# Engine Knock Prediction

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**Project ID: ACS110**

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# Overview

## Timeline

- Project start: 2/01/2016
- Project end: 1/31/2019
- Percent complete: 35%

## Barriers

- Increase the fuel efficiency of passenger cars
- Lack of modeling capability to accurately simulate engine knock
- Inadequate fundamental understanding of turbulence-chemistry interactions during engine knock

## Budget

- Total project funding: $715,933
  - DOE share: $643,839
  - Contractor share: $72,094
- Budget Period 1: $299,417
- Budget Period 2: $258,664

## Partners

- OSU (Lead)
- ORNL
- Convergent Science

# Relevance

**Project Objective**: Improving predictive capability for engine knock by developing a new, physics-based large eddy simulation (LES) combustion model

- Reproducing cycle-to-cycle variations
- Accurately predicting mean heat release/reaction rates during end gas ignition
- Using detailed (reduced) chemical mechanism (~100 species) in engine knock LES

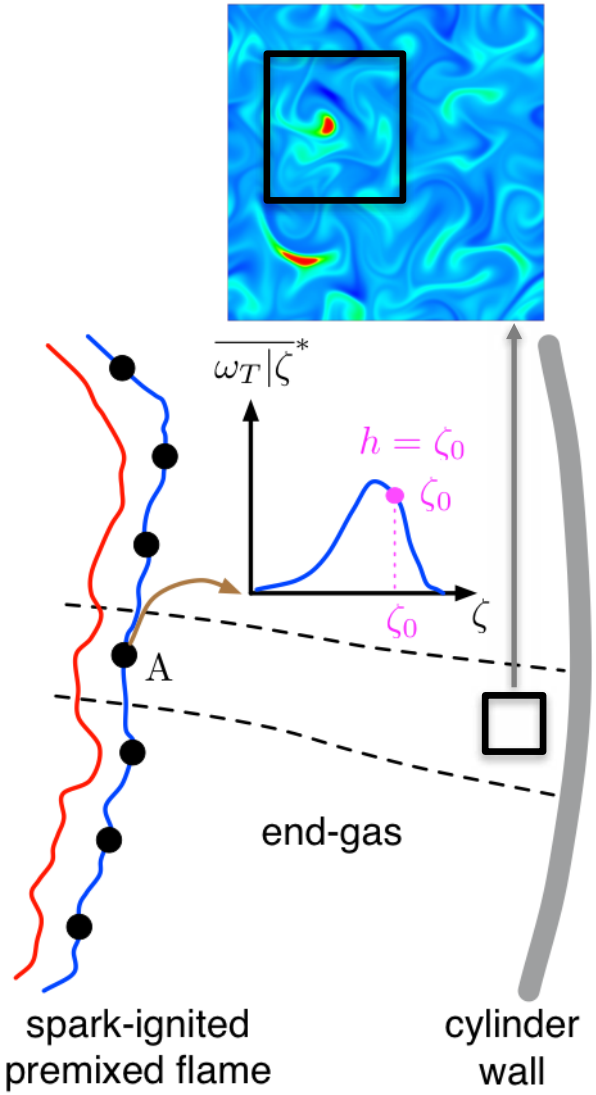
## Objectives in the Period of Feb. 2016-Mar. 2017

- Developing a base code
- Generating direct numerical simulation (DNS) data base for model validation
- Acquiring in-cylinder pressure data from laboratory engine experiments under knocking and knock-free conditions

# Approach: Model

## CMC-FPF: LES combustion model for knock

- CMC for end-gas ignition
  - Conditional Moment Closure: Klimenko and Bilger (PECS, 1999)
  - Accurate reaction rate prediction
    - Volume Avg. vs. Surface Avg.
    - Surface averaging in CMC preserves small-scale scalar structures and thus can lead to accurate reaction rate estimation
- FPF for SI premixed flame
  - Front Propagation Formulation: Kim (JCP, 2015)
  - Cycle-to-cycle variations in premixed burning rates
  - Reproducing the level set method in the flamelet regime
  - Applicable to broader premixed combustion regimes

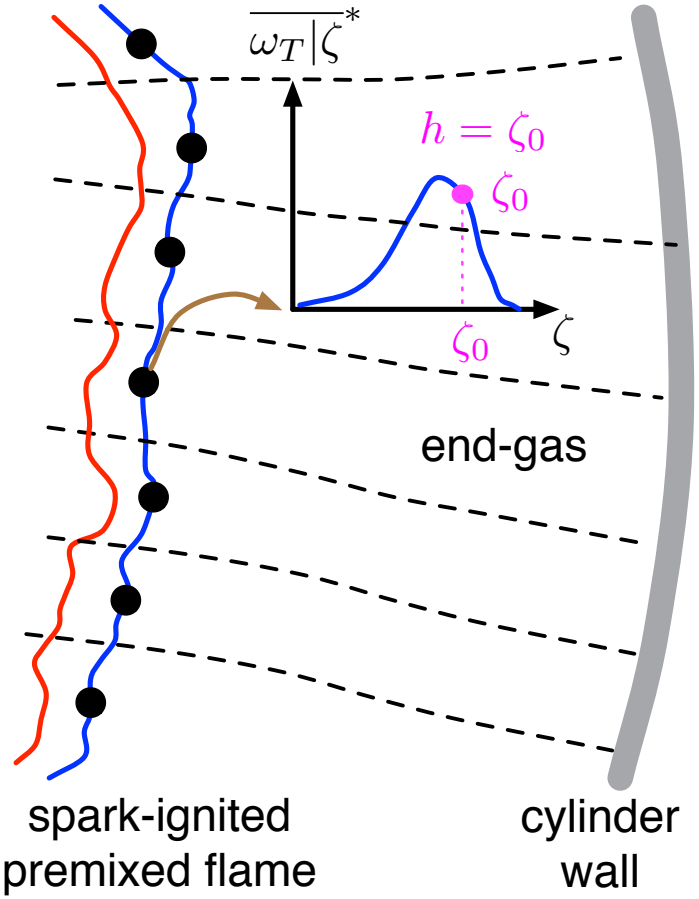


# Approach: Model

## End-gas ignition CMC can accurately estimate reaction rates in a computationally efficient way

- Small-scale scalar structures resolved in enthalpy space
  - Total enthalpy or sensible enthalpy
- Thus, the number of grid points in ignition CMC can be much smaller than the number of typical LES grid points
  - To be computationally more efficient than conventional LES where volume-averaged (filtered) species mass fractions and temperature are used to estimate reaction rates

$$\frac{d_\zeta \overline{Y_i|\zeta}^*}{dt} + T_{Y_i'} = \overline{N_h|\zeta}^* \frac{\partial^2 \overline{Y_i|\zeta}^*}{\partial \zeta^2} + \frac{\overline{\rho\dot{\omega}_i|\zeta}^*}{\rho_\zeta} - v_\zeta \frac{\partial \overline{Y_i|\zeta}^*}{\partial \zeta}$$



