HCCI – Update of Progress 2005

Tom Ryan

Scope of Activities in 2005

- Six Meetings Covered:
  - 2005 SAE Congress
  - 2005 SAE Spring Fuels and Lubes
  - 2005 DEER Conference
  - SAE ICE2005
  - SAE HCCI Symposium
  - 2005 SAE Power train and Fluids System Conference
- 100 Written Papers and 133 Presentations
- Topics include Basic Kinetics, Gasoline Engine Development, Diesel Fuel Engine Development, Alternative Fuels, Ignition Assisted HCCI, Fuel Property Effects, Mode Switching, etc

General Observations

- Continuing Problems with All Approaches to HCCI:
  - Mixture Preparation
  - Control of the Start of Reaction
  - Control of the Reaction Rate
- Volatile Fuels Reduce the Mixture Preparation Problems
  - Gasoline Boiling Range is Better than Diesel Fuel Boiling Range
  - Diesel Fuel HCCI will be Part Time, Light Load Option
- High-Speed, High-Load Operation Limited by the On-set of High Rates of Pressure Rise and Pressure Oscillations ("Knock")

SwRI Definition of HCCI

- Fuel Totally Vaporized Prior to Reaction
- Homogeneous, or Nearly Homogeneous Fuel Distribution
- Reaction Initiated by Compression Heating
- Main Reaction After TDC
- Operation for Low Emissions
  - Less than 15 ppm NOx
  - Zero Smoke
- Other Definitions Exist, but Generally Involve compromises in Emissions and Efficiency

Topics in this Presentation

- Fundamentals
- Stratification
- Fuel Advances

Fundamentals

Low Temperature Reactions
Delayed Reaction - Radical Survival
Heat release Rate Modeling
Homogeneous versus Stratified

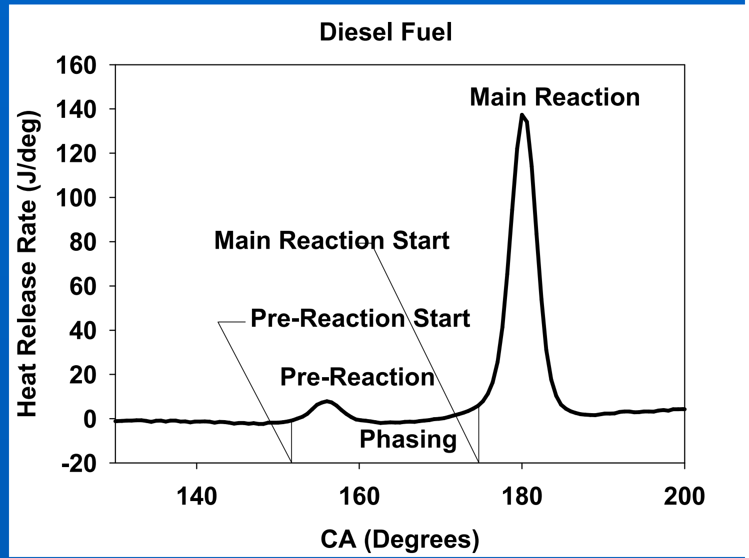
Reminder

- Ideally, a Homogeneous Fuel-Air Mixture is One in Which the Composition and the Thermodynamic Conditions are Uniform Throughout the Reaction Phase
  - Reaction Starts When the Thermodynamic Conditions are Sufficient to Initiate Chain Branching Reactions
  - Reaction Rates and Reaction Duration are Kinetically Controlled
  - Reaction Rates are thus Exponential Functions of the Local T

Cool Flame Chemistry – Low Temperature Reactions

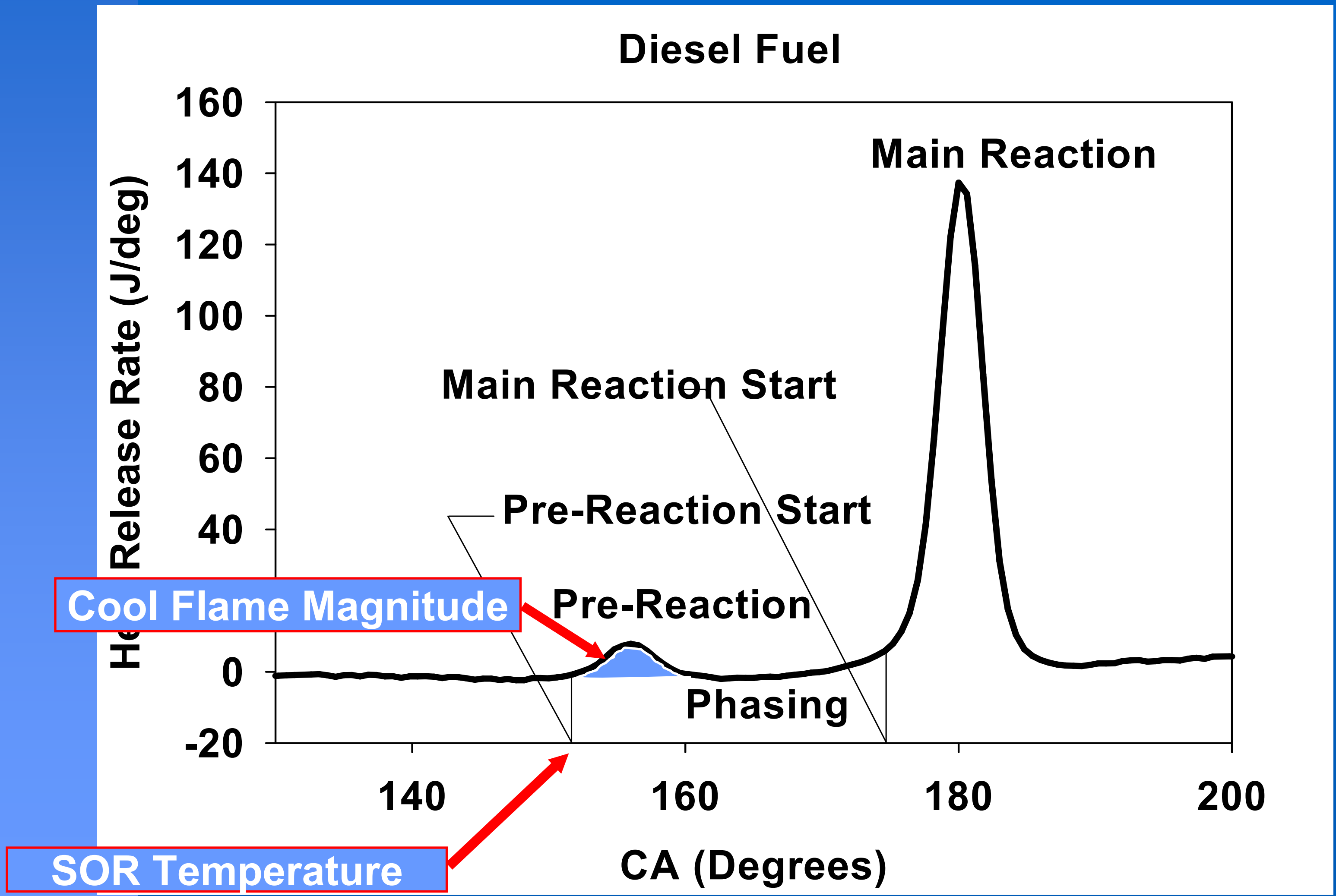
- Low Temperature Reactions are Important because they Define the Start of Reaction Temperature and Influence the Main Reaction Timing
- LTR Mechanism:

$$RH + O_2 \rightarrow R\bullet + HO_2 \quad (1)$$
$$R\bullet + O_2 \rightarrow ROO\bullet \quad (2)$$
$$ROO\bullet \rightarrow \bullet ROOH \quad (3)$$
$$\bullet ROOH \rightarrow \text{Carbonyl} + \text{Olefin} + OH\bullet \quad (4)$$
$$\bullet ROOH + O_2 \rightarrow \bullet OOROOH \quad (5)$$
$$\bullet OOROOH \rightarrow HOOR{=}O + OH\bullet \quad (6)$$
$$HOOR{=}O \rightarrow \bullet OR{=}O + OH\bullet \quad (7)$$



- LTR Ceases as T Increases Because Dissociation is Favored over Reaction 2, this is Called the Negative Temperature Coefficient Region because Reactions actually Cease as the T Increases

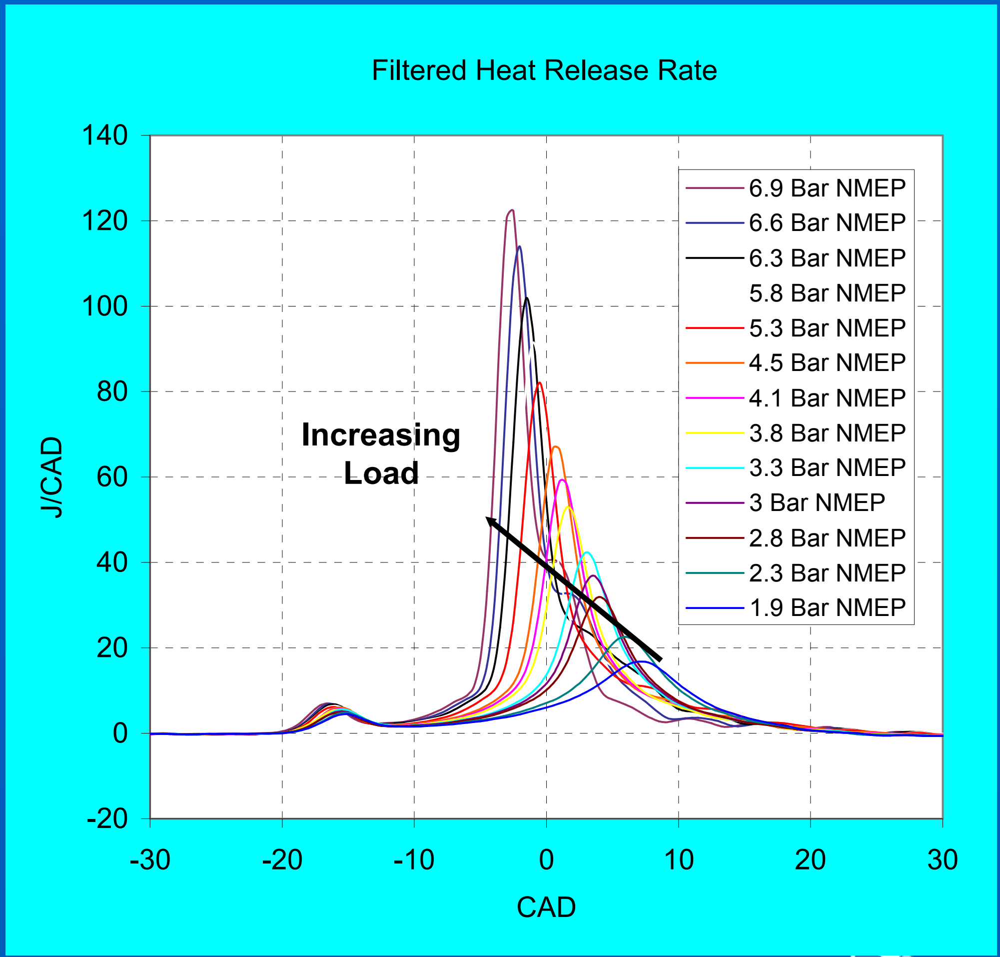
Definition of Terms



Factors Affecting Combustion Timing

- Fueling rate
  - Increasing load (fueling rate) tends to advance the combustion timing
  - This is typical of port-injected HCCI combustion

