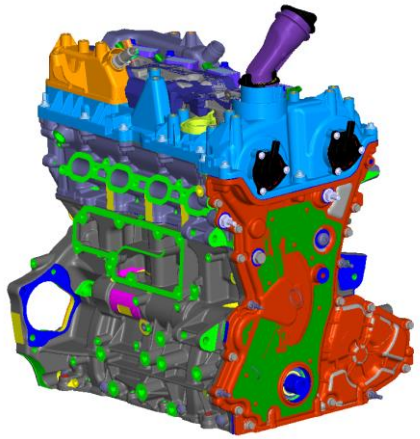
- Modern engine design
- High tumble combustion system designed for cooled EGR.
- Combustion can be improved via piston bowl design for LPG → leverage fuel characteristics to minimize heat losses and reduce burn duration.
- Experiments and simulations with multiple stroke-to-bore ratios to reduce friction uncertainty.

Generation 2 Prototype Characteristics

- Centrally mounted injector.
- Changing from hydraulically actuated valves to physical camshaft system for robustness and durability
- Production cylinder-head adapted into custom billet block and crankshaft.
- Updated design to be capable of stock to 1.5: 1 stroke-to-bore ratio



Stellantis Hurricane engine modification into Gen 2 LSE



Approach (fundamental simulations and design for updated engine)

Conceptual Understanding

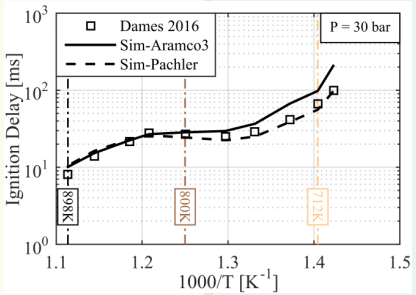
Fundamental Modeling

Model Free Approach – Direct Numerical Simulation (DNS)

Fundamental Ignition Simulations

Conceptual understanding of dilution effects on flame and ignition

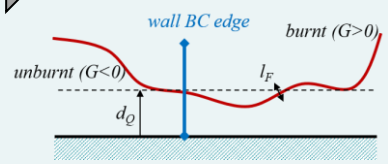
Chemical Kinetics Development

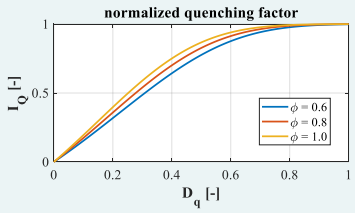


Prototype Hardware Demonstration

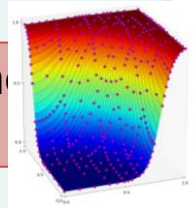
Applied Modeling

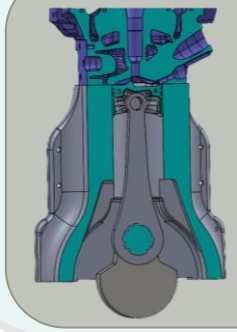
Sub-Model Development





Combustion System and Engine Design Optimization

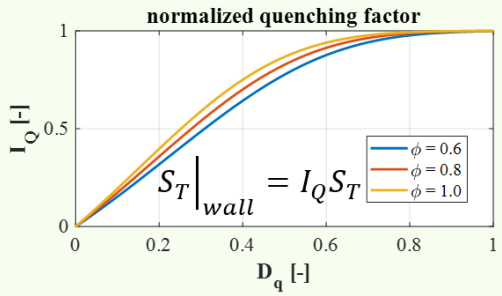


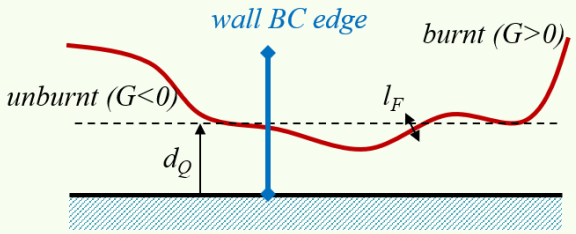


Gen 2 Long-Stroke Engine

Sub-model development needed to improve predictive capability towards optimization of geometry

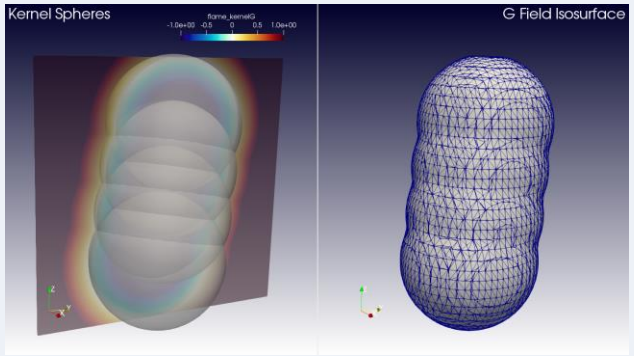
Wall Quenching Model





- Improved hydrocarbon emissions predictions
- Allows prediction of squish-driven quenching