# Approach: Milestones

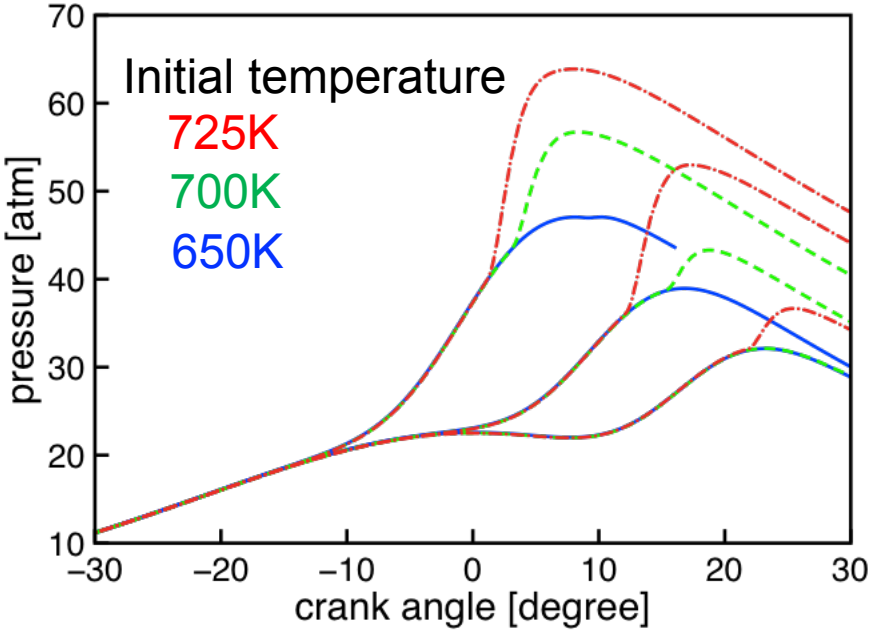
## Model development supplemented by direct numerical simulation (DNS) and engine experiments

### Milestones

- Developing a CMC solver for end-gas ignition (Y1Q2)
- Developing a base CMC-FPF solver (Y1Q4)
- Experimental campaign I (Y1Q4)
- DNS of end-gas knock (On-going)
  - Detailed chemistry ignition 2-D DNS: Reaction rate estimation
  - Two-step-chemistry ignition 3-D DNS: Scalar dissipation
  - Premixed flame DNS: Premixed flame modeling
- Validation of CMC-FPF with DNS data (On-going)
- Base engine simulations – knock-free (Started)
  - Premixed model to be implemented as UDF of Converge CFD

# Developed base knock CMC code

- Transient, 1-D transport in enthalpy space, and reaction
- Time integration
  - Stiff ODE solvers
    - CVODE, DVODE (Lawrence Livermore National Laboratory)
    - Plan to include other solvers
- Transport in enthalpy space
  - Second-order finite difference
- Chemistry
  - CHEMKIN compatible
  - Use of CHEMKIN II (Sandia National Laboratory)
- Adaptive mesh refinement

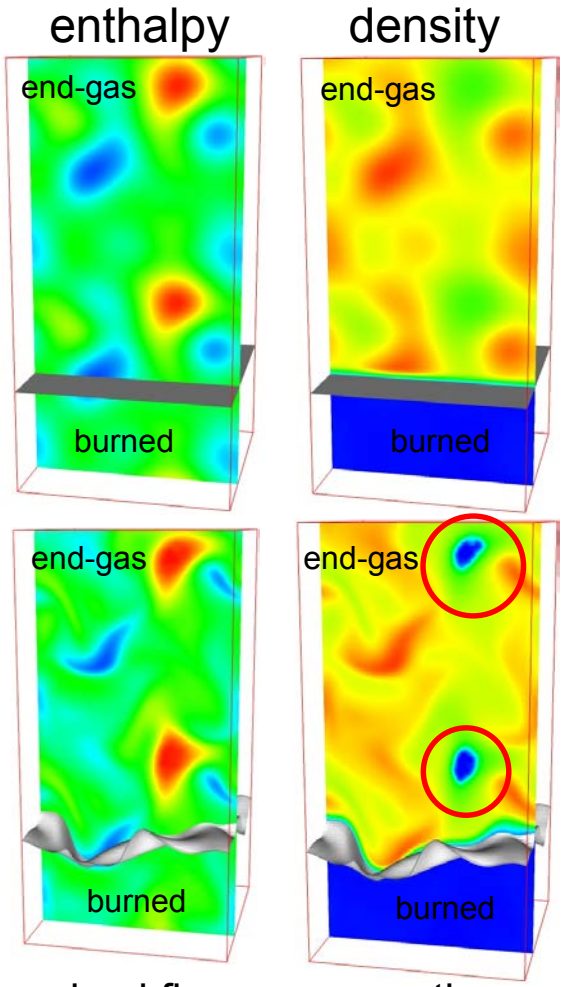



End-gas ignition in engine-like pressure evolution (Stoichiometric iso-octane/air mixture; 116 species reduced mechanism for PRF, Luong et al. CnF 2013; imposed thermal stratification; three spark timings)

# Model Development

## Developed initial interface module to couple CMC-FPF solver with an LES solver

- CMC-FPF combining
  - Knock CMC
    - Base solver described before
    - Included transport in physical space: operator splitting, high-order TVB finite difference
  - Premixed Flame FPF
    - Fifth-order WENO scheme (Jiang and Shu JCP 1996) for regularized Delta function
- Coupling with an LES solver
  - Initial interface module developed
  - Coupled with low Ma flow solver, NGA (Desjardins et al. JCP 2008)