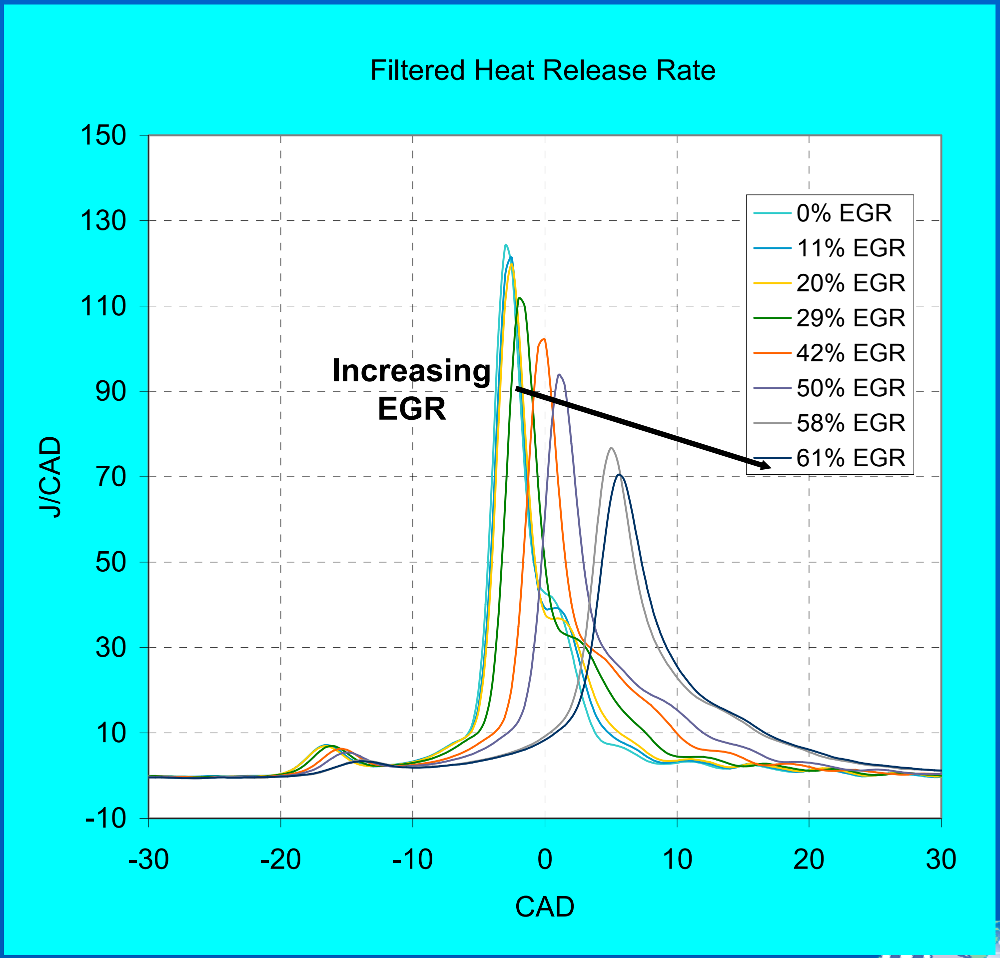
1300 RPM



Factors Affecting Combustion Timing (cont.)

- EGR
  - Increasing EGR will retard the combustion timing
  - EGR also tends to moderate the heat release rate, and is regularly used during high load operation

1300 RPM, 7 bar NMEP



Observations

- Increasing load results in increased T (higher surface and gas T due to higher heat flux), resulting in earlier start of reaction and higher HRR
- Delaying the start of reaction lowers the HRR due to reaction during expansion (lower and decreasing T)
- Start of reaction can be delayed by lowering T (MAT, CR, etc), using more EGR (more third body interactions), or changing fuel (less cool flame=lower reactivity)

Delaying Reaction

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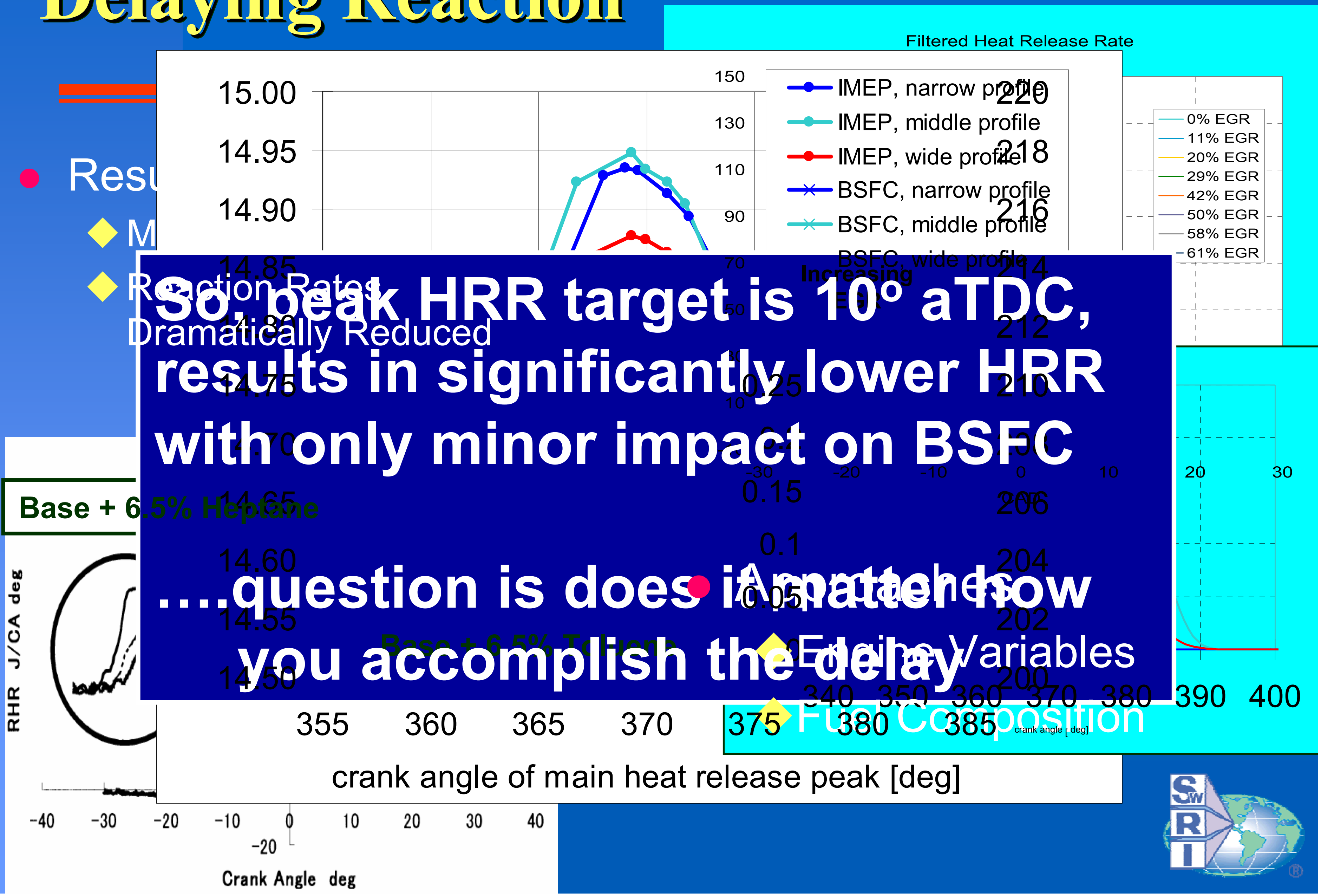
  - M
  - Reaction Rates Dramatically Reduced

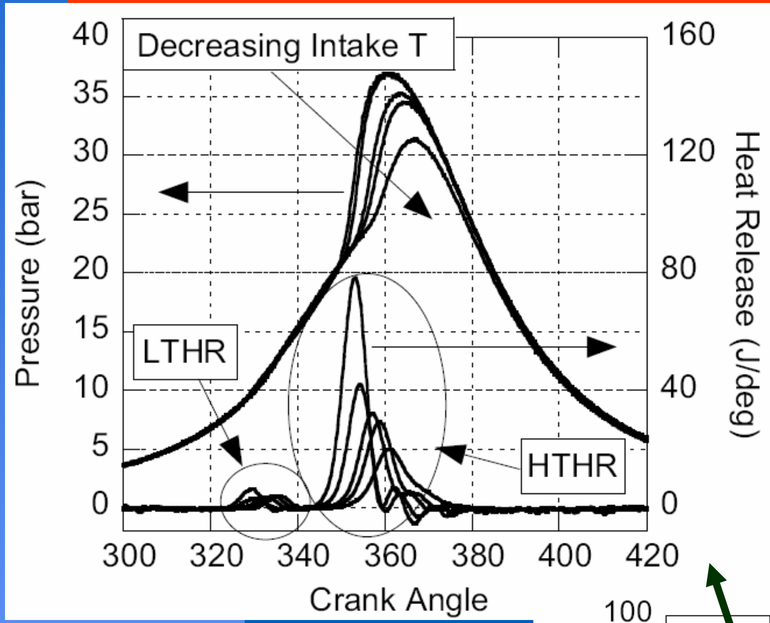


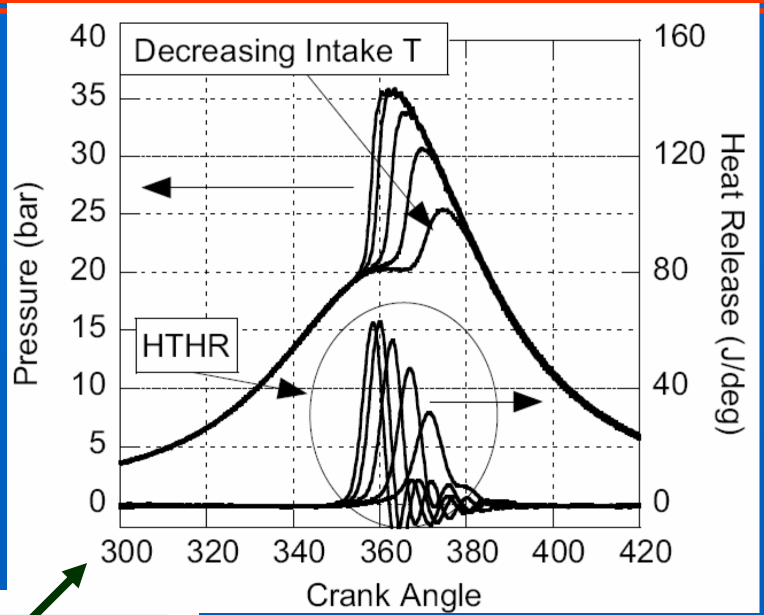
So, peak HRR target is 10° aTDC, results in significantly lower HRR with only minor impact on BSFC

