HCCI Combustion Fundamentals: In-Cylinder Diagnostics and Kinetic-Rate Computations

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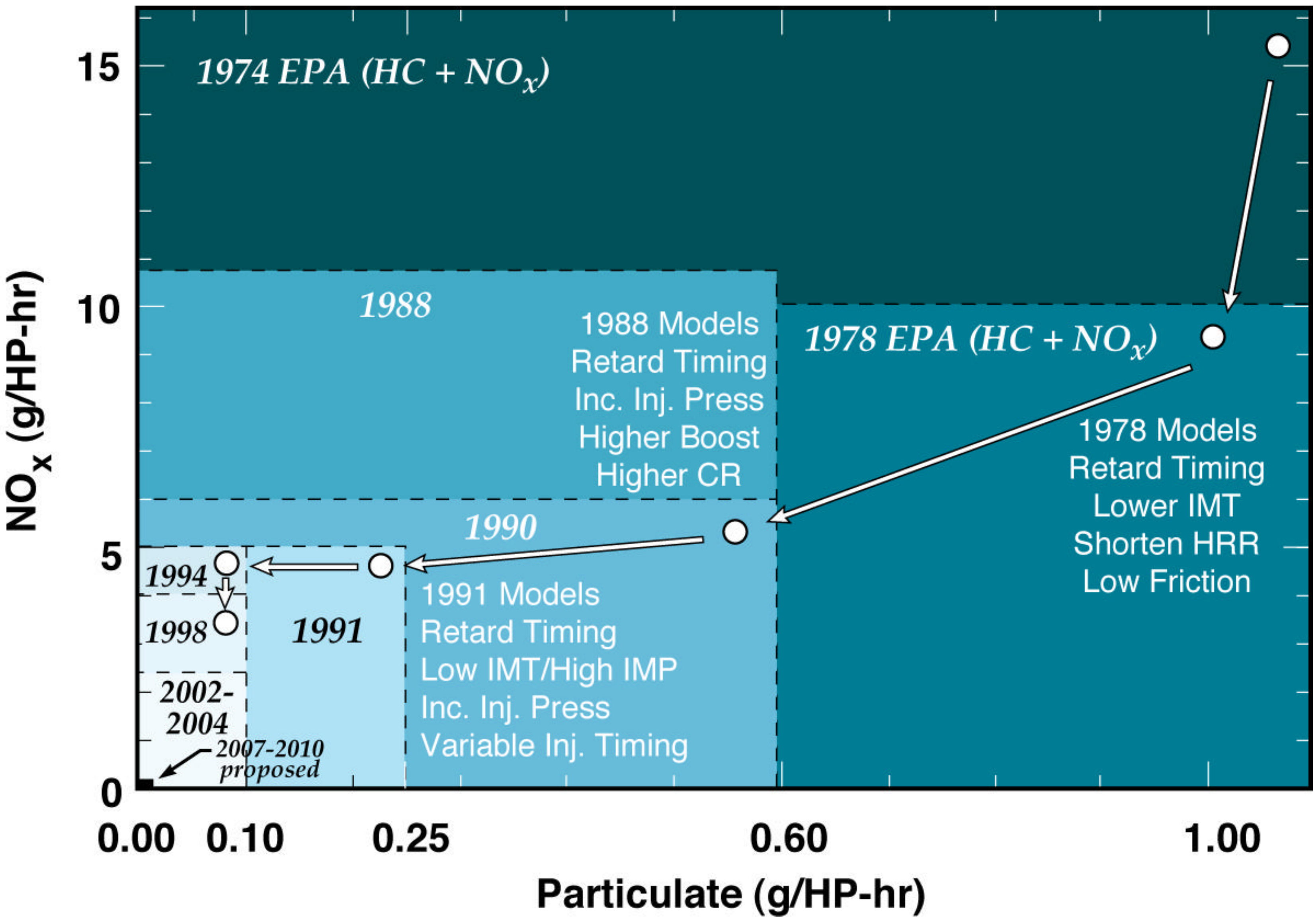
Introduction

- Substantial progress has been made in reducing emissions and improving the performance of Diesel engines.
  - Appears to be a lower limit for engine-out NO_X of about 1 g/hp-hr.
  - Serious difficulty in meeting Tier II or newly proposed H-D standards.