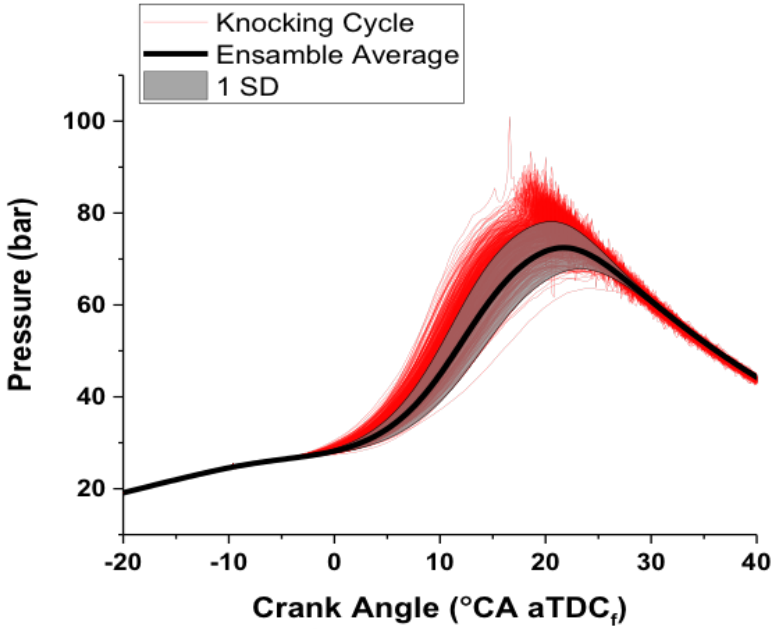



Premixed flame propagation and end-gas ignition in constant volume configuration

# Experiments

## Single-cylinder engine laboratory used to identify knocking conditions by statistical analysis

- 2007 GM LNF 2.0L Ecotec Single cylinder
  - 9.2:1 compression (stock)
- Conditions
  - Fuel: Iso-octane
  - 2000 r/min
  - CA50 from knock to 50 $aTDC_f$
  - Intake temp from 35°C to 135°C
  - Constant airflow (4 levels) all positive gauge pressure
  - 0 and 15% EGR
- Knocking cycles identified as 1 bar KI

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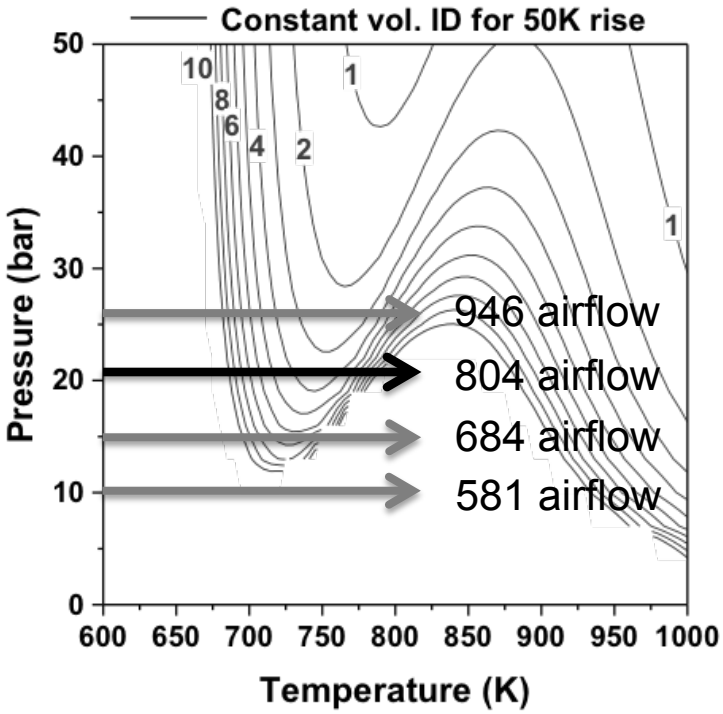
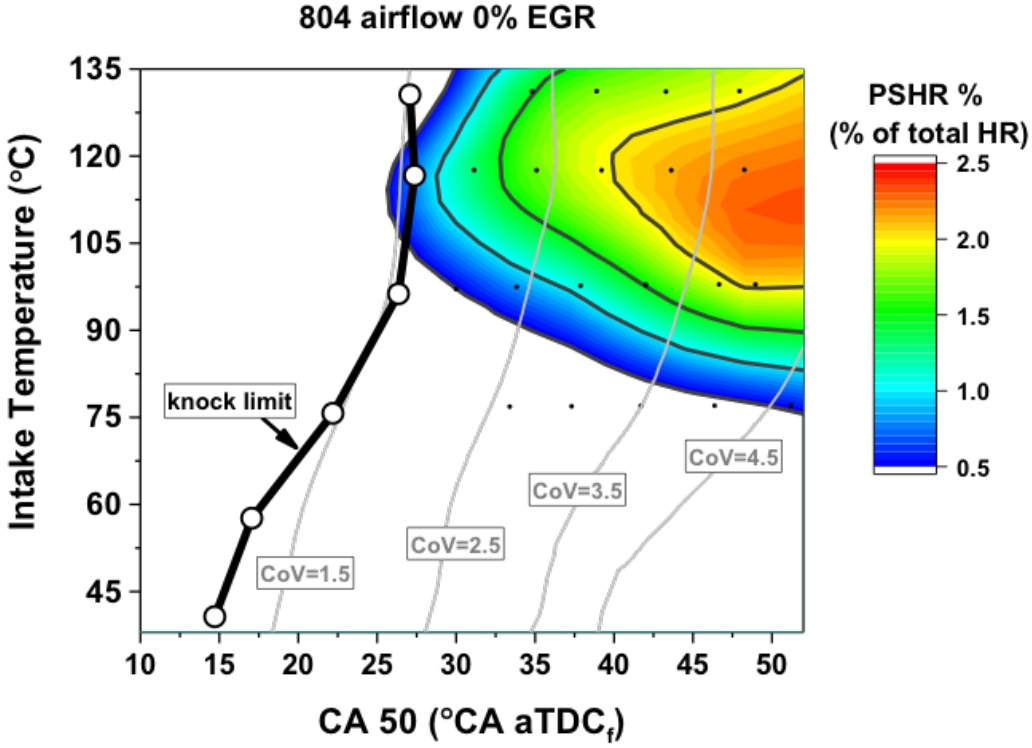
# Experiments

## Experimental conditions "slice" through ignition delay regions for each boost condition using intake temp.

- Experimental conditions varied
  - Intake temperature, boost, and EGR rate (0% and 15%)

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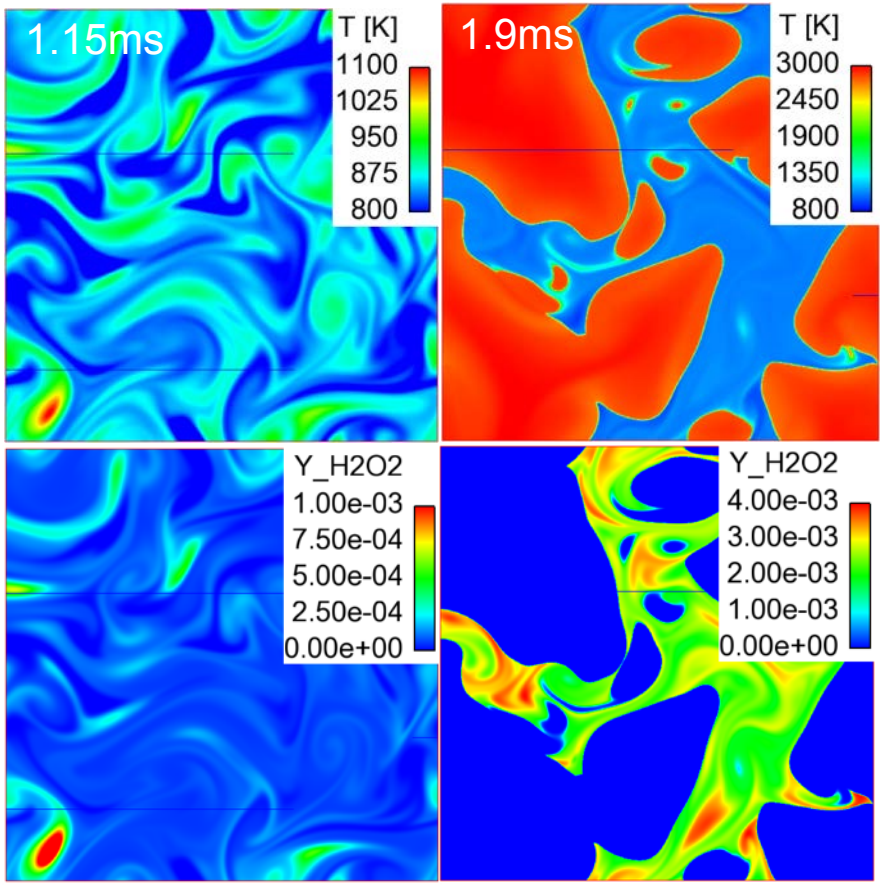
# DNS: Detailed Chemistry