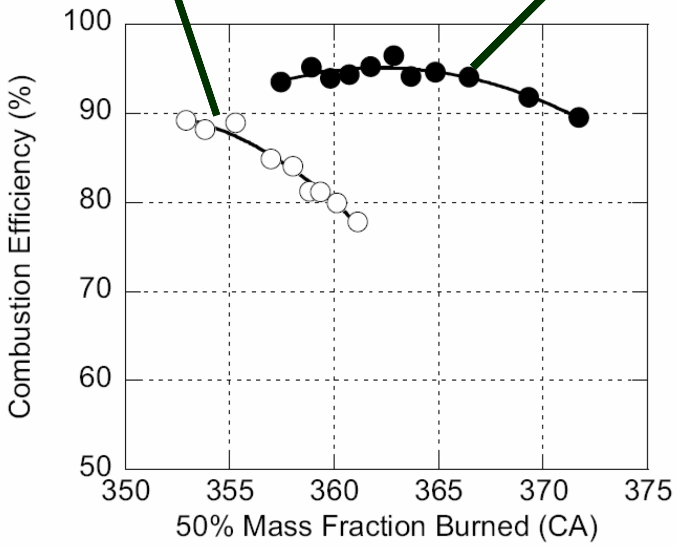
….question is does it matter how you accomplish the delay

- Approaches
  - Engine Variables
  - Fuel Composition

Low Temperature Reactions – Less is Better?
SAE 2005-01-3737



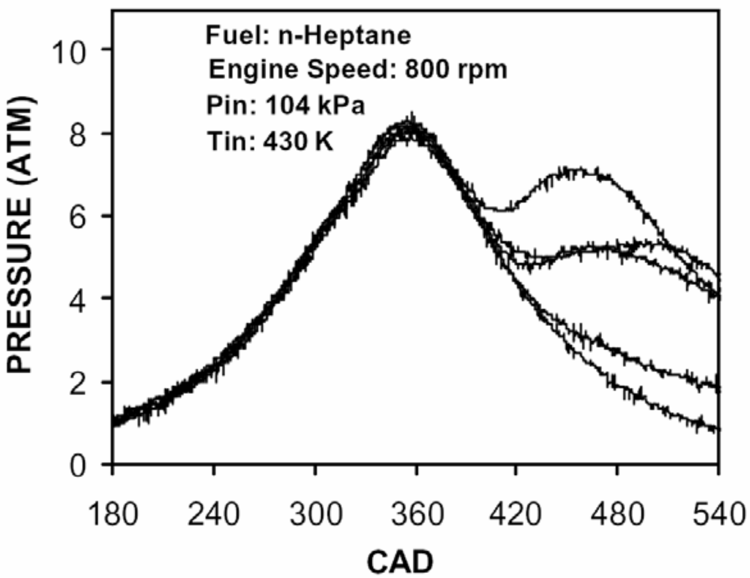


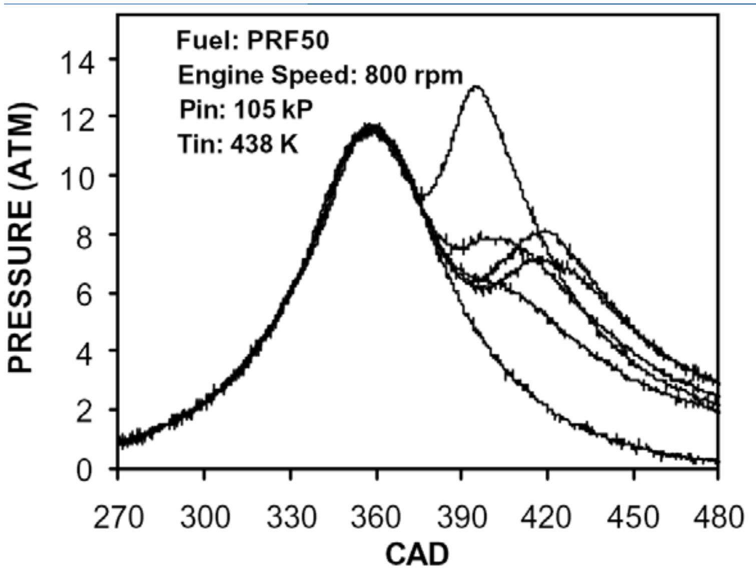


Delayed Reaction Produces Lower Rates of Pressure Rise, but CE is Affected

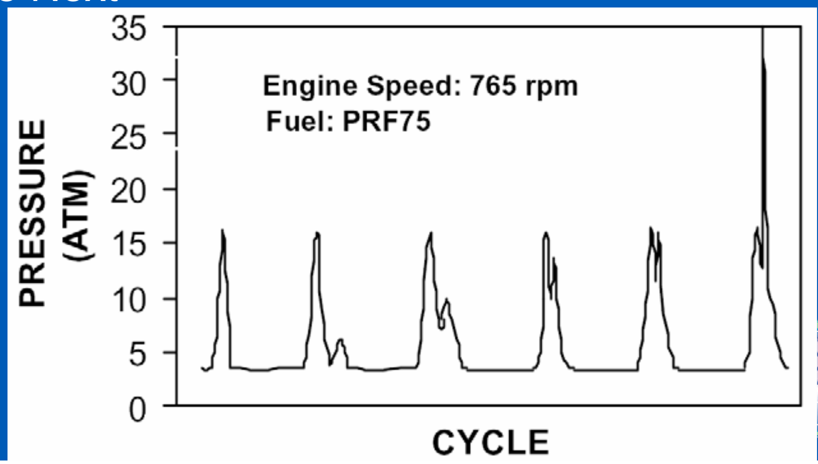
Presence of LTR Initiates Early Reaction but CE Is Poor and Worsens With Delayed Main

Delayed Reaction
2005-01-0178





- One Approach for Reducing Peak Reaction Rate (and the resulting peak rates of pressure rise) is to Delay Main Reaction to After TDC
  - Previous Work at SwRI Indicates that the Ideal Timing for the peak Heat Release Rate is 10-15° ATDC
- Literature Data Demonstrates very Late Reaction in the Presence of Massive EGR
- Occasional, but Regular, Main Reactions Occur at Temperatures well Below the Normal High Temperature Reaction Limit
  - Suggests that Partial Reactions Create Radicals that Survive in the Residuals from One Cycle to the Next



Heat Release Rate Model
2005-01-0183

- Cycle Simulation Models Typically use Empirical Heat Release Rate (HRR) Models
- Work in Progress on HRR Model for HCCI