- Homogeneous charge compression ignition (HCCI) is an alternative IC engine combustion process that has the potential to:
  - Provide diesel-like or higher efficiencies.
  - Very low engine-out NO_X due to low combustion temperatures.
  - Very low particulate (PM) emissions.

- HCCI engine combustion is not well understood, and research is required to resolve technical barriers, including:

Evolution of H-D Diesel Emission Regulations



Sandia HCCI Project

- **Objective**: Provide the fundamental understanding needed for industry to develop/optimize practical HCCI engines.

- Establish a laboratory to investigate HCCI combustion.
  - All-metal engine
    - Measure - ignition timing, combustion rates, emissions
    - Establish operating points and develop combustion-control methods.
    - Compare results with kinetic-rate computations.
  - Optically accessible engine
    - Apply optical diagnostics to develop an understanding of: the nature of HCCI combustion, the effects of fuel/air/residual mixture, partial stratification of charge mixture and temperature, wall quench, etc.

- Chemical-kinetics calculations
  - Guide engine design, operating-point selection, combustion-control strategies, etc.

Scope of Interest in HCCI

- Most major automobile and diesel-engine manufacturers have initiated research and development efforts in HCCI or HCCI variants.

- A wide range of HCCI-type combustion is being investigated
  - Automotive engines
  - Heavy-truck engines
  - Gaseous fuels
  - Gasoline-like fuels
  - Diesel-like fuels
  - Premixed-fueling
  - Port injection
  - Direct injection

- Sandia HCCI facility should be sufficiently flexible accommodate most potential operating modes.