Kernel Formation and Development Model

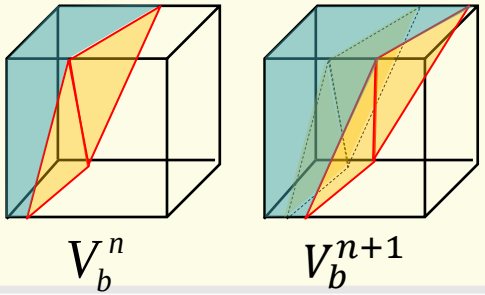


- Fuel and EGR stratification

Program's Improved G-Equation Simulation Approach

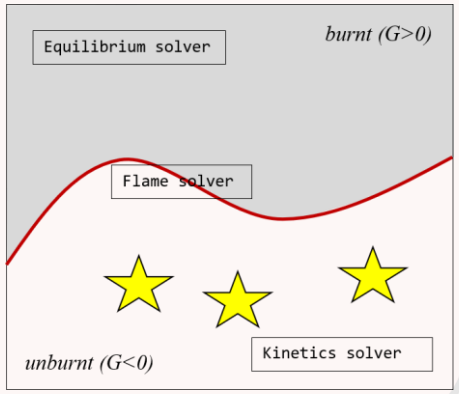
Swept volume approach for G-Equation

- Improved flame propagation predictions



Fast End-gas auto-ignition model

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



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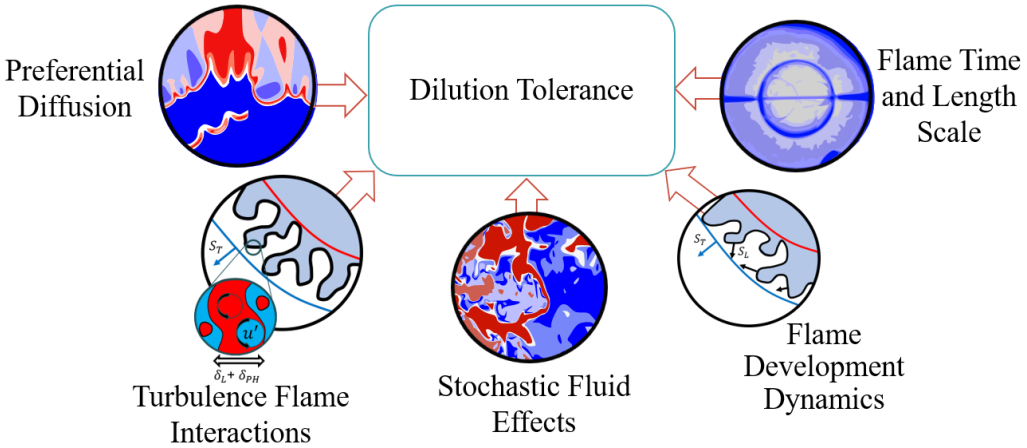
Three factors from experiments identified as key to achieving diesel-like efficiency: dilution tolerance, knock resistance and fast burn duration

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

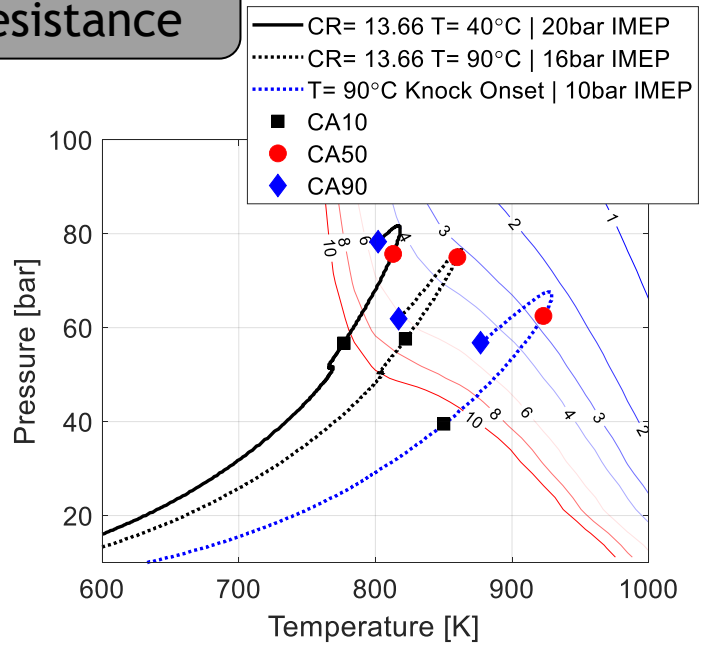
High Efficiency Stoichiometric Spark Ignition

EGR Dilution



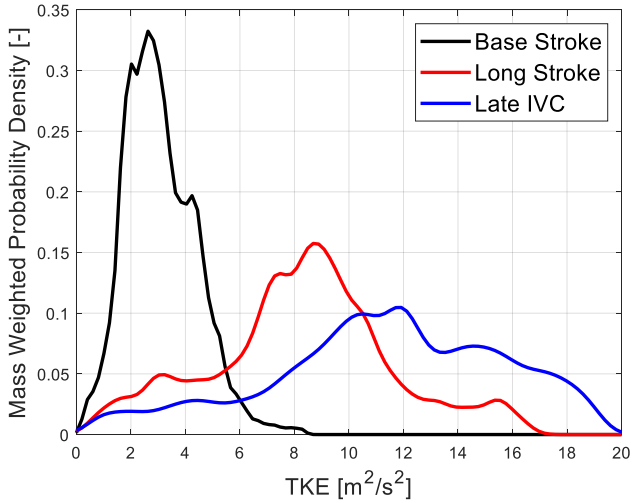
- Program will investigate factors affecting dilution tolerance
  - Comprehensively understand physical-chemical processes and opportunities
  - Includes ignition through late-cycle quenching phenomena

Fuel Knock Resistance



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

Fast Burn (turbulence)



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

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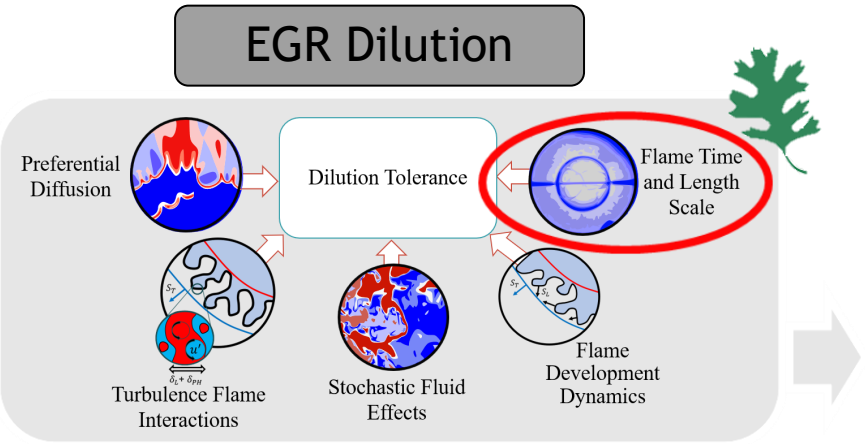
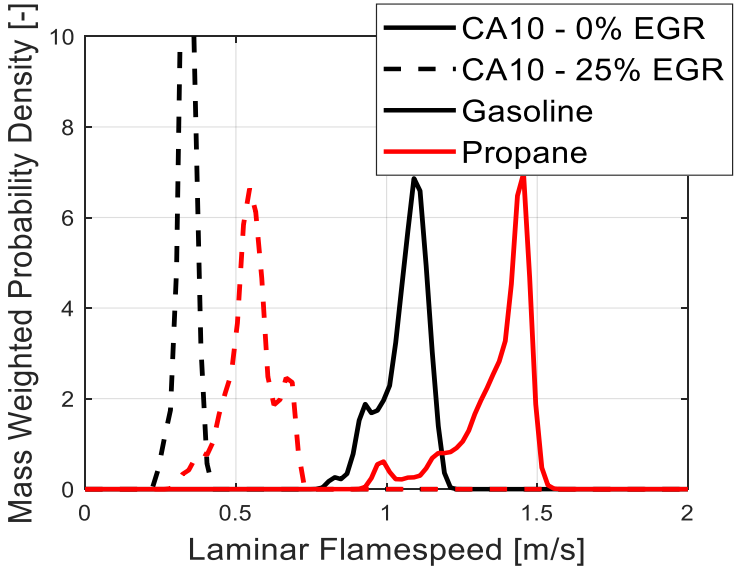
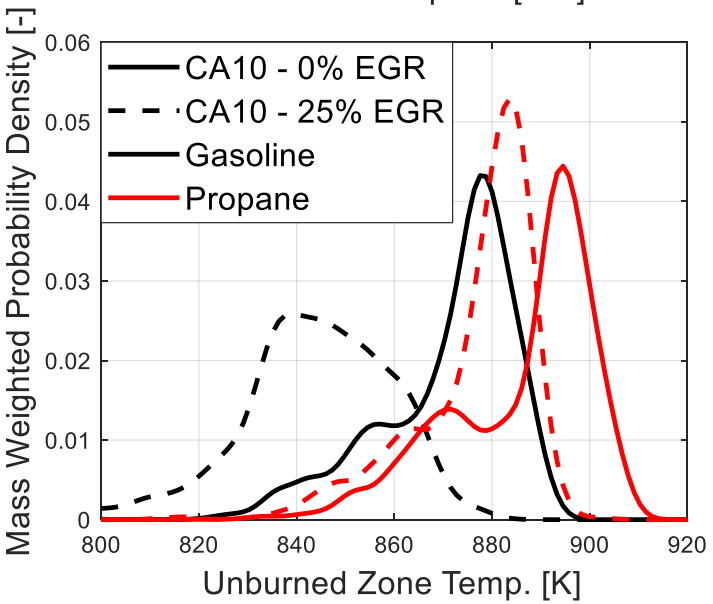
Fundamental fuel properties of LPG enable improved EGR tolerance