$$X_{MFB-PreComb} = A + B\exp\left(-\frac{\theta}{C}\right)$$

$$\ln A = a_2 + b_2 / n^{1.5} + c_2 / f_{rg}{}^2$$

$$a_2 = -7.8946$$

$$b_2 = 1021019.3$$

$$c_2 = -31700260.0$$

$$B = a_3 + b_3 * n^2 + c_3 / f_{rg}{}^2$$

$$a_3 = 0.00344$$

$$b_3 = 4.15745E-08$$

$$c_3 = 62.054$$

$$C = a_4 + b_4 * n^{2.5} + c_4 * f_{rg}{}^3$$

$$a_4 = -3.4486$$

$$b_4 = -2.4334E-08$$

$$c_4 = 4.5184E-10$$

$$X_{MFB-mainComb} = 1 - (1 - \tau^{c_{p1}})^{c_{p2}}$$

$$\tau = \frac{\theta - \theta_{10\%MFB}}{\Delta\theta}$$

$$c_{p1}{}^{-1} = a_5 + b_5 * f_{rg} + c_5 * f_{rg}{}^{1.5}$$

$$a_5 = 1.9935$$

$$b_5 = -0.086227$$

$$c_5 = 0.0081414$$

$$c_{p2} = a_6 + b_6 / n + c_6 * f_{rg}$$

$$a_6 = 317.26057$$

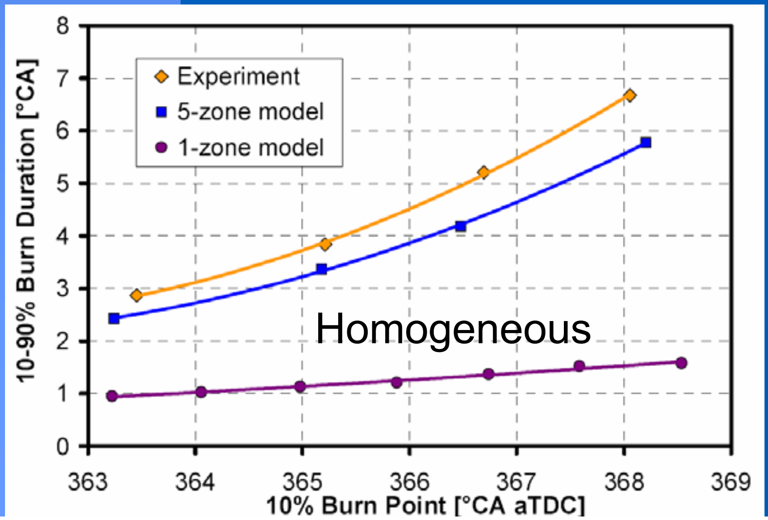
$$b_6 = -110321.03$$

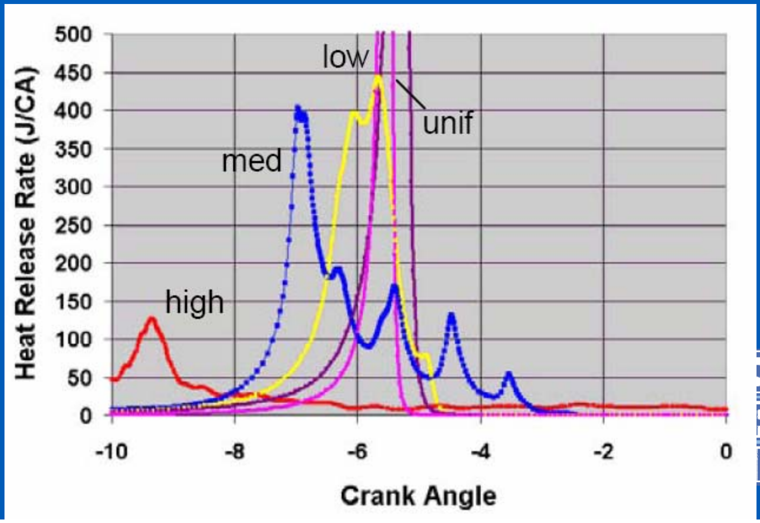
$$c_6 = -3.5212194$$

$$\Delta\theta = 58.9 - 383112.0 / n^{1.5} - 2.76 * \lg(f_{rg})$$

Homogeneous Reaction

- HCCI Reaction in Totally Homogeneous Mixtures are very Fast, on the order of the Kinetic Rates
  - Dec (SAE 2005-01-0113)Predicts 10-90% Burn Durations of 1°CA
  - Grenda (SAE 2005-01-3722) Predicts 10-90% Burn Durations of 1°CA
- Stratification is the Reason for Actual Observed Reaction Rates and Combustion Durations



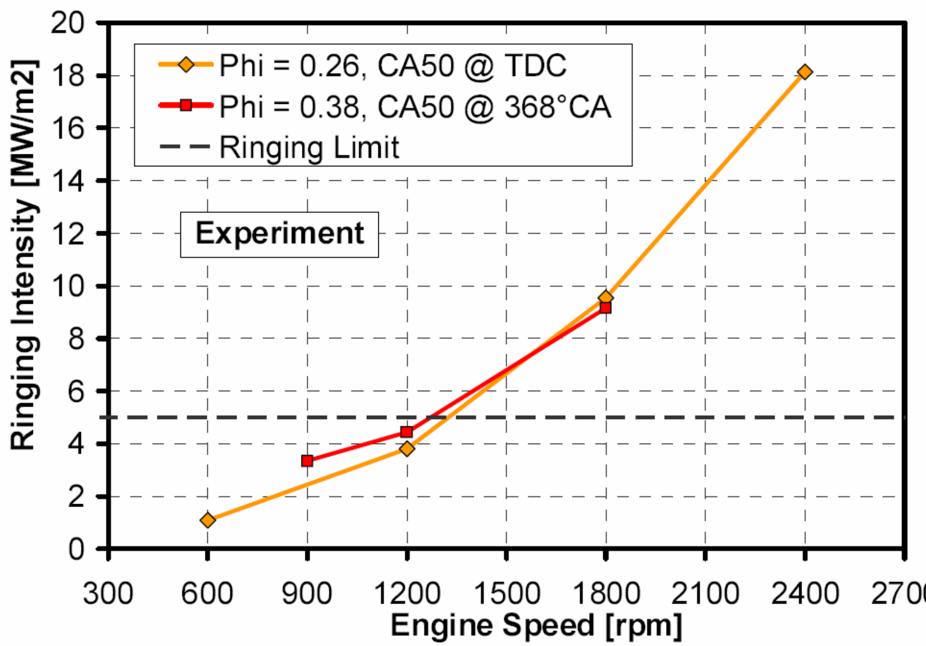


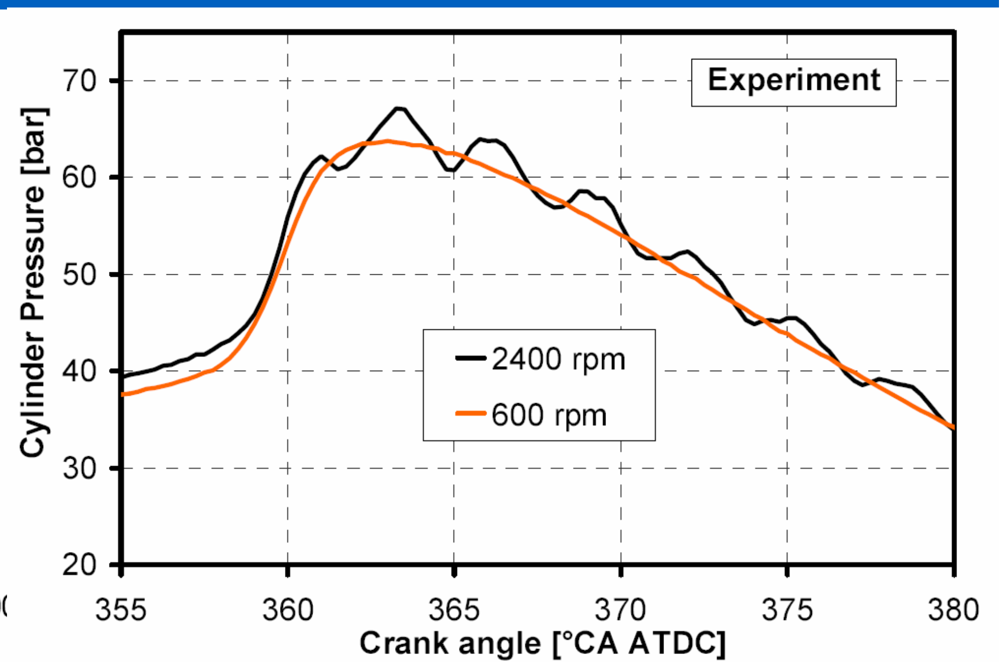
Stratification

Combustion Pressure Ringing

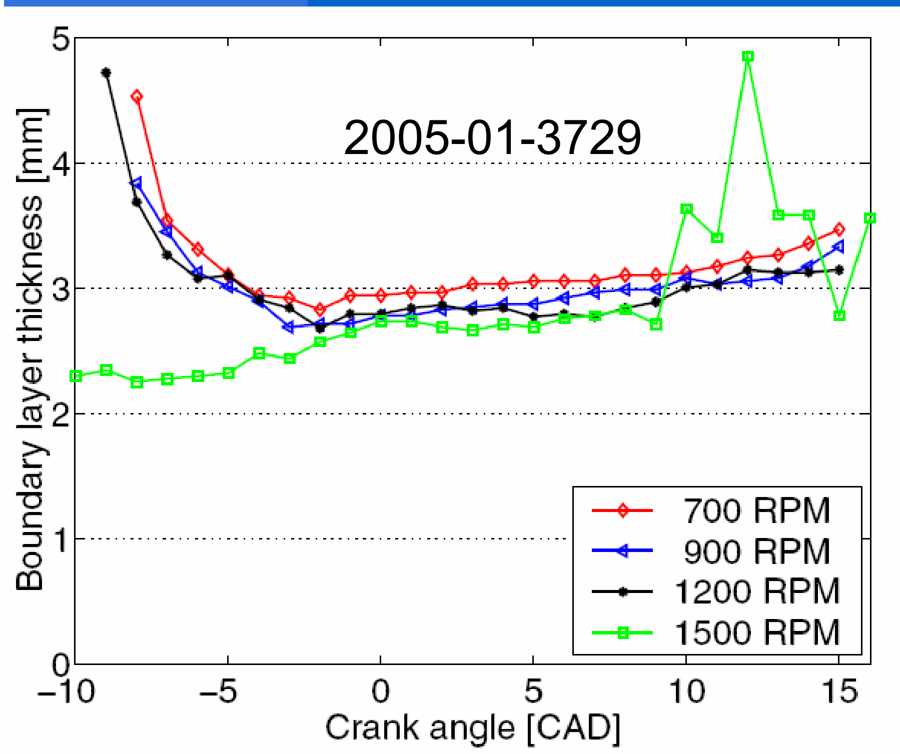
2005-01-2125

- HCCI Engine Speed and Load Range Limited by Pressure Rise Rates (Ringing)
- As Speed and Load are Increased Reaction Advances and Becomes more Rapid
- Likely Reasons are Increased Temperatures and Decreased Stratification