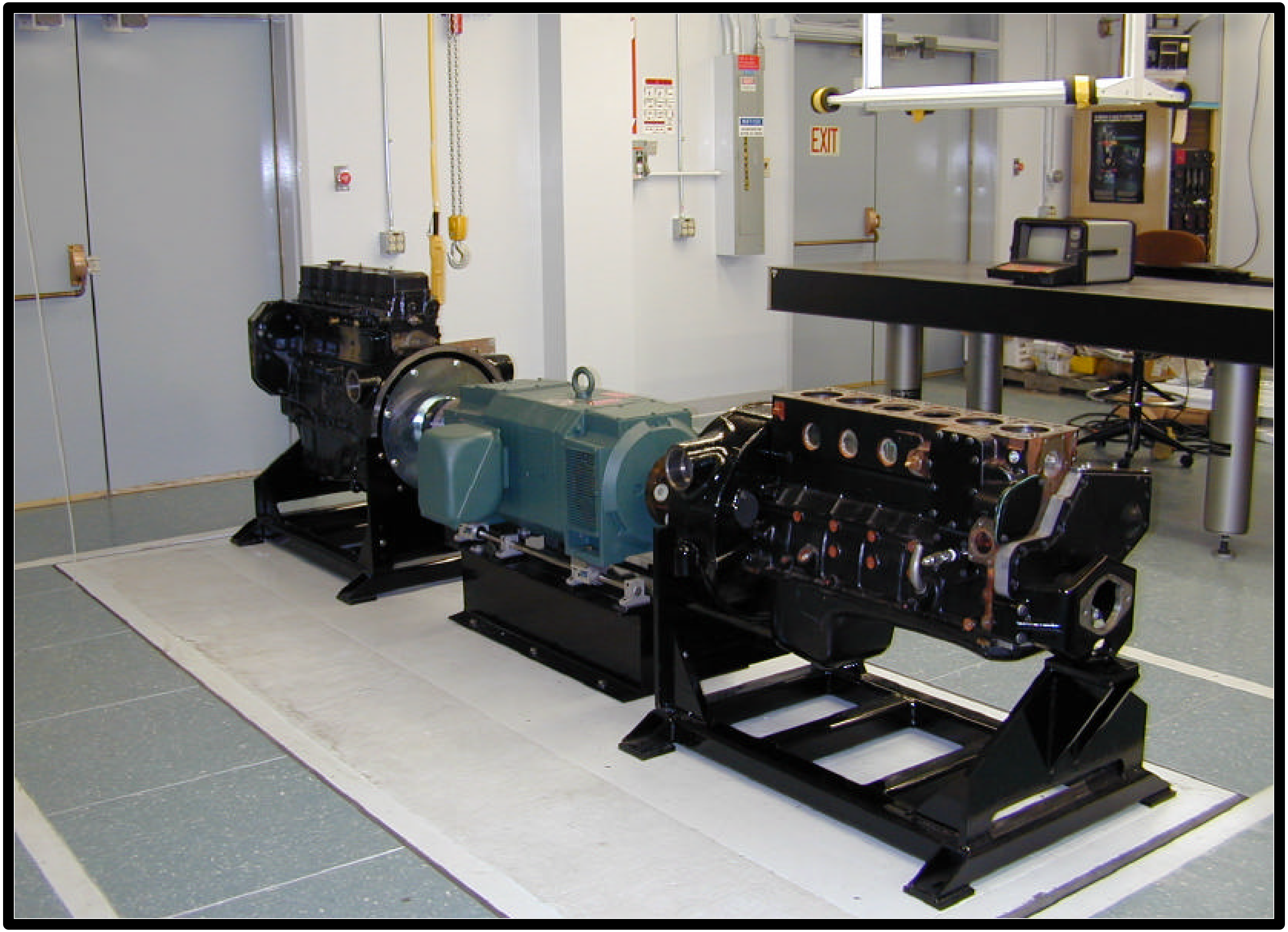
Sandia HCCI Research Engine

- Base engine: Cummins B-series
  - Intermediate size: 0.98 liters/cylinder
  - Speeds >3600 rpm - adequate to study speed effects relative to automotive-sized engines.
  - Very rugged engine - should easily withstand knock, etc.
- Accommodate various fuel-types and mixing techniques.
  - Fully premixed - gaseous fuels and vaporized more-volatile liquid fuels
  - Port fuel-injection - liquid fuels
  - Direct injection - liquid fuels (future experiments).
- Compression ratio variable by mechanical adjustment.
- Variable swirl via custom intake-port system.
- Full control of intake conditions: temperature, pressure, and simulated EGR.