## Performed detailed-chemistry 2-D DNS to generate database for model validation

- Low Ma, second-order kinetic energy conserving scheme (NGA)
  - Combined with CHEMKIN and TRANSPORT package
- 116 species PRF reduced mechanism
- Isotropic turbulence with thermal stratification
- Conditions
  - PRF80/air, 20-30bar, 800-970K, 0.8-1 equivalence ratios
  - $u'$ ~ 1.2m/s, $l_t$~1.2mm, $T_{rms}$~40K
- Focusing on reaction rate estimation during ignition

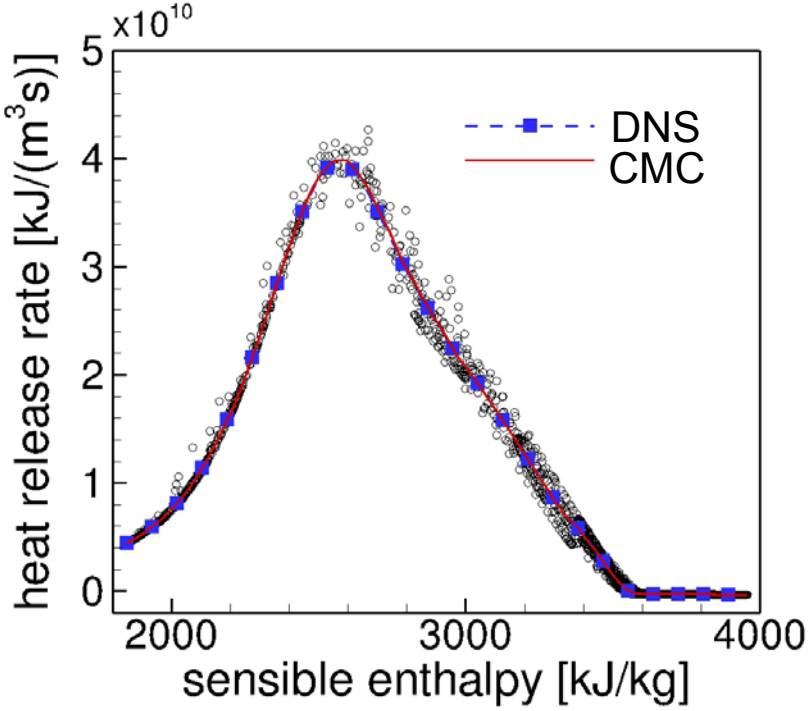


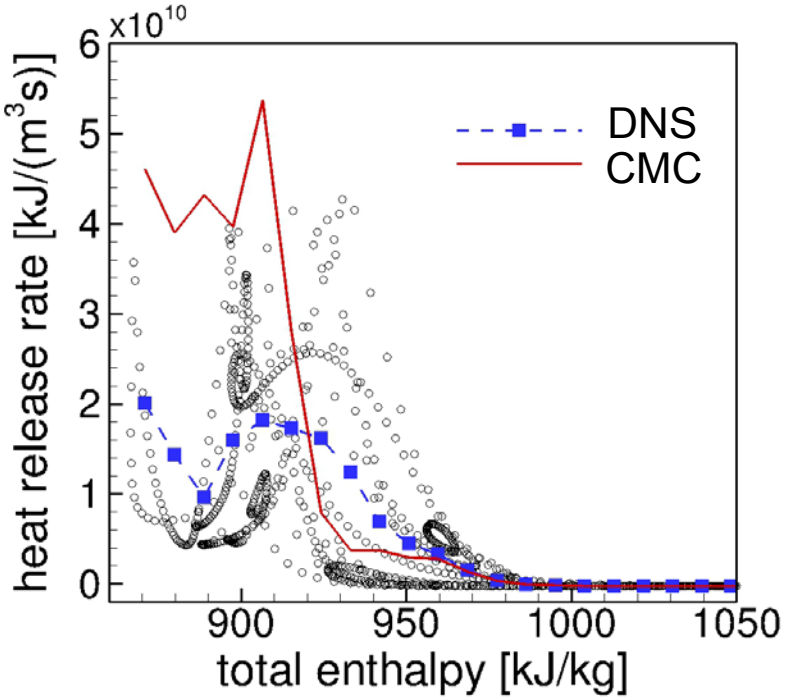

Temperature and $H_2O_2$ mass fraction fields during end-gas ignition ($T_0$=850K, $P_0$=30bar, stoich. PRF80/air, 5mm$^2$, 1024$^2$ grid points). Refined grid DNS (3072$^2$) in progress.