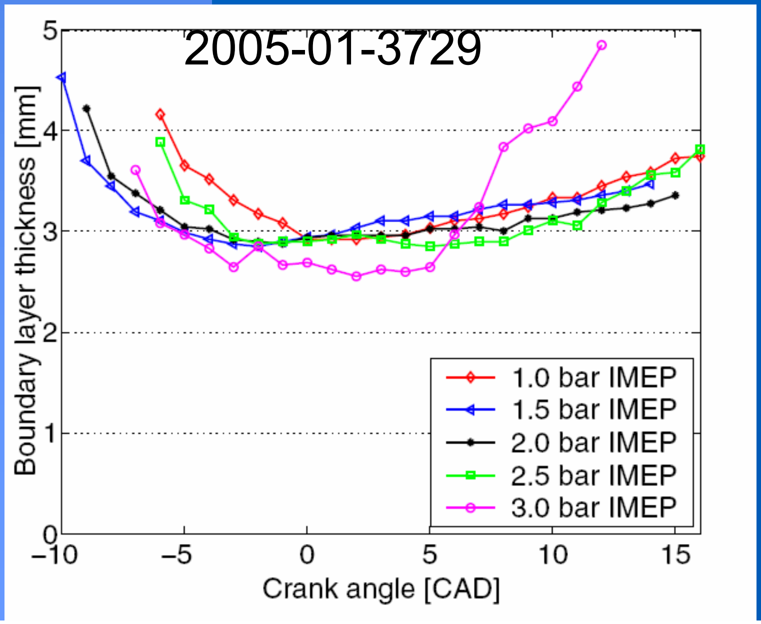
Effects of Engine Speed

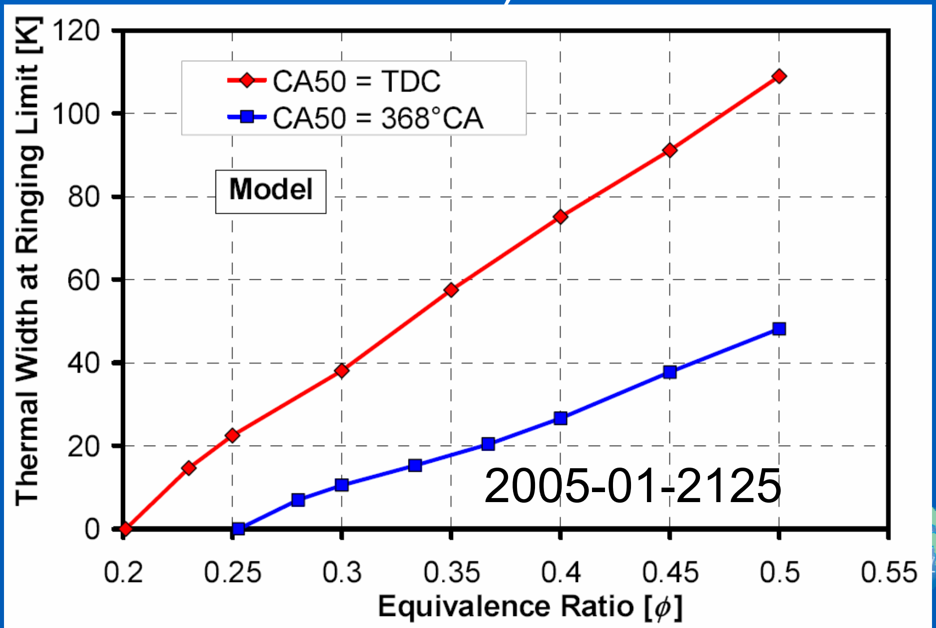


- Engine Speed Affects Turbulent Flow, Heat Transfer, and Heat Flow Through the Engine, affecting:
  - Surface Temperatures
  - Boundary Layer Thickness
  - Mixture Stratification (Composition and T)
- Boundary Layer Effect Shown in Figure on Left
  - Boundary Layer Thickness Decreases with Increased Engine Speed

Engine Load Effect

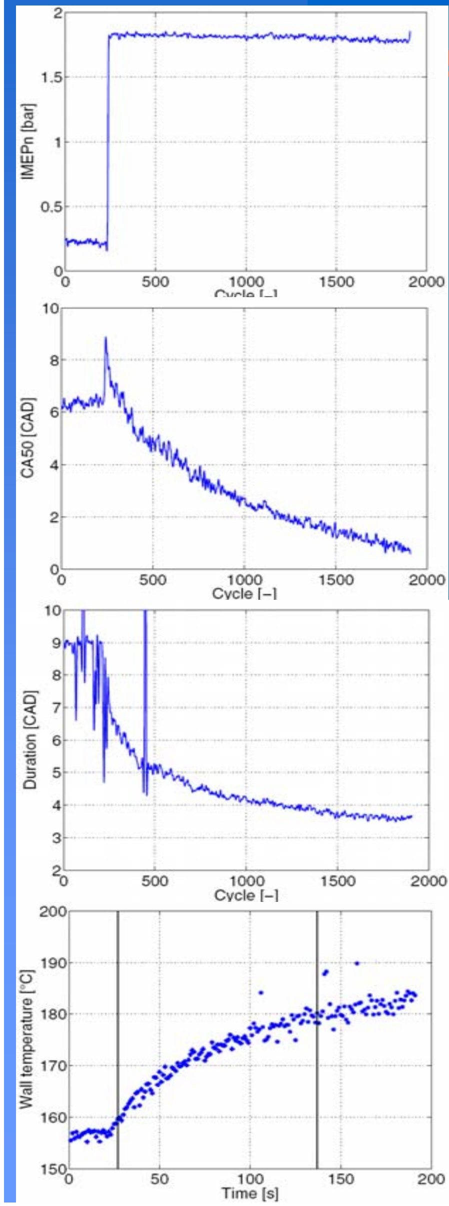
- At Fixed Speed, Heat Flow Through the Engine Increases with Increased Load
  - Boundary Layer Thickness is not Affected
  - In-Cylinder Temperatures Increase
    - As Indicated by the Need for Larger T Gradients (represented by Dec as the Thermal Width)



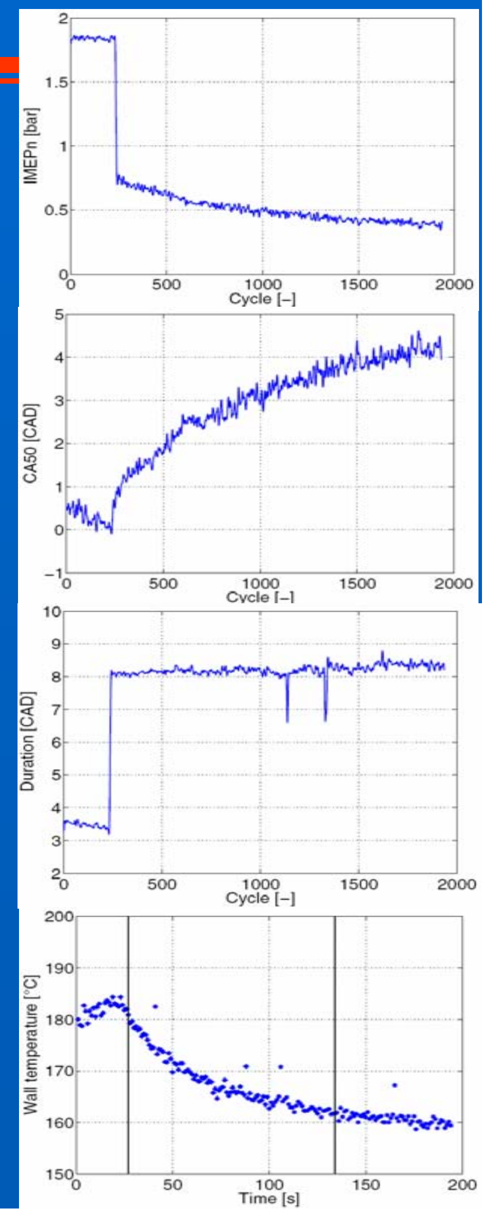


Engine Load Effect on Wall Temperature

2005-01-3731

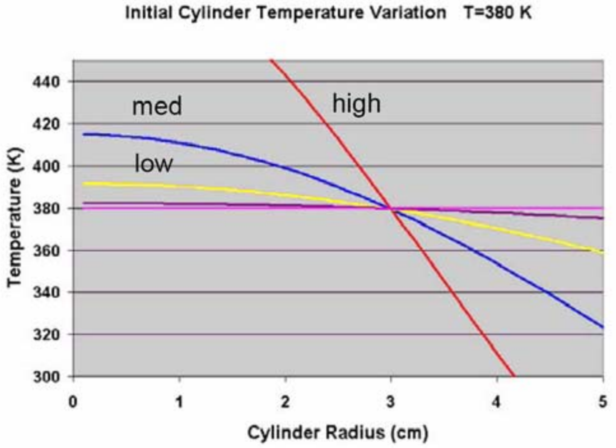


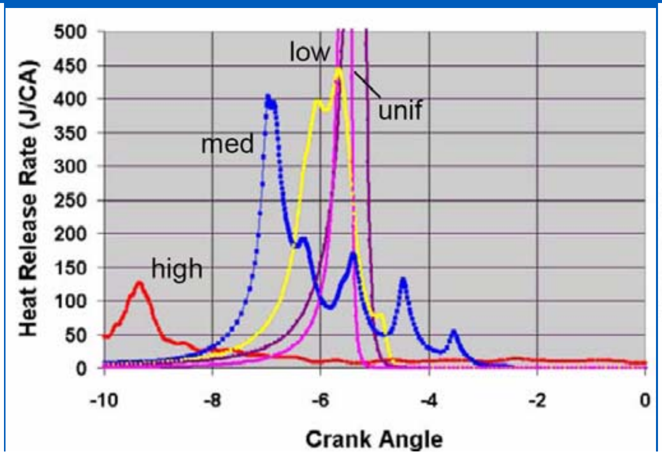
- Step Increase in Load Advances Reaction Timing, Decreases Reaction Duration, and Increases T_{wall}
  - Decrease in Duration is Gradual due to initial Impact of Fuel Cooling
- Step Decrease in Load Retards Reaction Timing, Increases Reaction Duration, and Decreases T_{wall}
  - Reaction Duration Effect is Instantaneous due to Instantaneous Fuel Rate Change

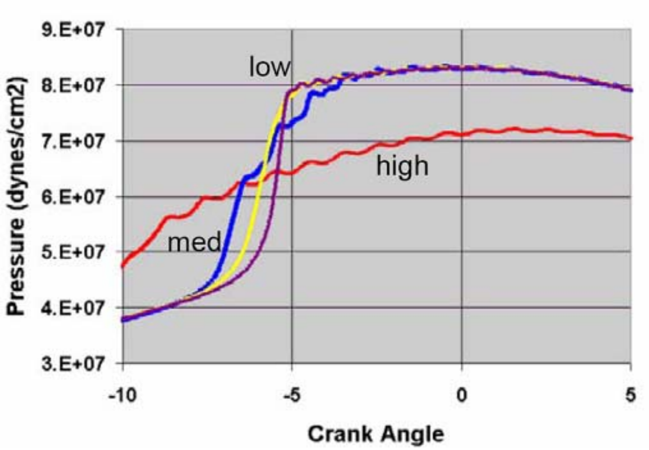


High Speed, High Load Operation
Model Predictions
2005-01-3722

- Stratification of the In-Cylinder Mixture is one Approach to Achieve High Speed and High Load
  - Temperature Gradients
  - Composition Gradients
- Model Results Indicate that both Work to Reduce Peak HRR
- T Stratification Results Below Show that while Peak Pressure is reduced at this Initial Average T, Reaction Advances due to Higher T in the Center, Leading to Pressure Oscillations