Facility

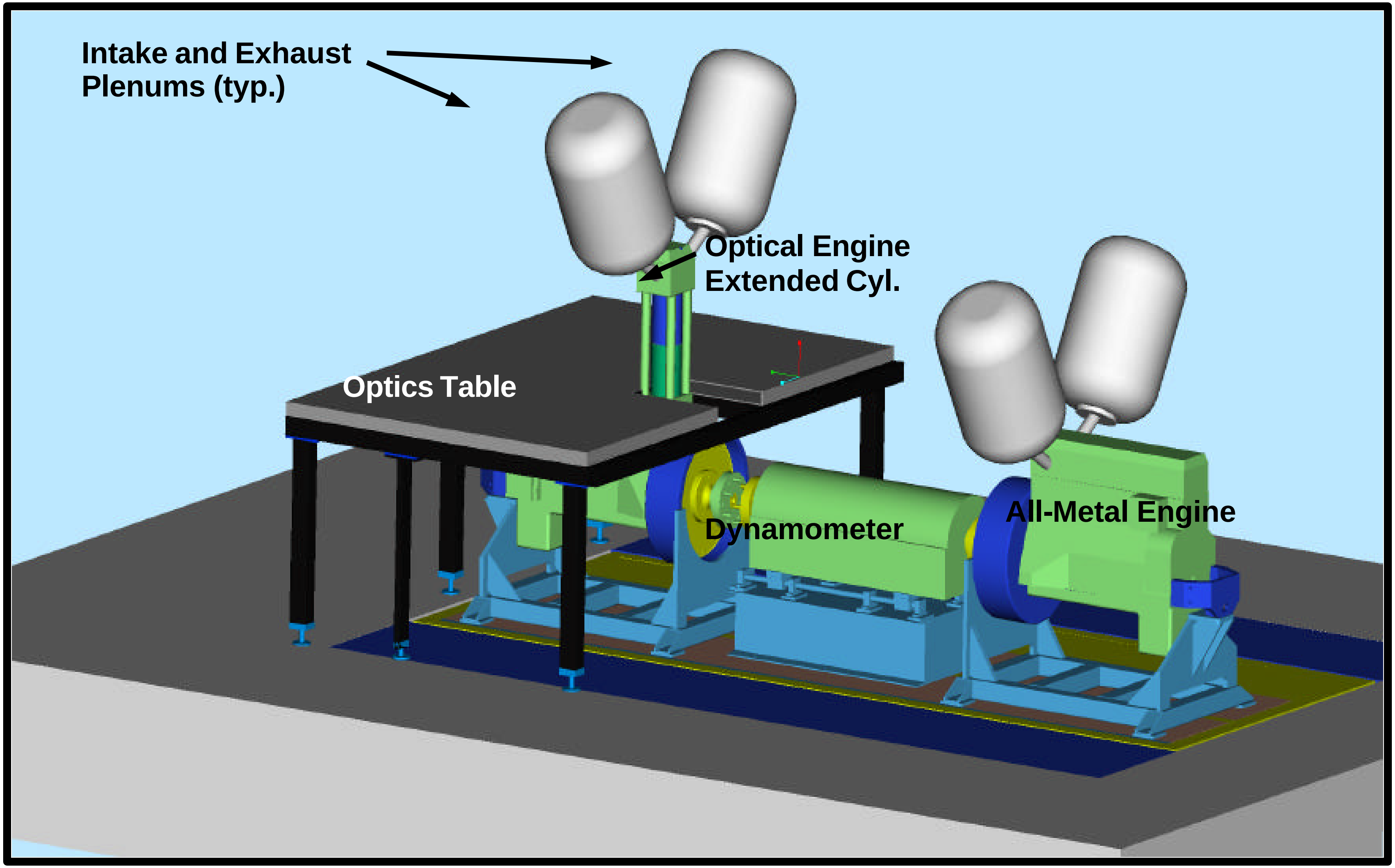
- Laboratory room/facility
  - Vibration-isolation pad, overhead crane, intake-air supply compressor, and gas-supply system, and major electrical modifications.
- Double-ended dynamometer and two B-series engines.
- Engine modifications for laboratory operation.
  - Conversion for balanced single-cylinder operation.
  - Cylinder-head modifications for variable swirl.
  - Numerous minor modifications (oversized flywheels, hand-crank system, shaft encoders, external water and oil supply, etc.)
- Engine subsystems
  - Intake gas metering and conditioning
  - Fuel/air mixing
  - Oil and water heating and circulating systems

HCCI Laboratory - May 2000



Layout of Engines, Dynamometer, and Optics Table

Installation as per this schematic is underway.