Initial study targeting understanding of flame and time scales.







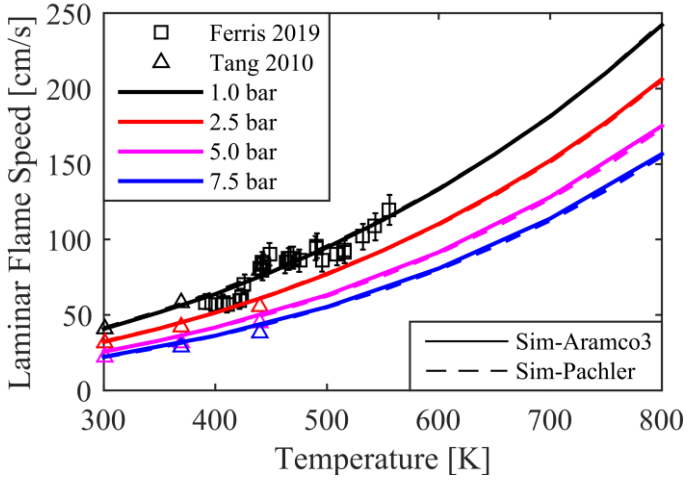
3-D CFD results using **RANS turbulence model and G-Equation** approach for flame suggest that LPG's enhanced dilution tolerance is a result of laminar flame speed effects:

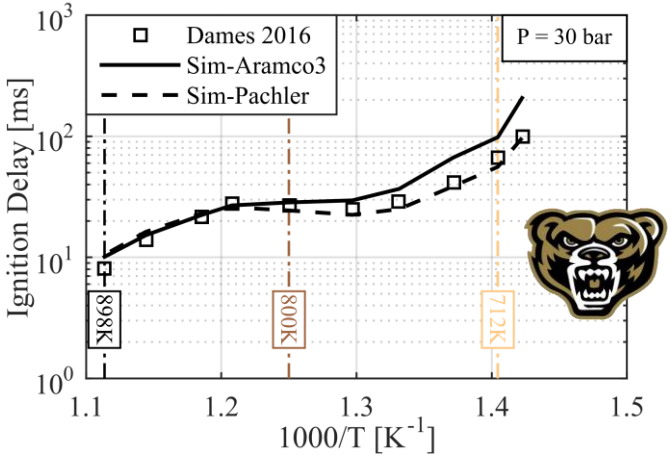
- Higher laminar flame speeds than gasoline
- Higher end-gas temperatures due to gamma effect of LPG vs. gasoline → Even higher effective flame speed.

SAE 2021-01-0483

Chemical response of LPG can change significantly with changes in impurities, kinetics needed for fundamental simulations

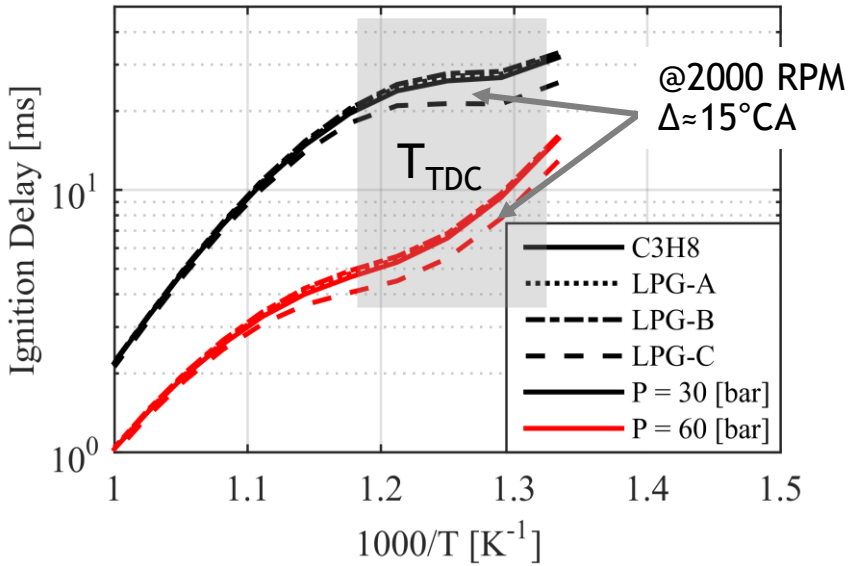
- Development of an improved chemical mechanism validated for mixtures of LPG.
  - Enables DNS of LPG flames and reactions (fundamental affecting EGR dilution)
- Literature survey of existing mechanisms has identified potential starting points:





Aramco 3.0 [572 species 3037 reactions] (Too large for DNS)
Pachler et al. [70 species 352 reactions] (Suitable size for DNS)

Fuel	C_3H_8	LPG-A	LPG-B	LPG-C
Propane, C_3H_8	100%	96%	92%	92%
Ethane, C_2H_6	0%	2.5%	6.5%	1.5%
Iso-Butane, iC_4H_{10}	0%	1.0%	0.0%	0.0%
n-Butane, nC_4H_{10}	0%	0.5%	1.5%	6.5%

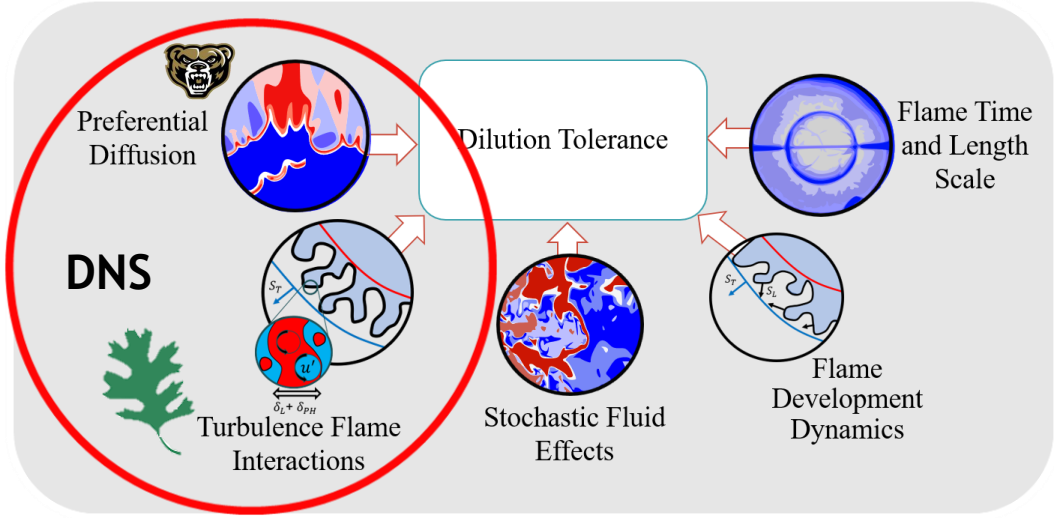


References

1. Ferris, A., et al., Combustion and Flame 205 (2019), https://doi.org/10.1016/j.combustflame.2019.04.007
2. Tang, C., et al., Energy Conversion and Management, 51:2, (2010), https://doi.org/10.1016/j.enconman.2009.09.024
3. Dames, E. E., et al., Combustion and Flame 168 (2016), https://doi.org/10.1016/j.combustflame.2016.02.021
4. Zhou, C-W., et al., Combustion and Flame 197 (2018), https://doi.org/10.1016/j.combustflame.2018.08.006
5. Pachler, R. F., et al., Fuel 172 (2016), http://dx.doi.org/10.1016/j.fuel.2015.12.044

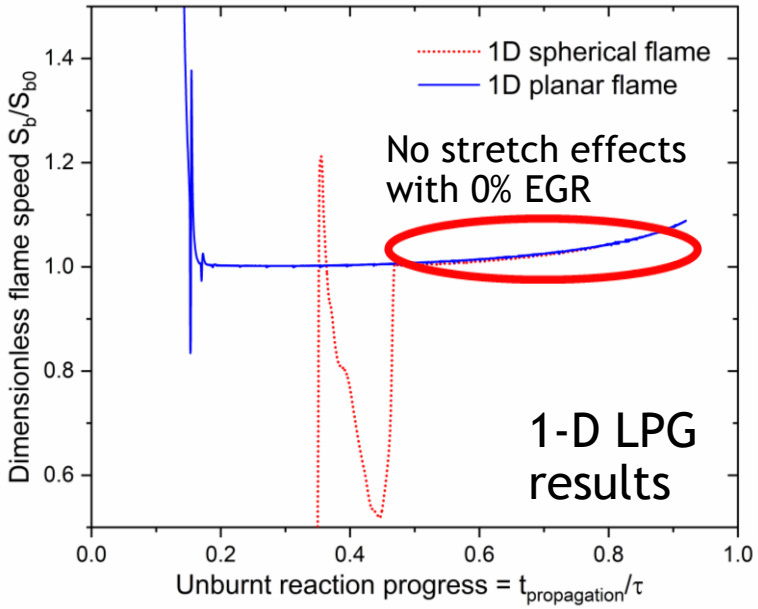
Direct Numerical Simulations (DNS) are a model free approach to study the effect of preferential diffusion and auto-ignition on dilution tolerance

- Fundamental reason for improved EGR with LPG 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 (**preferential diffusion**) show no flame stretch effects **with 0% EGR.**

- Thermal and mass diffusivity are similar and LPG itself is not intrinsically affecting flame processes (Lewis number is unity)
- **EGR analysis ongoing**

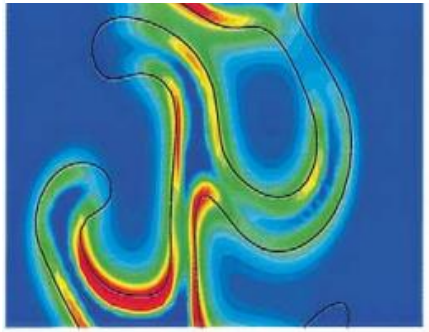


Flame regime analysis in backup slides

DNS results will elucidate fundamental sources of LPG dilution tolerance (opportunity for engine development)

1-D results & Kinetics used in DNS approach

2-D DNS concept



DNS study of preferential diffusion (Hydrogen-Air flames)
Hong and Chen. 2002. Combustion and Flame, 131(3)

Responses to previous Years Reviewer's Comments

- This project has not been reviewed previously

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 LPG blends.
  - **University of Tennessee - Knoxville** (Formerly of Oakland University) – Sub recipient: 1-D spherical flames and stretch effects.
  - **Katech** – Sub recipient: Engine design integration for Gen 2 prototype and Fuel system
  - **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

- Development of Gen 2 prototype engine with fully integrated variable camshaft system and belt driven LPG pump.
  - Integration of Stellantis stock head on custom build billet block.
  - Integration of variable camshaft system on custom platform.
  - Development of belt driven LPG pump that avoids cavitation issues.
- Understand the chemical effect of impurities in the LPG composition such as butane and ethane.
  - Can have strong impact on knock performance of fuel.
- 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.