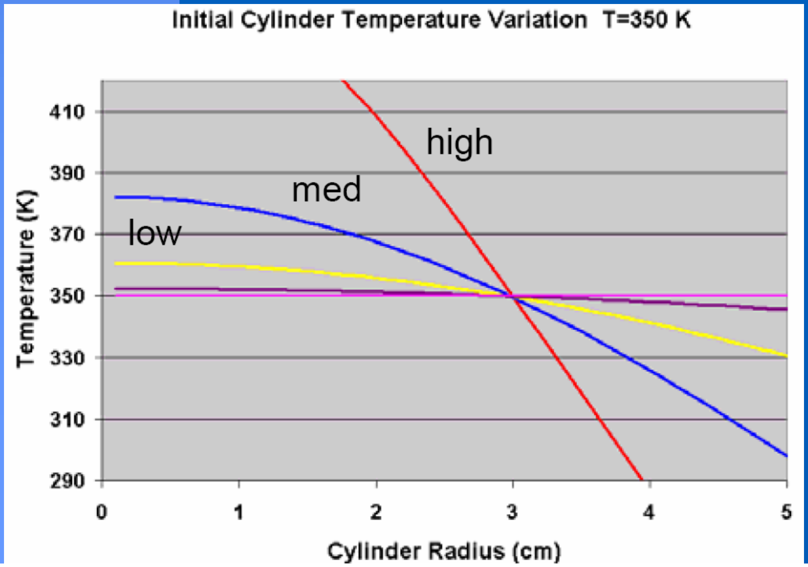


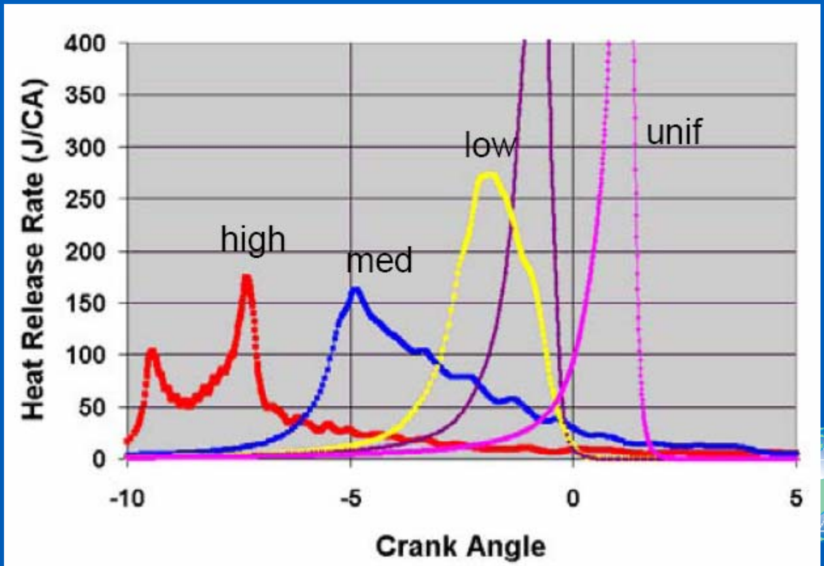




High Speed, High Load Operation
Model Predictions
2005-01-3722

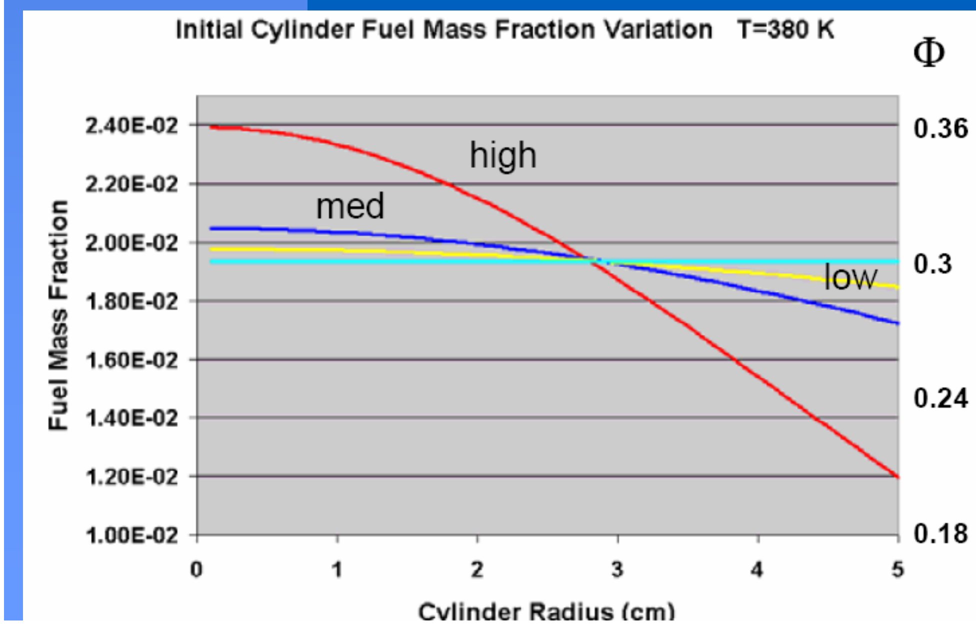
- Delaying Reaction, to Accomplish the Main Heat Release During Expansion, Increases Reaction Duration and Lowers the Peak HRR
- Model Results with Delayed Reaction and Different Levels of T Stratification, Demonstrate the Reduced Peak HRR

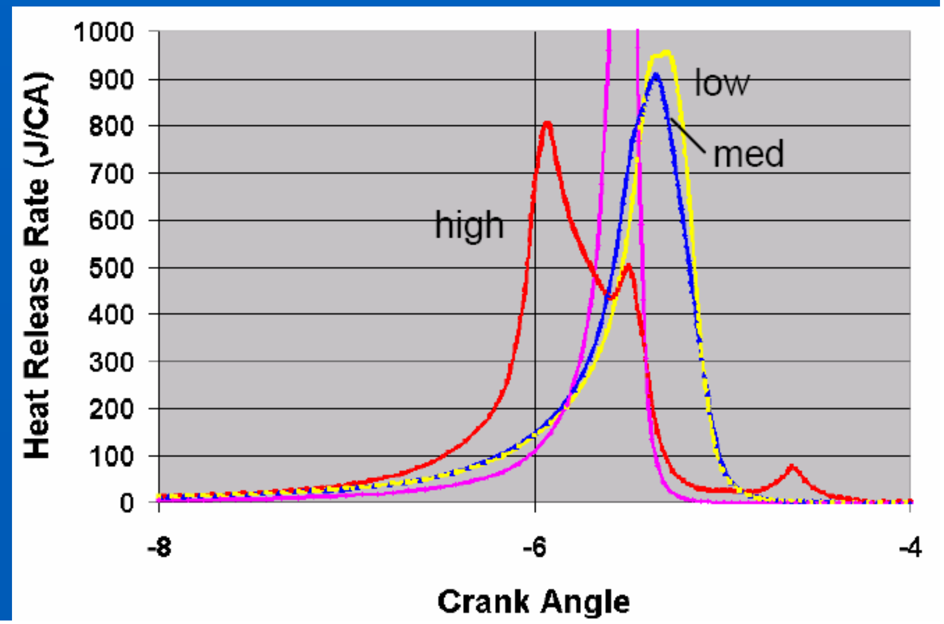




High Speed, High Load Operation
Model Predictions
2005-01-3722

- Stratification of the In-cylinder Mixture Composition is another Approach to Reduce the Peak HRR
- Model Results indicate that Peak HRR is Reduced but Reaction does Advance due to the local A/F effect