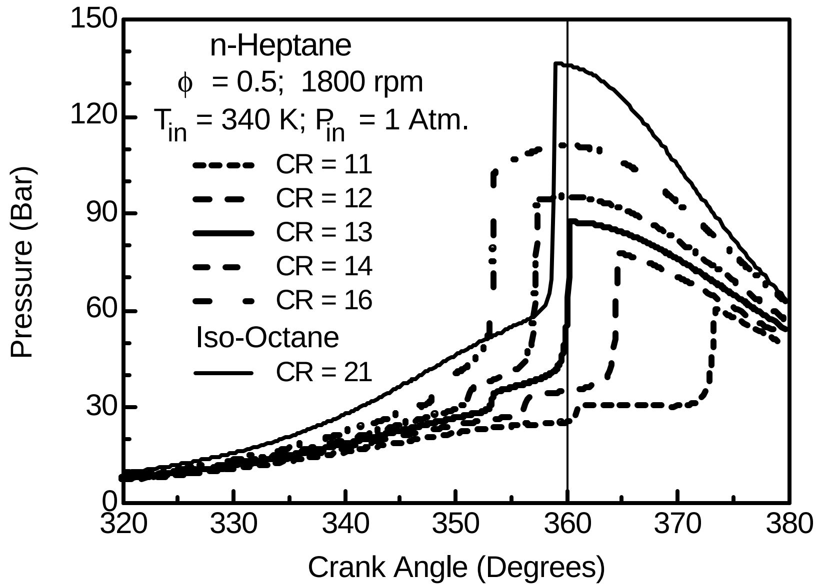
Ignition Timing Computations

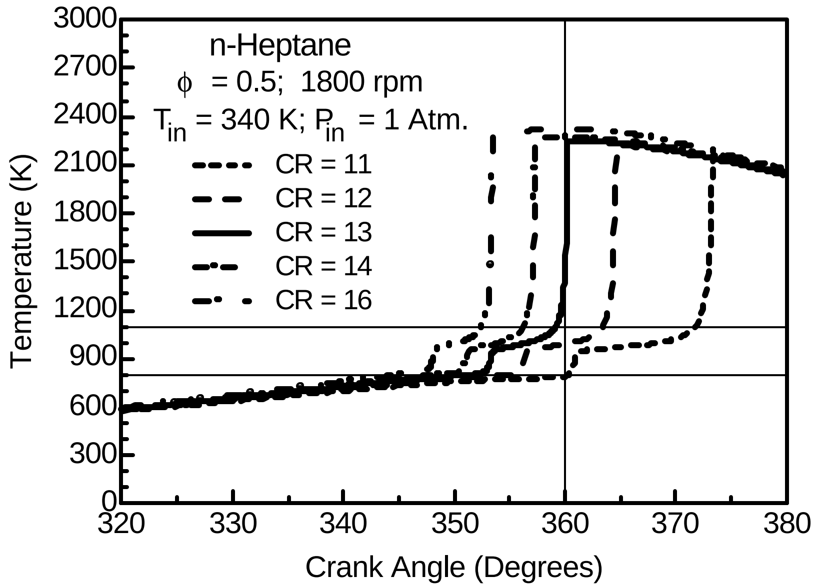
- Use CHEMKIN kinetic-rate code.
  - Full chemistry mechanisms for *n*-heptane and iso-octane - from LLNL (gasoline reference fuels, ON from 0 to 100).
  - Code is zero-dimensional but allows time-varying compression.
    - > Good indication of ignition timing, less accurate at true heat-release rate.

- Have conducted a comparative study of HCCI ignition timing for diesel-like and gasoline-like fuels across a range of operating parameters.
  - Investigate the effects of CR, intake conditions, equivalence ratio, engine speed, and EGR.
  - <u>Diesel-fuel surrogate</u>: *n*-heptane, CN = 56.
  - <u>Gasoline surrogate</u>: iso-octane, ON = 100 (ON = 87 is similar).