# Model Validation

## Assessed accuracy of reaction rate estimation

- Sensible-enthalpy or total-enthalpy can be used as a conditioning variable (for surface averaging)
- Sensible-enthalpy CMC accurately estimates heat release rates, while total-enthalpy CMC leads to substantial errors
- More investigation for a wider range of conditions is necessary



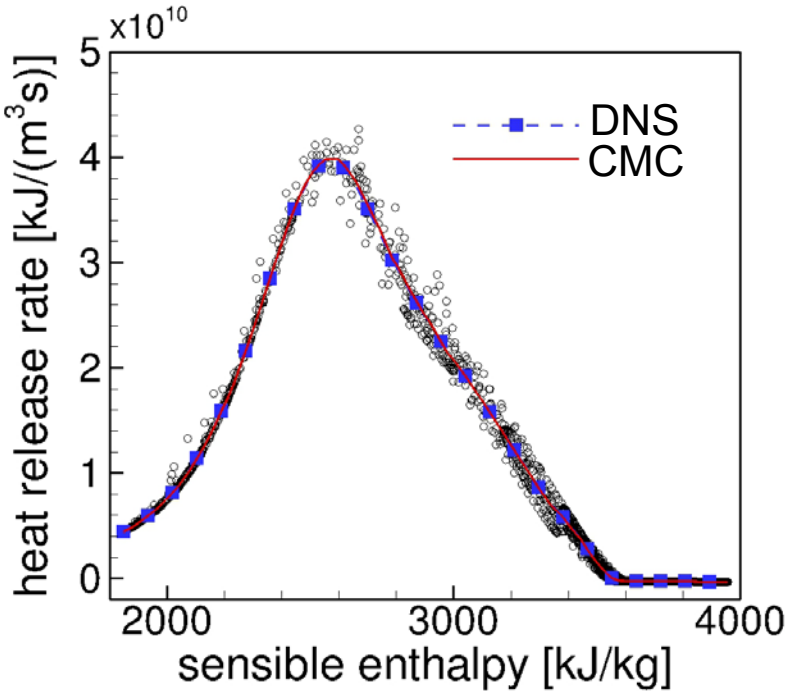



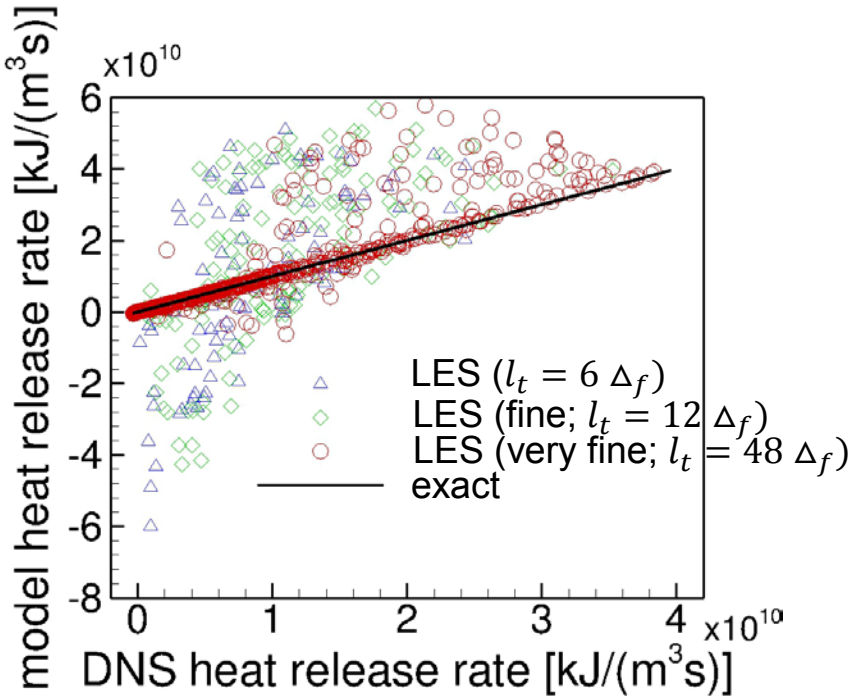

(data from the case with $T_0$=850K, $P_0$=30bar, stoich. PRF80/air, 3.2mm$^2$ 2048$^2$ grid points; at the time of the maximum heat release)

# Model Validation

## Assessed accuracy of reaction rate estimation

- Conventional LES where volume-averaged (filtered) species mass fractions and temperature are used to estimate reaction rates leads to substantial errors



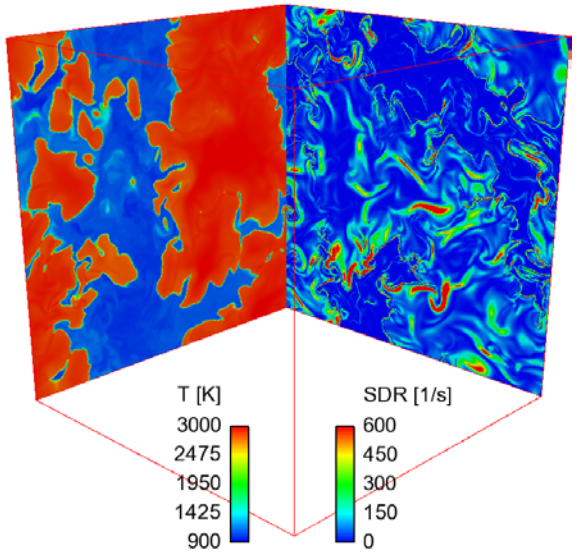



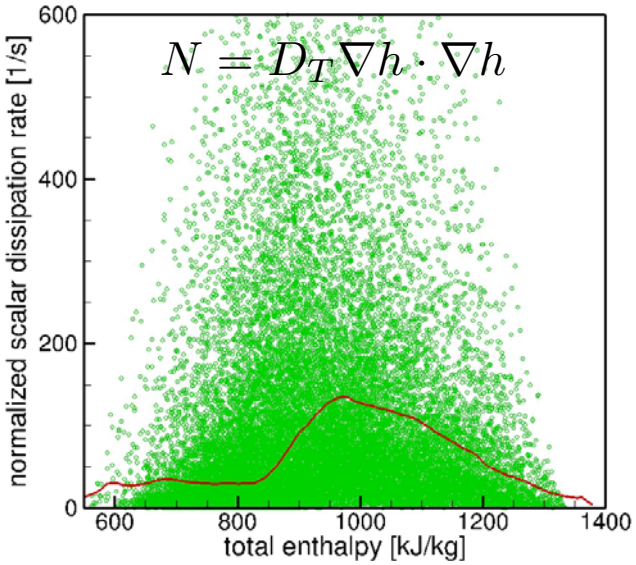

(data from the case with $T_0$=850K, $P_0$=30bar, stoich. PRF80/air, 3.2mm$^2$ 2048$^2$ grid points; at the time of the maximum heat release)

# DNS: Mixing Statistics

## Two-step chemistry 3-D DNS to extract scalar dissipation statistics under way

- Two-step chemistry
  - Iso-octane oxidation step/CO-$CO_2$ conversion (Misdariis *et al.* PCI 2015)
- Conditions
  - Stoich. Iso-octane/air
  - $P_0$: 30bar, $T_0$: 970K, initial $T_{rms}$~50K
  - Isotropic, forced turbulence/thermal-energy
  - Taylor-scale Reynolds number~96
  - Turbulence intensity~3.2m/s
  - 3.2mm$^3$, 512$^3$ grid points (planning a case with 1536$^3$ grid points)
- Extracting statistics of scalar dissipation rates and FDF for total enthalpy and sensible enthalpy
  - Models needed for CMC