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Proposed Future Research

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

FY21

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

II. **Gen 1 Experiments with 1.25 stroke-to-bore**
   I. Assessment of stroke-to-bore effects and generation of validation data

III. **1-D Flame Stretch Simulations**
   I. Effect of EGR on flame stretch effects.

FY22

I. **Chemical kinetic development for LPG mixtures**

II. **Design integration of Stellantis Hurricane engine with custom built block and crankshaft.**

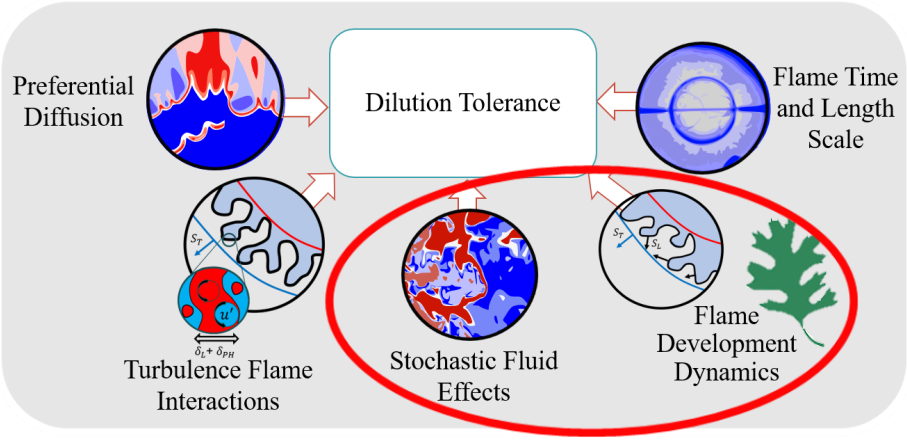
III. **Fuel system development with belt driven pump and high flow injectors**

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

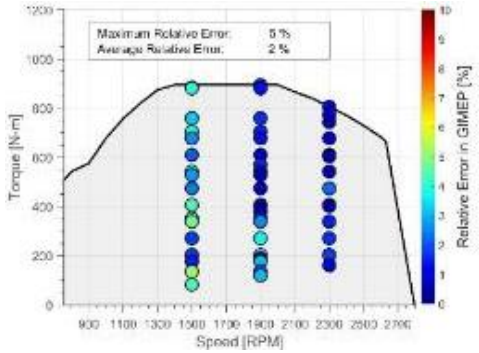
FY23

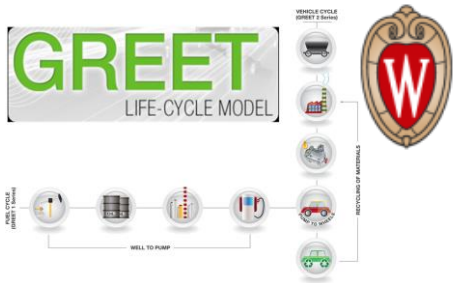
I. **Demonstration of Gen 2 prototype efficiency**

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



III. **System and life-cycle analysis**





Summary

Relevance

- Program is in line with 21st Century Truck partnership research roadmap of increasing propane engine efficiency with no cost premium.
- Program supports USCAR Priority 1 goals of mitigating knock and increasing EGR dilution

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

- Initial experiments identified three aspects of the engine performance: dilution tolerance, knock and burn rate.
- Initial 3-D CFD results using RANS turbulence and G-Equation models suggest that propane’s superior dilution tolerance is driven by its higher laminar flame speed and ratio of specific heats
- Initial 1-D spherical flame simulations did not observe stretch effects on the flame propagation speed of propane
- Literature surveyed for propane mechanisms and potential starting points were identified.

Collaborations

- Collaboration of 3 universities, industry, and a national laboratory to develop high efficiency LPG engines.