Comparison of Pressure and Temperature Plots

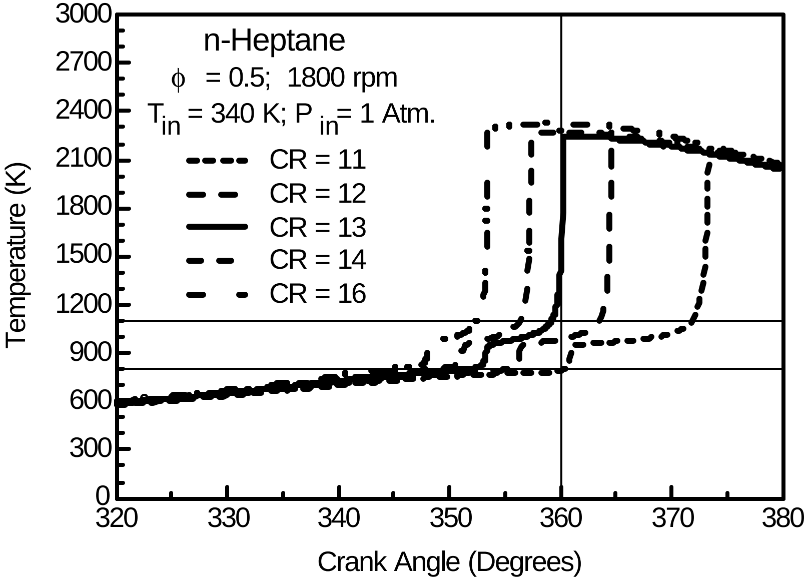
Vary Compression Ratio; n-Heptane

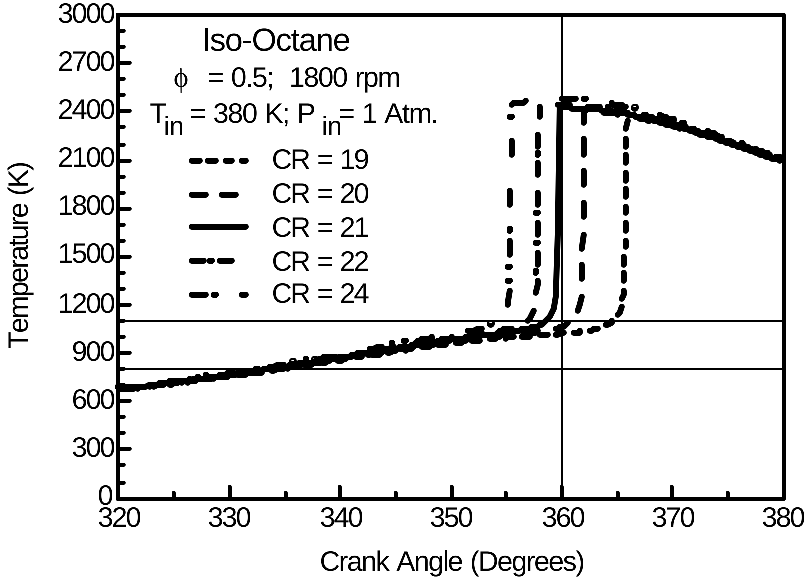




- Both pressure and temperature give a good indication of ignition timing.
- Pressure plots illustrate efficiency advantages, *i.e.* potential to do work.
- Temperature plots provide a better understanding of ignition chemistry.
  - Note the 2-step ignition - characteristic of diesel-fuel autoignition.
    - > First step occurs at a fairly low temperature, about 800 K.
    - > Second step occurs at about 1100 K - main “ignition”.

Vary Compression Ratio





Diesel-fuel surrogate: CN = 56

- "Cool" combustion chemistry easily activated - induces "hot" chemistry.
  - Note 2-step reaction.
  - Ignition occurs with a fairly low temperature, ~800 K.
- Prevents the use of high, diesel-like compression ratios, limiting efficiency.
  - Ignition too early for CR > 13:1