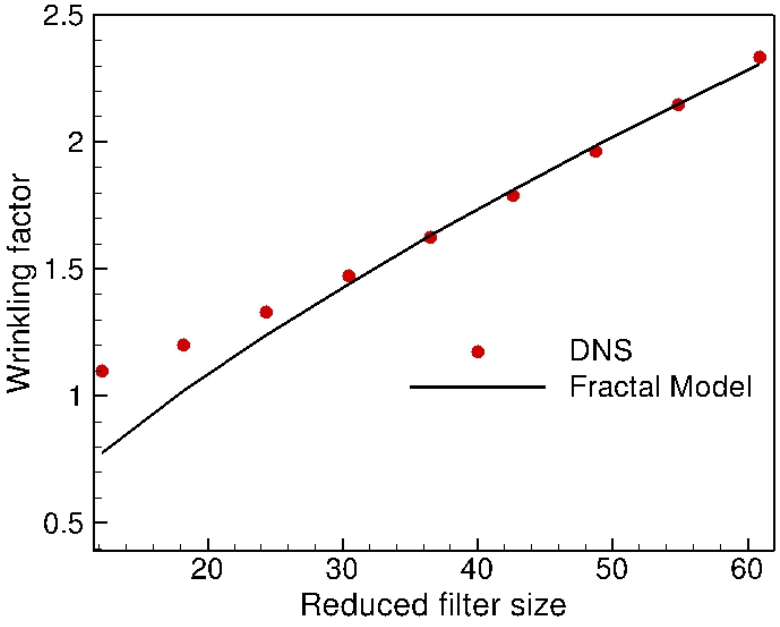


# DNS: Premixed Flame

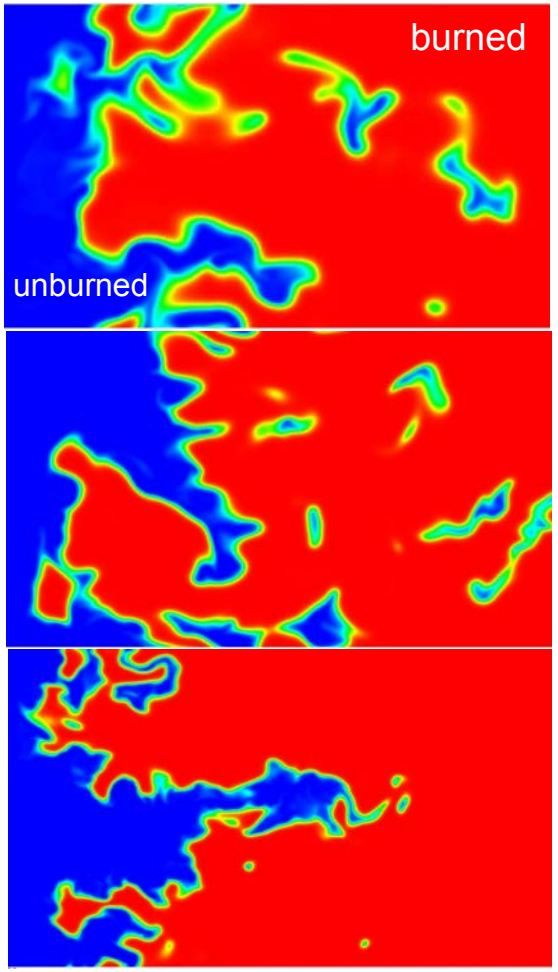
## Performed single-step chemistry 3-D DNS to validate and refine premixed flame modeling

- DNS with varying Reynolds numbers in the thin reaction zones regime
- Extracting flame wrinkling characteristics and validating subfilter flame speed models used in FPF




**DNS Conditions**
Taylor-scale Reynolds number: 52, 68, 100 (one more planned: ~150)
22M-420M grid points
Karlovitz number~4
$u'/s_L$~ 5 - 7.7

Reaction progress variable



# Responses to Previous Year Reviewers' Comments

- This is the first annual merit review of the project

# Collaborations

- Ohio State University
  - Model development and validation
- Oak Ridge National Laboratory
  - Experiments and assist in engine simulations
- Convergent Science
  - Converge CFD
- Oak Ridge Leadership Computing Facility
  - DD allocation
- Ohio Supercomputer Center

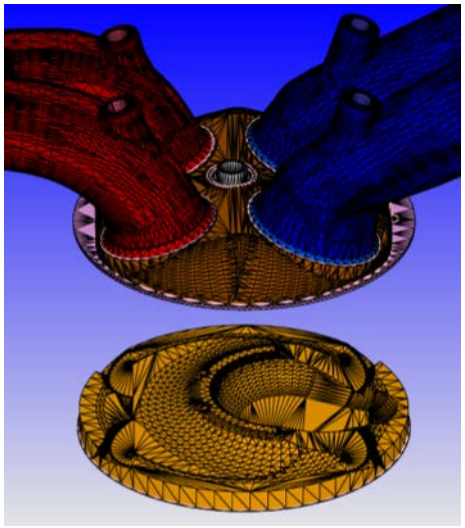
# Remaining Challenges/Barriers

- Development of a submodel for scalar dissipation rates of sensible enthalpy (reacting scalar)
  - Many studies for conserved scalar (total enthalpy), few for reactive scalars (sensible enthalpy) in the context of LES
- Coupling with commercial CFD software
  - Coupling with Converge CFD (implemented as UDF)

# Proposed Future Research

- Validating/developing reaction rate estimation and scalar dissipation models using end-gas ignition DNS data (Year 2)
  - Complete larger-scale DNS cases
  - Further assess total-enthalpy-based and sensible-enthalpy-based approaches
  - Develop/validate scalar dissipation models
- Engine simulations for knock-free conditions and validating premixed flame modeling (Year 2) – Basis of Year 3 efforts for knocking engine simulations
- Engine experiments (Year 2)
  - Complete acquiring in-cylinder pressure and gas sampling data for a range of knocking and knock-free operations