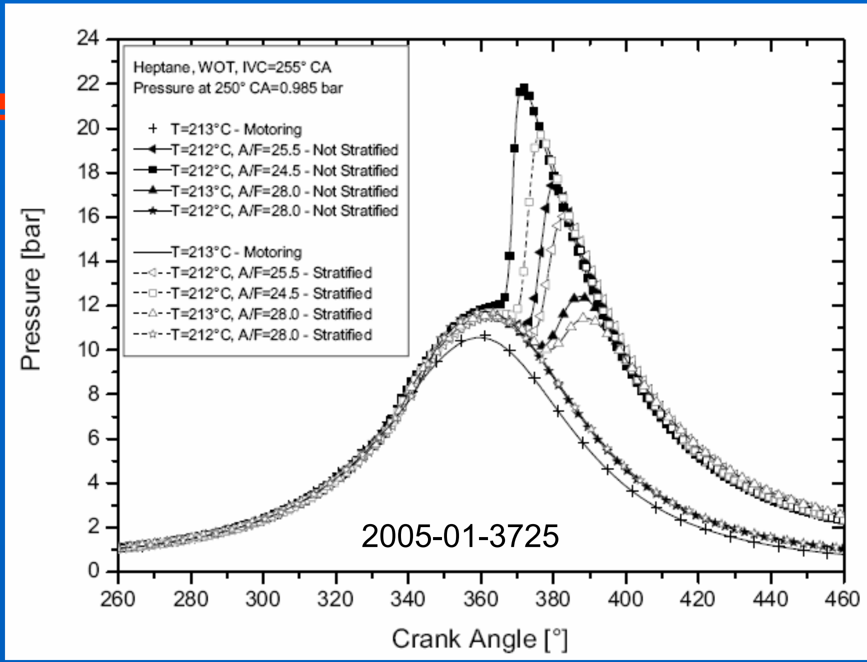


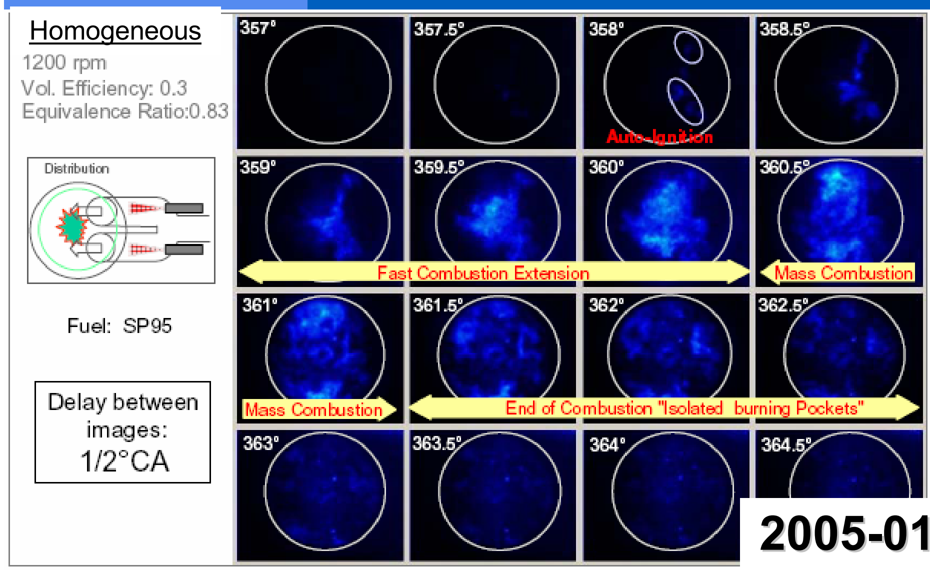


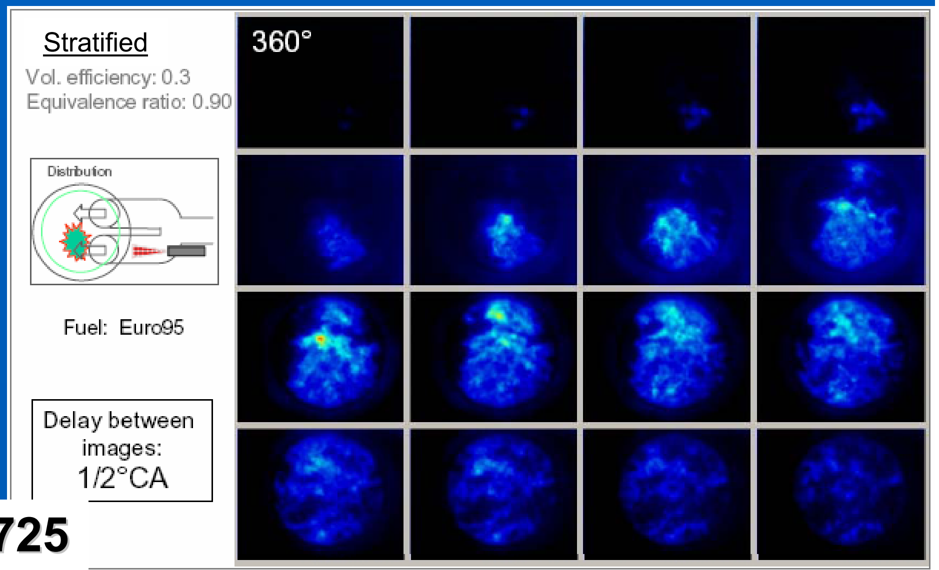
High Speed, High Load Operation

Measurements

- Fuel Distribution can be Accomplished using Individual Port Injectors
- Fuel Distribution does Affect the HRR





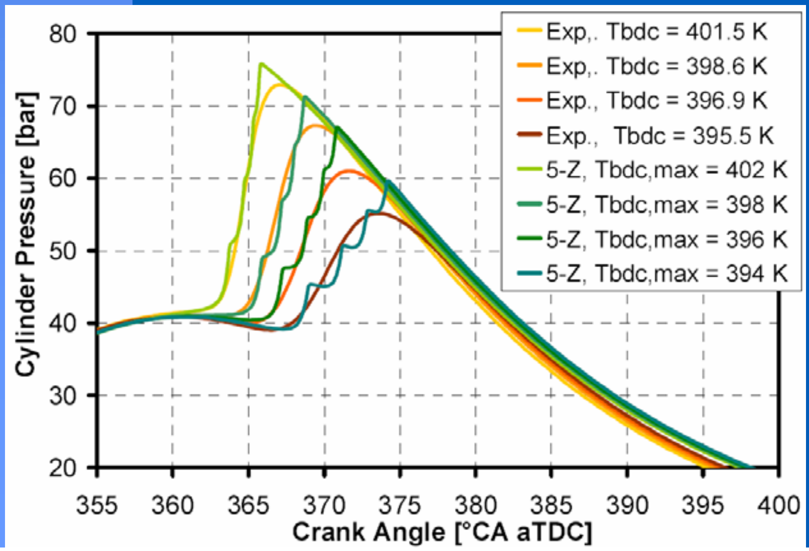


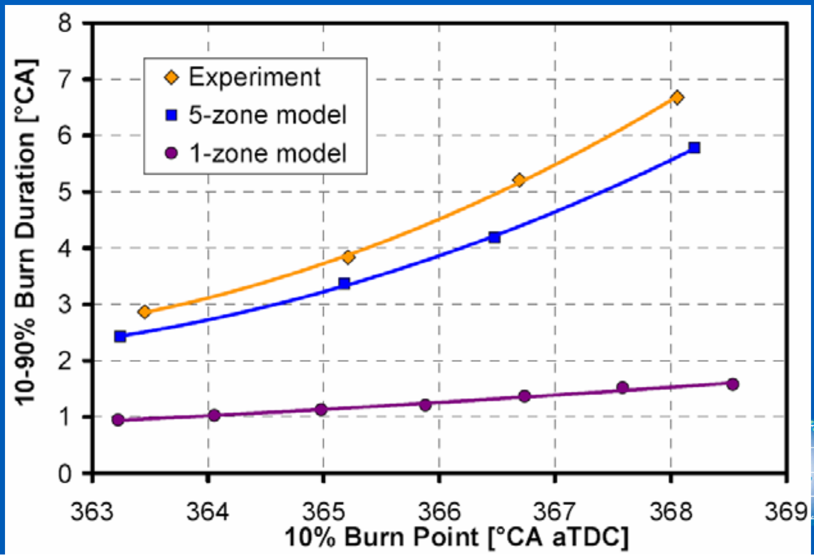
2005-01-3725

High Speed, High Load Operation

2005-01-0113 and 205-01-2125

- Dec Defined a Parameter Called "Thermal Width" (TW) to Characterize the T Stratification
- Dec Uses a Multi-Zone Model to Predict the Heat Release in each Zone, where the Zones are Based on a Uniform Distribution of the TW
- Total Heat Release is Integrated Across all of the Zones to Arrive at the Total Predicted Heat Release and Pressure Rise
- Issue Reduces to Defining the Required Thermal Width to Arrive at the Target Speed, Load, and Still Stay Below the Limit on the Pressure Rise Rate

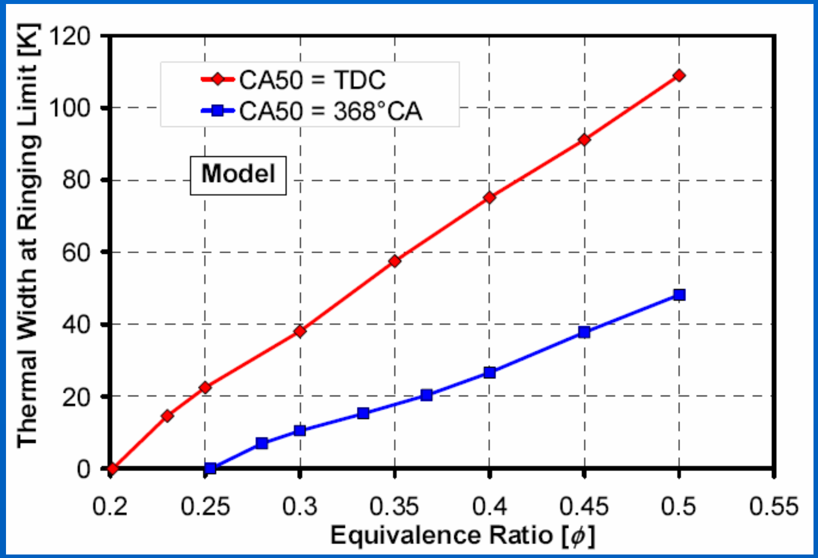


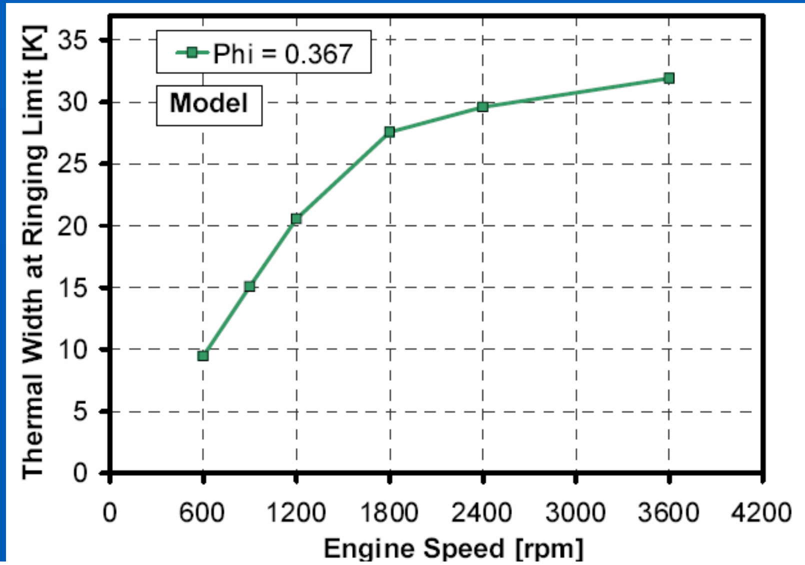


High Speed, High Load Operation

2005-01-0113 and 205-01-2125

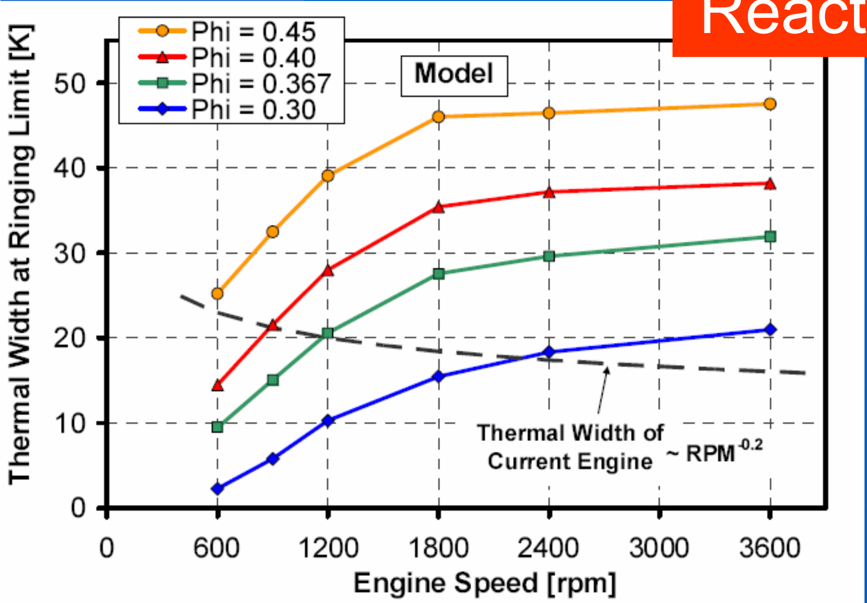
- TW, as a Parameter used to define T Stratification, can be used to Determine the Limits for Acceptable Rates of Pressure Rise
- Ringing Intensity, Defined by Eng, Gives a Measure of the Impact of High Rates of Pressure Rise
  - $$\text{Ringing Intensity} \approx \frac{1}{2\gamma} \cdot \frac{\left(0.05 \cdot \frac{dP}{dt,\max}\right)^2}{P_{max}} \cdot \sqrt{\gamma R T_{max}}$$
  - Maximum Acceptable Ringing Intensity is in the Range of 5 MW/m^2
- Acceptable TW Varies with the Target Reaction Timing, Load, and Engine Speed