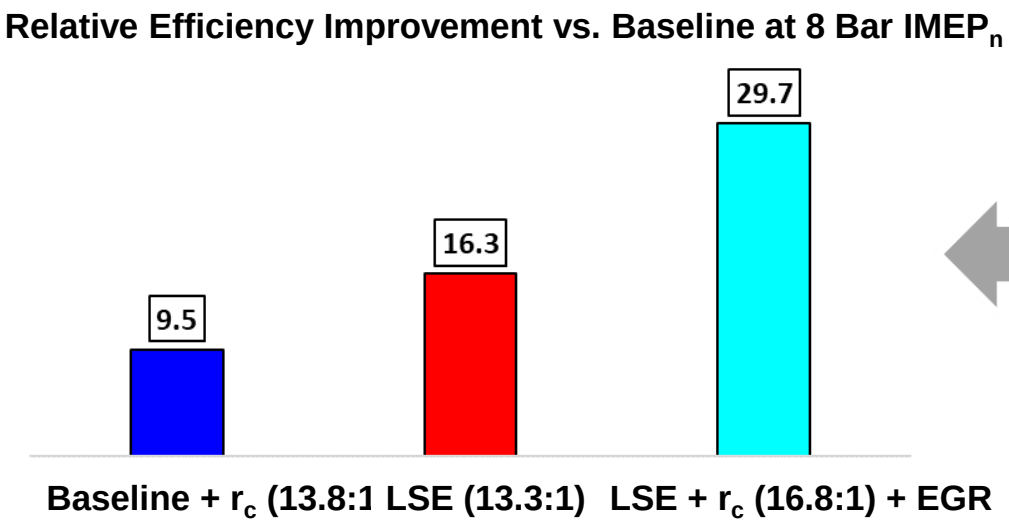
Future Work

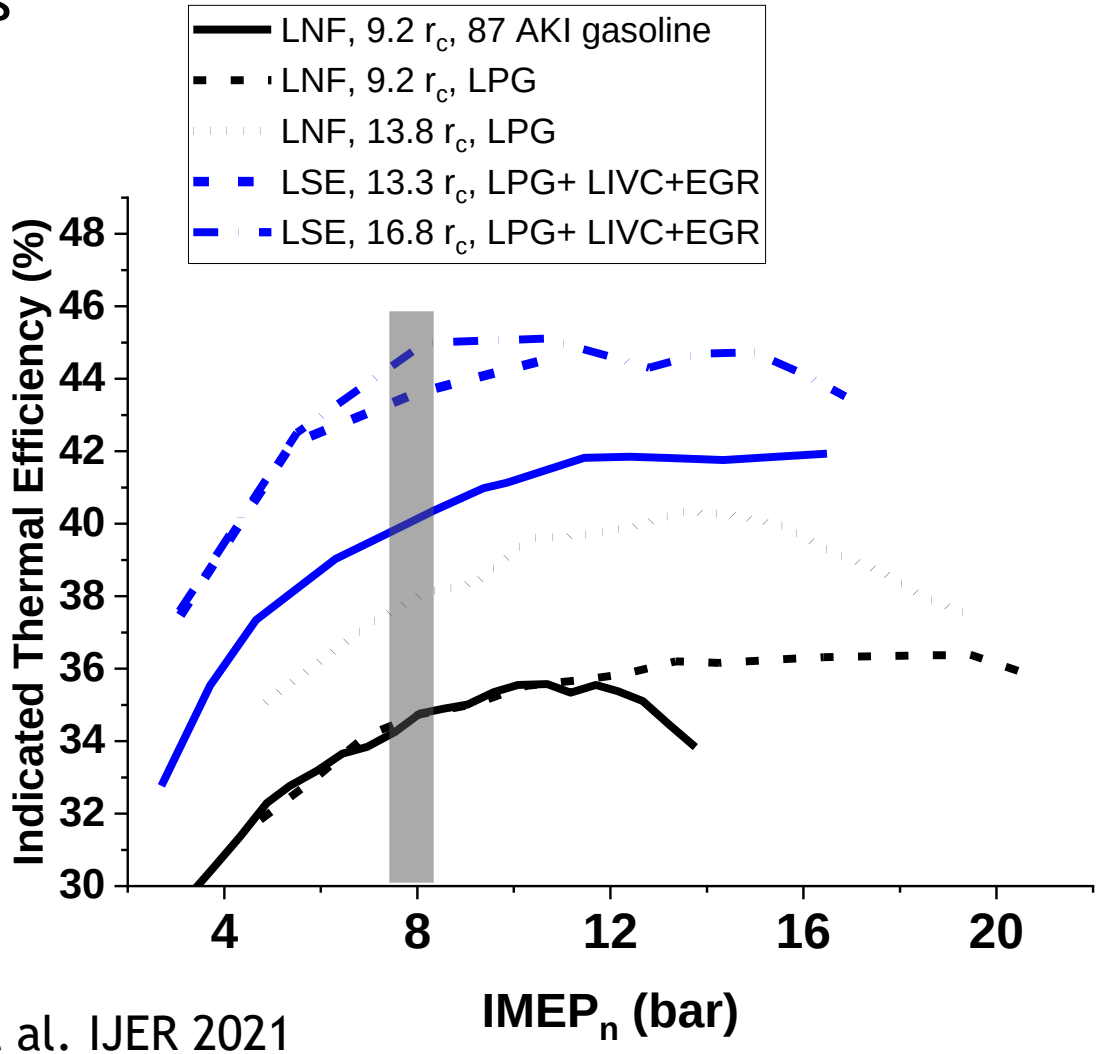
- Reduced stroke Gen 1 engine experiments to provide validation data for chemical kinetic and CFD development
- Computationally guided Gen 2 engine development and integration with Stellantis Hurricane base platform
- 1-D Flame stretch simulations to assess the effect of preferential diffusion on dilution tolerance
- Development of belt driven pump and high flow fuel system

Technical Back-Up Slides

Combined fuel properties and engine design highlight promising pathways for diesel engine efficiency parity

- Systematic approach illustrates pathway towards diesel engine efficiency parity
- High EGR, late IVC, with high compression ratio (16.8:1)
- Stoichiometric operation possible at high compression ratios (3-way catalyst)





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Prior work is informing pathways for this program

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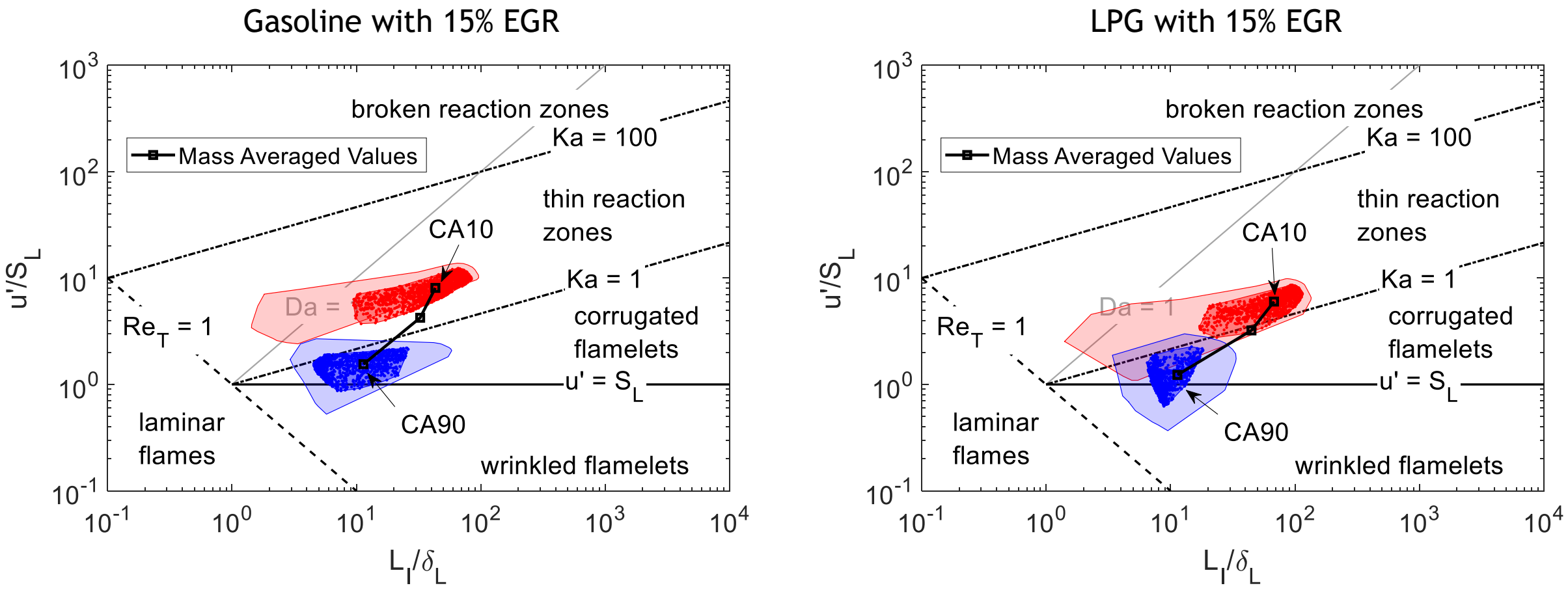
Flame Regime analysis Highlights Improved Reaction and Flame Stability of LPG vs. Gasoline with EGR