Geometry model of engine from scanned hardware



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

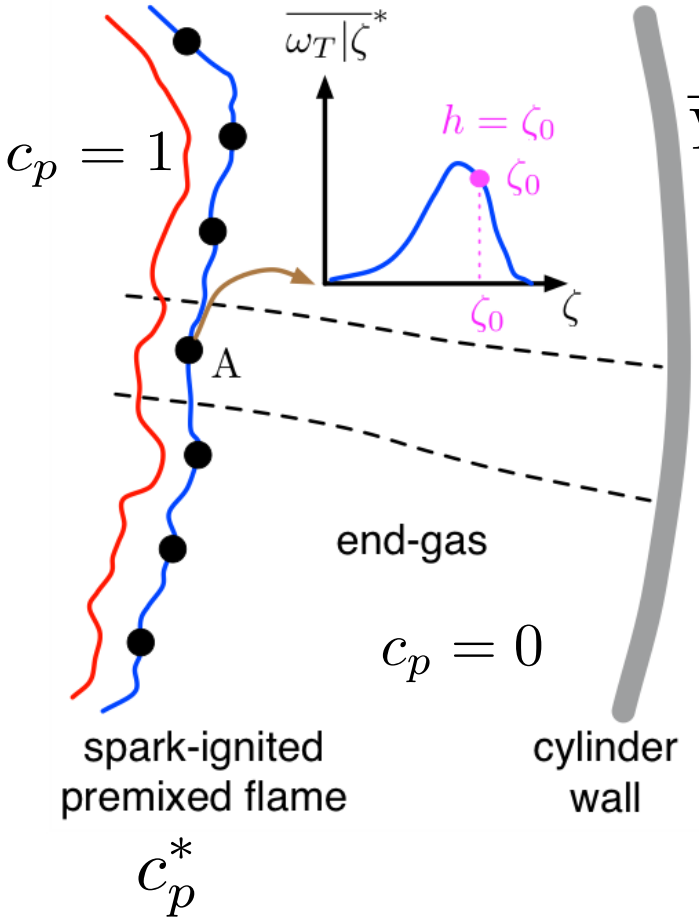
# Summary

- CMC-FPF consistently combines CMC for end-gas ignition with FPF for SI premixed flame propagation
  - LES-based knock prediction employing detailed chemistry
- Base code and validation data made available
  - Developed base CMC-FPF code
  - Generated DNS and experimental data for validation
- In Year 2, continuing model validation
  - Continuing generation of DNS and experimental data
  - Submodel development/validation using DNS data
  - Knock-free engine simulations with premixed flame FPF model - serving as a basis of Year 3 efforts for knocking engine simulations and model validation

# Technical Backup Slides

# Approach: Model

## Knock CMC




**Conditional moment**

$$\overline{Y_i|\zeta}^* = \frac{\int_V \rho Y_i \delta(h-\zeta) H(c_p^* - c_p) F(\mathbf{x}-\mathbf{x}')d\mathbf{x}'}{\int_V \rho \delta(h-\eta) H(c_p^* - c_p) F(\mathbf{x}-\mathbf{x}')d\mathbf{x}'}$$

samples taken for mixture with a particular value of enthalpy (h) in the end-gas region

Enthalpy~temperature~reaction rate

Mapping of scalar structures in physical space (x) to enthalpy space enabling accurate estimation of reaction rates

# Approach: Model

## FPF for SI Premixed Flame

Solving the conventional transport equation for the reaction progress variable (end-gas indicator)

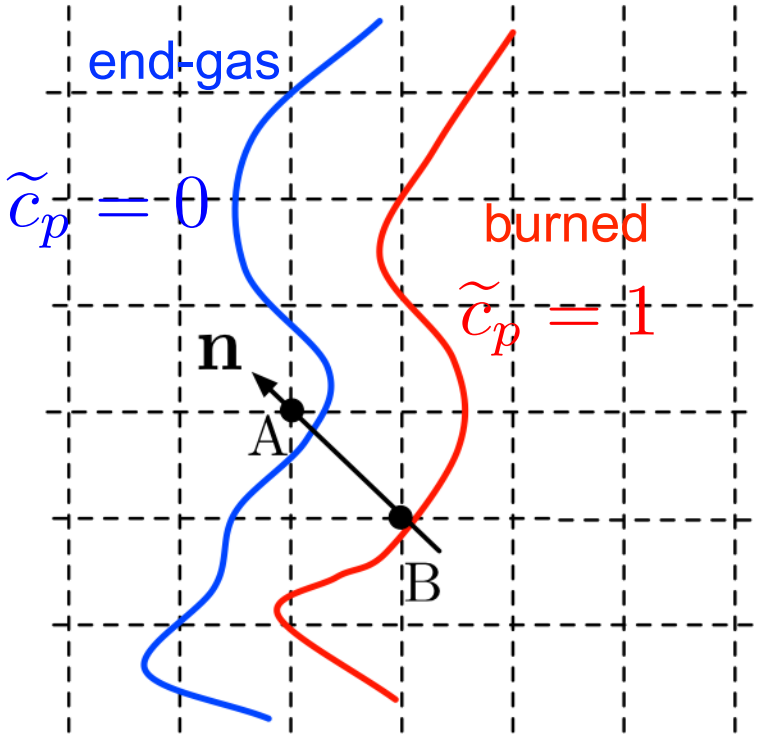
$$\frac{\partial \overline{\rho}\widetilde{c_p}}{\partial t} + \nabla \cdot \left(\overline{\rho \mathbf{v} c_p}\right) = \nabla \cdot \left(\overline{\rho D \nabla c_p}\right) + \overline{\rho}\widetilde{\omega_{c,p}} + \overline{\omega_{sp}}$$

With reaction rates designed to reproduce a specified propagation speed of the flame regardless of resolution levels

$$\overline{\rho}\widetilde{\omega_{c,p}} = \rho_u s_t \delta_\Delta\left(\mathbf{n} \cdot \left(\mathbf{x} - \mathbf{x}_s\right)\right)$$