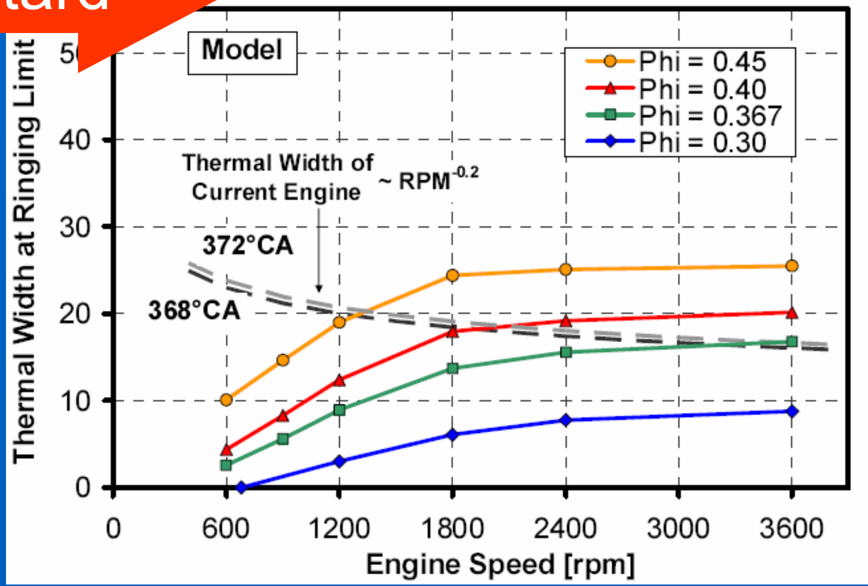


High Speed, High Load Operation

2005-01-0113 and 205-01-2125



Reaction Retard

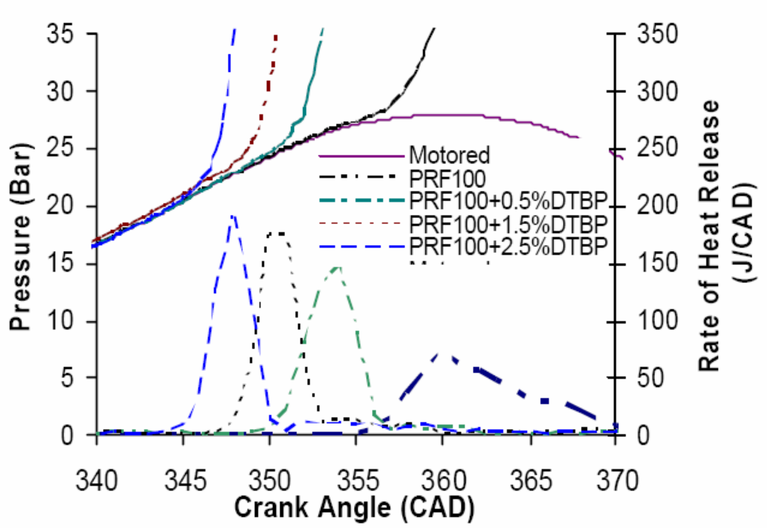


- Required Thermal Width (TW) (Temperature Gradient) Increases with Speed and Load, and Decreases with Delayed Ignition Timing

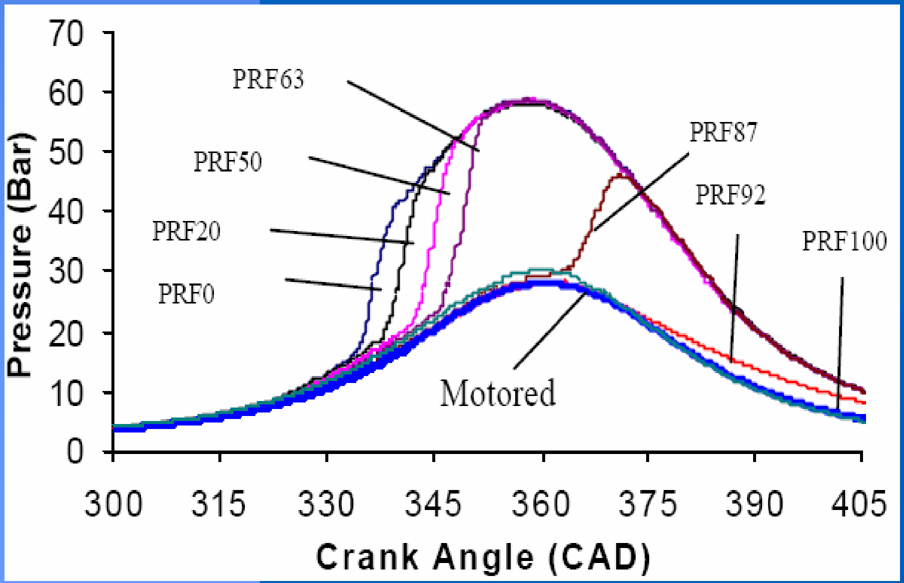
Fuel Advances

Fuel Additive Idea

2005-01-3740



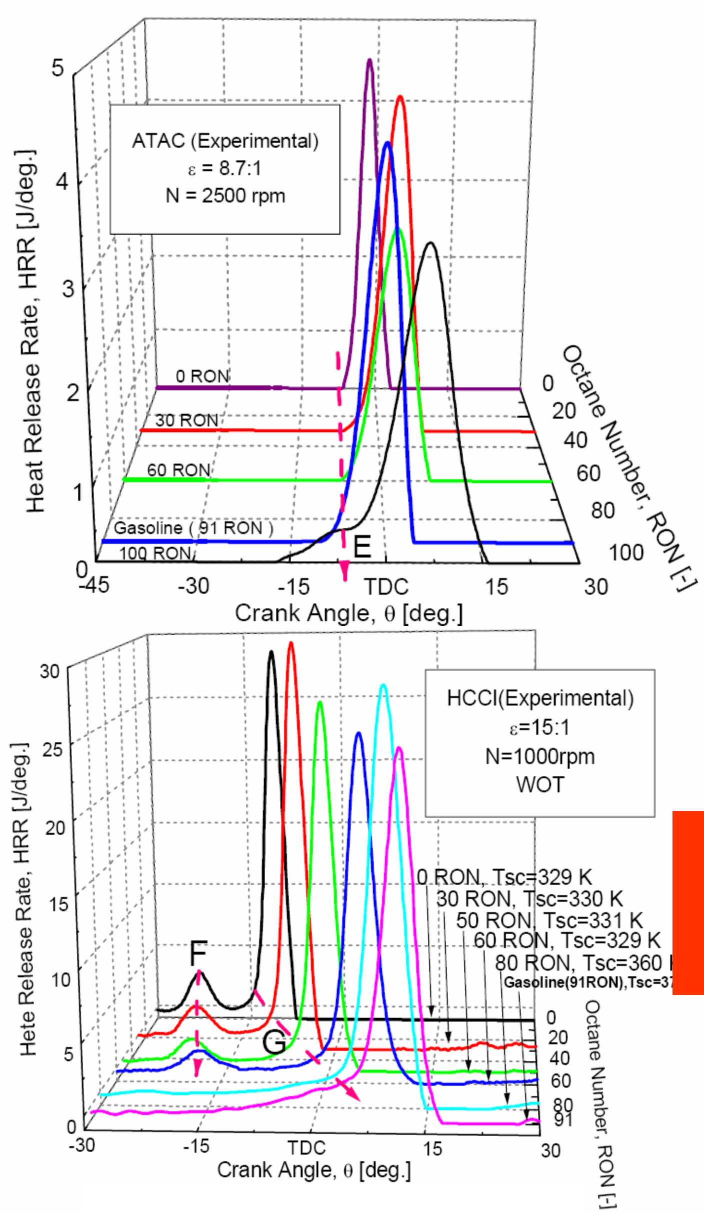
- Fuels have Different "HCCI Reactivities" Depending on the Chemical Composition
  - ◆ Reactivity Refers to the Propensity of the Fuel to React, as a Function of Temperature
  - ◆ Reactivity Indicated Relatively by ON and CN



- Additives can be used to Increase a Fuels Reactivity, it is not Likely that Acceptable Additives can be used to Decrease the Reactivity
  - ◆ CN Improvers in Gasoline to Lower Reaction T is Possible
  - ◆ ON Improvers in Diesel Fuel to Increases Reaction T are not Likely

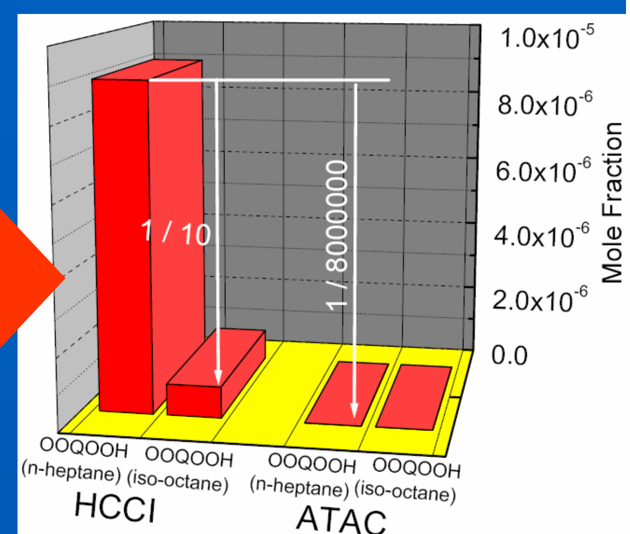
ATAC versus HCCI

2005-01-3732



- ATAC first Reported in 1979, involves Hot Residual Gas Initiated Auto-Reaction
  - Typically used in 2-Stroke Engines at Light Load and Low Compression Ratio
  - Typically does not Involve Low T Reactions
  - Not Sensitive to Fuel Ignition Characteristics

Difference in ATAC and HCCI
n-Paraffin versus iso-Paraffin
Cool Flame versus None



Additional General Observations

- Most of the Literature Focused on Gasoline Like Fuels and Development of HCCI Engines for these Fuels
- Stratification is being Extensively Examined
- Fundamental and Practical Models are being Developed and Advanced
- Large Body of Work in 2005 on the Application of VVA in HCCI for T control
  - Effective Compression Ratio Control
  - Residual Gas Control
- Full Time Gasoline HCCI more Likely than Full Time Operation on Diesel Fuel

Thank you

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