Chuahy et al. SAE 2021-01-0483

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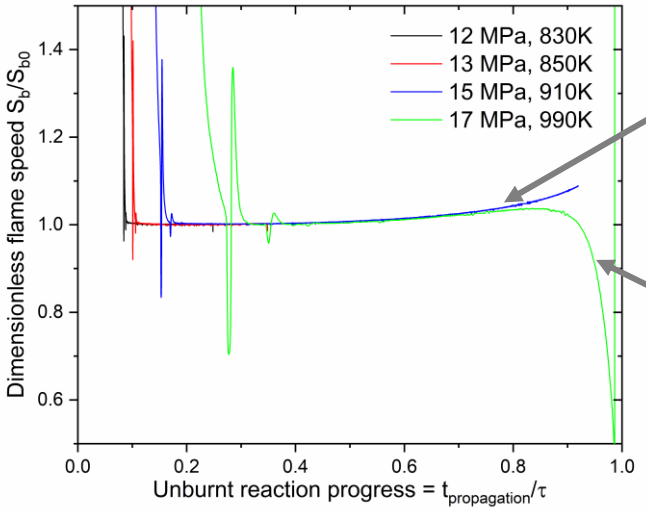
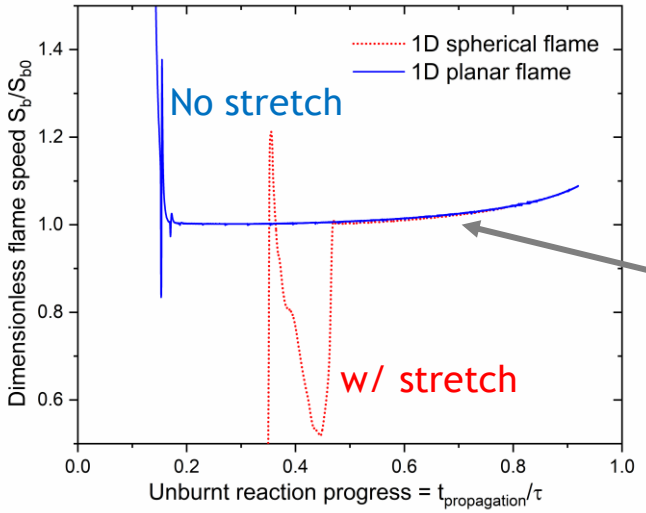
Fundamental Ignition simulations give insight on the impact of stretch and auto ignition

- Use of robust, open-source validated platform "reactingFOAM-SCT" [1-4]
- Allows the study of 1-D unsteady flame initiation in planar (effect of reaction progress) and spherical (includes flame stretch) configurations.
- Goal is to study the effects of dilution on auto-ignition/diffusion coupling and effect of flame stretch on flame propagation.



Coupling between ignition and diffusion to enhance flame speed.

Pressure wave from auto-ignition subduing flame speed.



Initial simulations with no dilution show no effect of stretch on flame speed → Stratification and dilution need to be investigated.

[1] Q. Yang, P. Zhao, H. Ge, reactingFoam-SCI: An Open Source CFD Platform for Reacting Flow Simulation, Computers & Fluids, 190 (2019) 114-127.
[2] Q. Yang, P. Zhao*, "Minimum ignition energy and propagation dynamics of laminar premixed cool flames", Proc. Combust. Inst., 38 (2021) 2315-2322.
[3] M. Tao, Q. Yang, P. Lynch, P. Zhao*, "Auto-ignition and reaction front dynamics in mixtures with temperature and concentration stratification", Frontiers in Mechanical Engineering, 6 (2020) 68.
[4] Q. Yang, Z. Chen, A.J. Susa, R.K. Hanson, P. Zhao*, "Over-driven flame and its role in the negative-temperature dependence of iso-octane flame speed at elevated temperatures", Combust. Flame, 223 (2021) 65-76.

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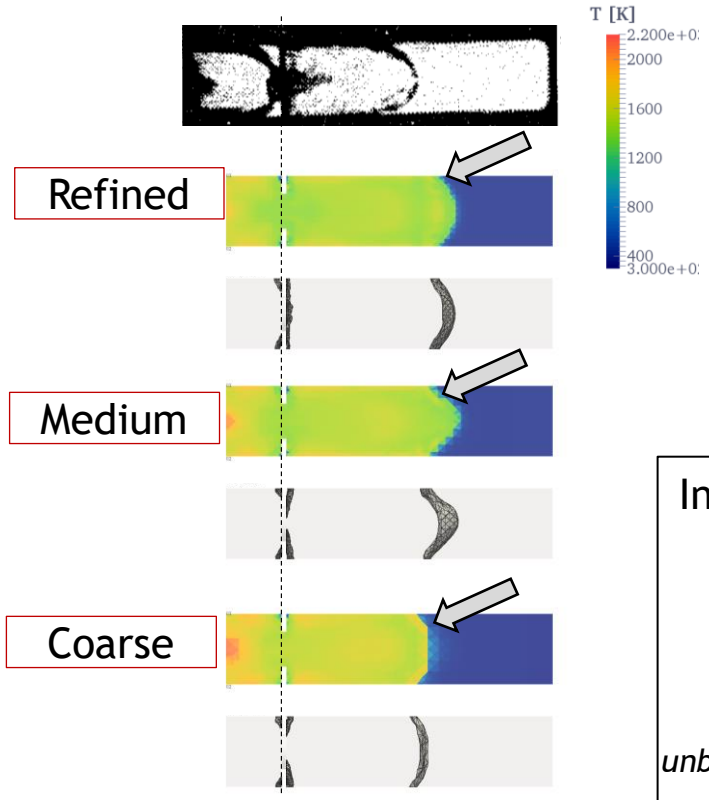
Flame-wall interaction submodel requires improvement for understanding emissions and efficiency penalties