Sub-filter flame speed

Regularized delta function

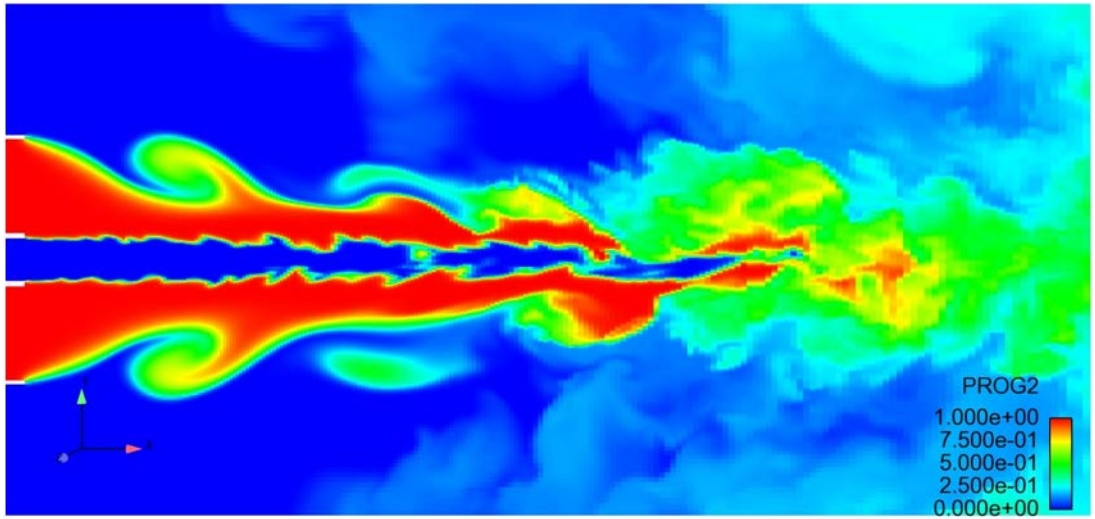



Premixed flames are typically under-resolved in LES

*Kim, J. Comput. Phys. (2015)*

# Model Development

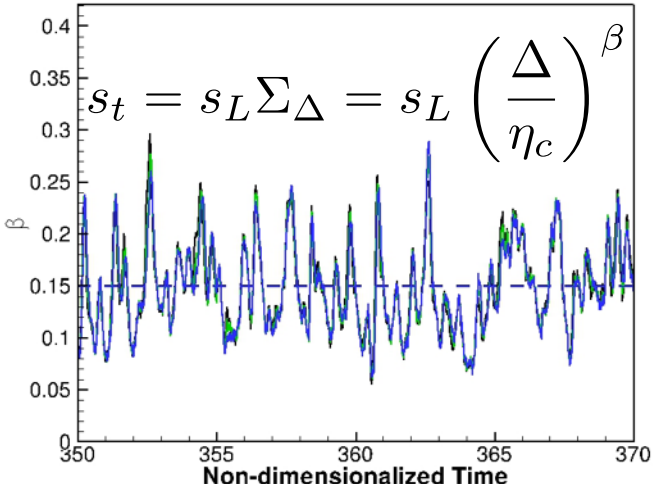
## Premixed flame FPF validation under way

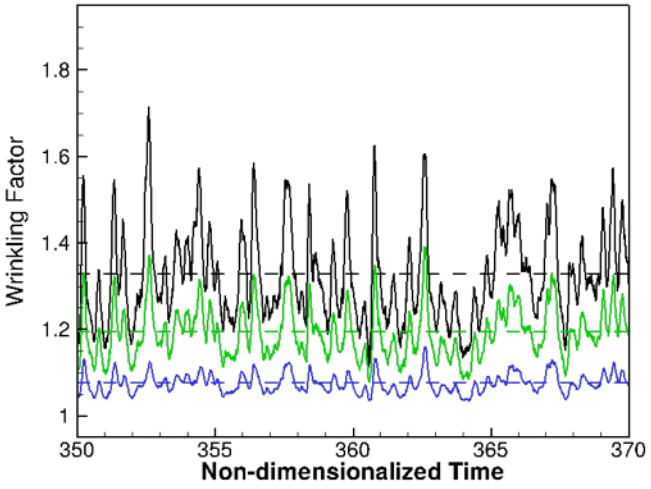



LES of a premixed jet flame
(F3 Flame of Chen et al. CnF 1996)

- Needing models for
  - Sub-filter flame speed
  - Regularized delta function
- Assessment of sub-filter flame speed model in progress

Dynamic fractal model

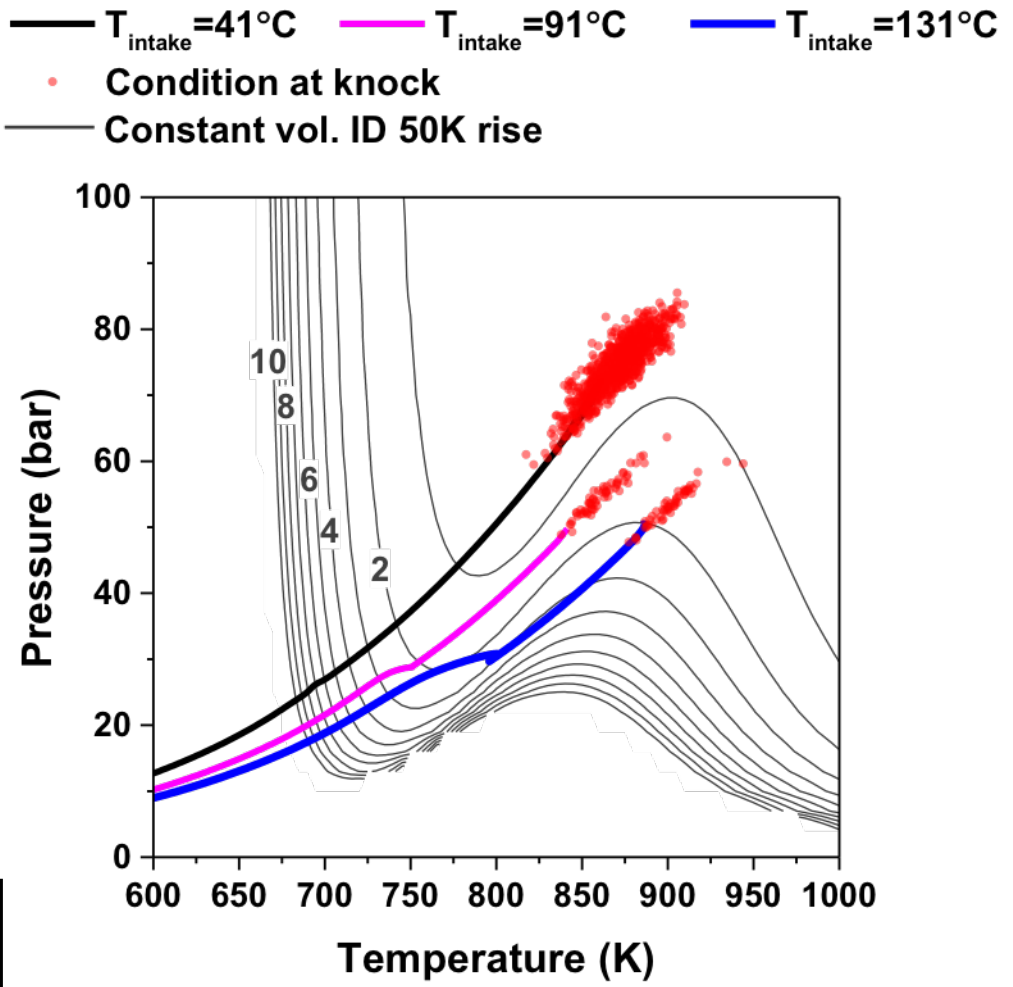


# Experiments

- Coupled experimental measurements of in-cylinder thermodynamics with simulated constant volume ignition delay
- 2-zone model for experimental data
- Indicate measured bulk-gas state at knock
- Determine cycle-by-cycle ignition exposure at knock

$$ignition\ exposure\ (-) = \left[\frac{1}{encoder\ resolution\left(\frac{\theta}{CA}\right) * RPM * \frac{360\ (CA)}{60000\ (ms)}}\right] * \int_{IVC}^{knock} \frac{1}{const.vol\ ID\ (ms)} d\theta$$

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# Experiments

## Effects of Low-Temperature bulk as reactions on knock observed in experiments

- Increased low temperature reactions (PSHR) reduced time to knock
- EGR independent
- Reduced variability with PSHR
  - Thermal or chemical effect?
  - will be studied in simulation effort