State-of-the-art G-Equation models do not capture near-wall quenching



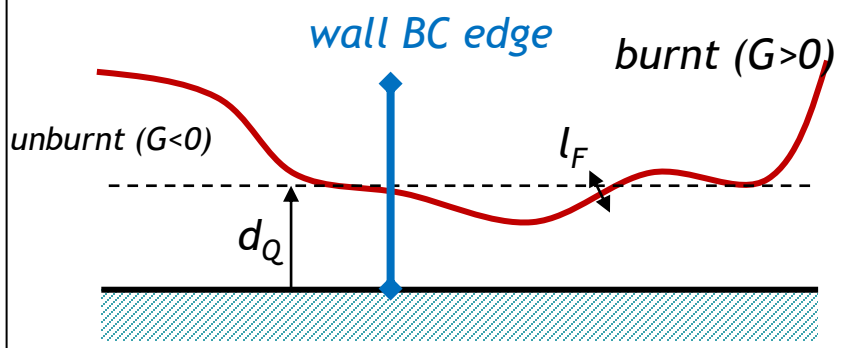
exp: 3.3 ms
sim: 3.0 ms

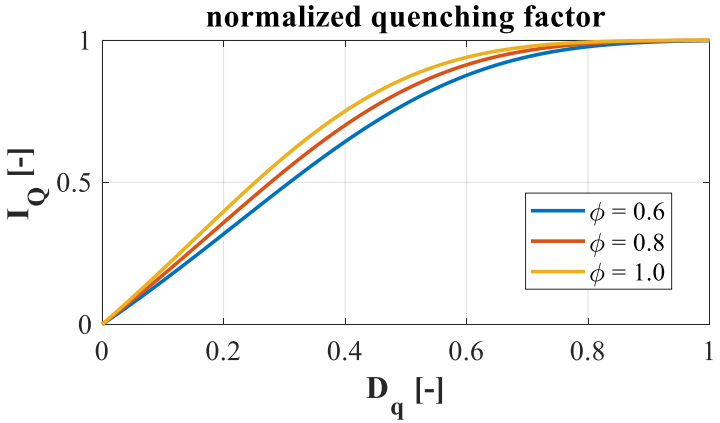
Sonic flame through orifice
(*Furukawa and Gomi, JSME 1982*)

- Some bending/quenching at the wall is captured due to temperature/tke gradients affecting the turbulent flame speed (SAE J. Eng. 9(3),1409-1424)
- But, near-wall modeling is not improved by increasing mesh resolution
- Combustion efficiency and heat transfer predictions are affected

Introduce a **near-wall quenching zone:**

$$S_T\Big|_{wall} = I_Q S_T$$





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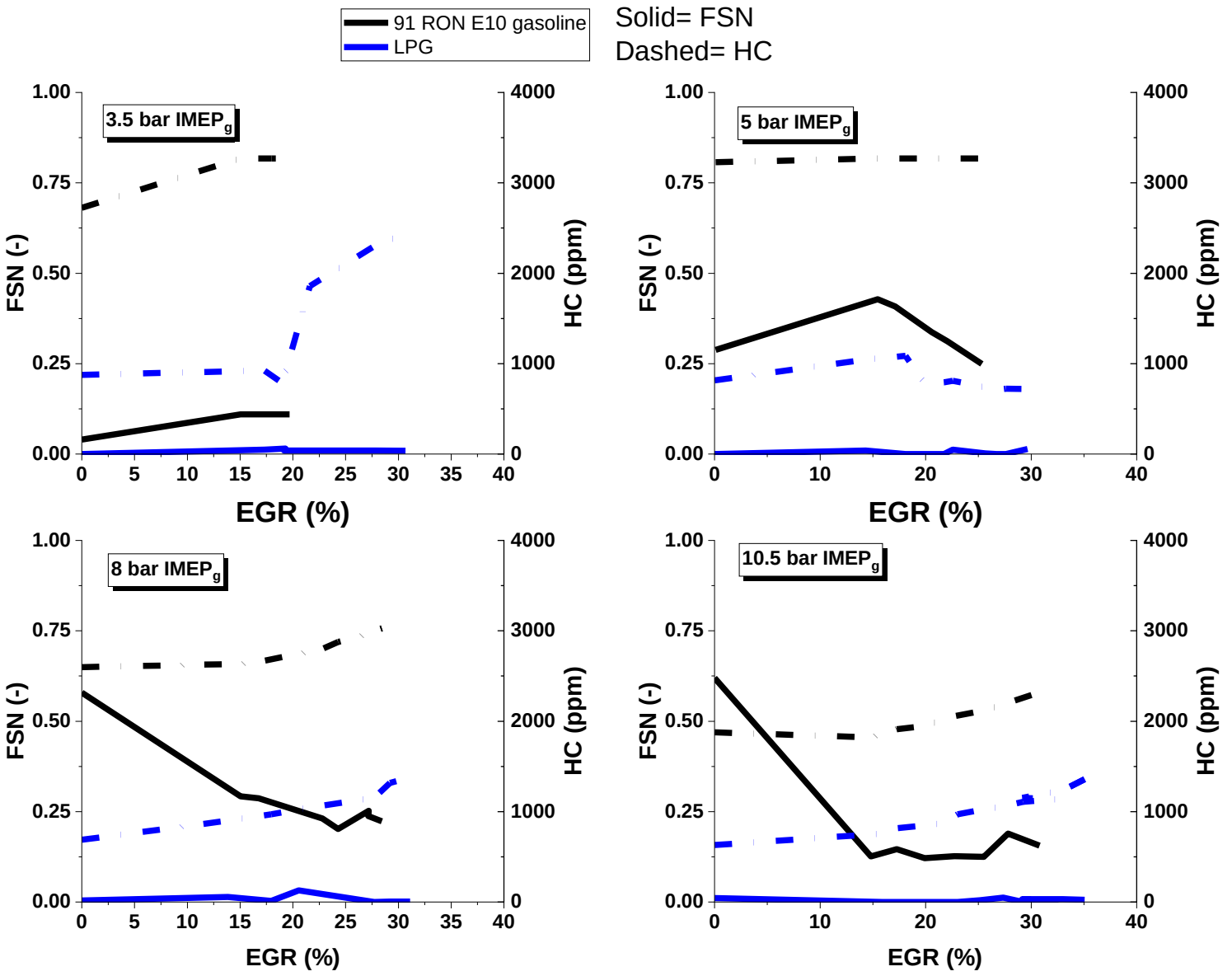
High volatility of LPG shows near-zero FSN and large HC reductions

- LPG shows ~2-3X reduction in HC for a given conditions
- At measurement detection limit for FSN for LPG
- Opportunity for engine geometry redesign could be possible (HC and Soot behavior different)
  - Follow on programs and areas could be possibility for further efficiency improvements.



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