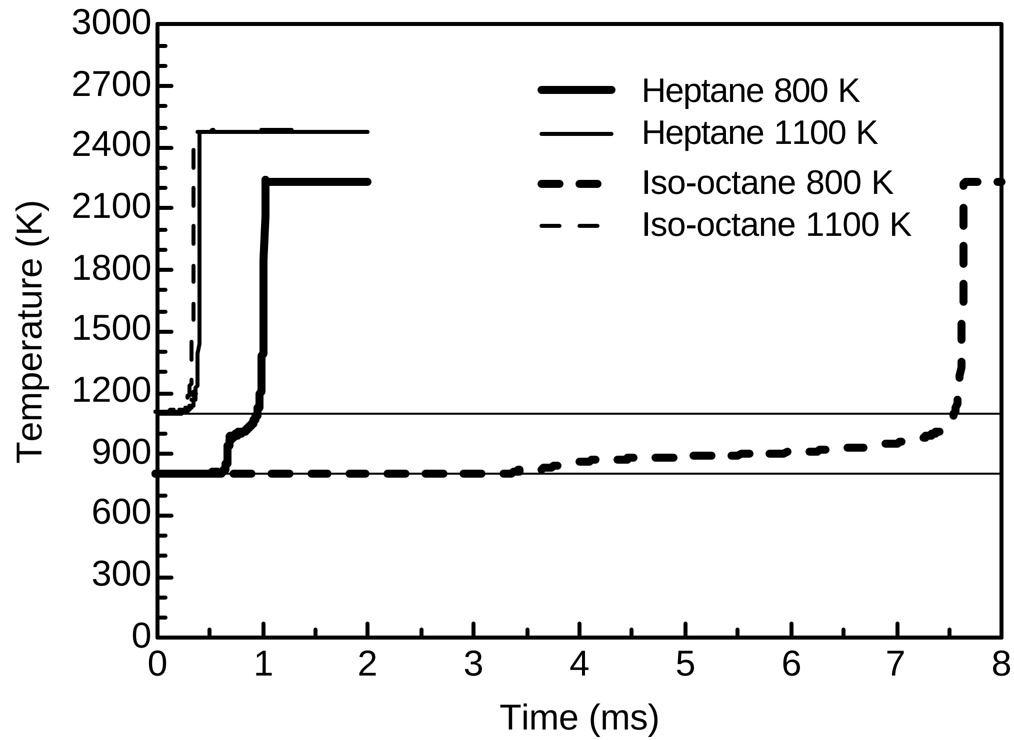
Gasoline surrogate: ON = 100

- "Cool" chemistry is minimal.
  - No evidence of 2-step reaction.
- Allows diesel-like compression ratios
  - High, diesel-like efficiencies
- Need to boost intake temperature by mixing with hot EGR, or use CR~24:1.
  - Effect is less for gasoline, ON = 87.

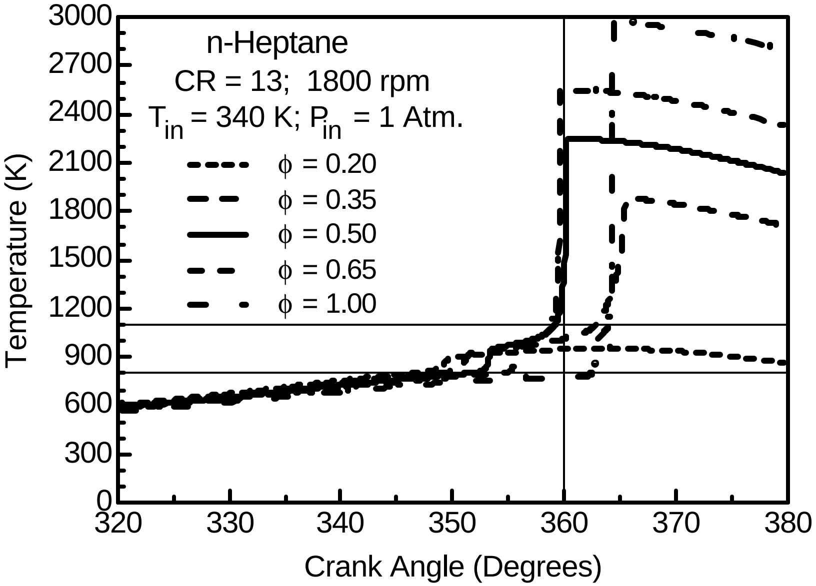
Constant-Volume Ignition of *n*-Heptane and Iso-octane

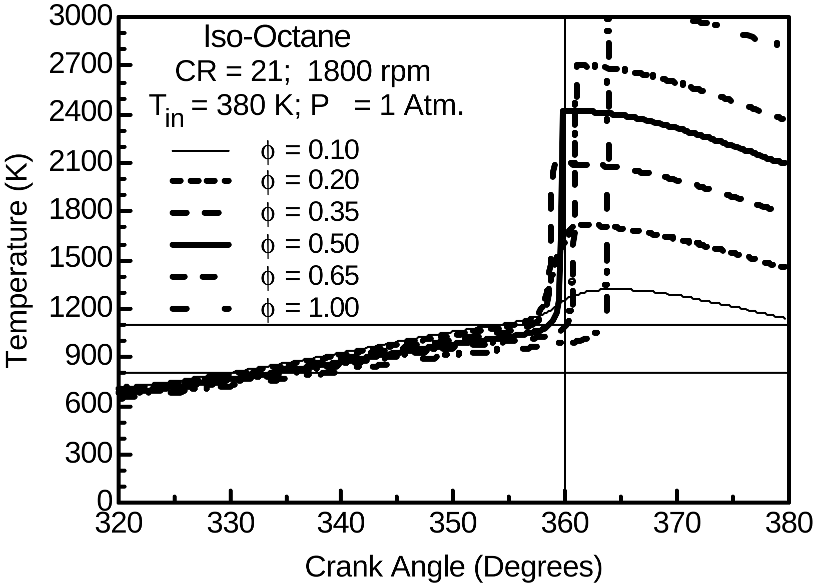
- *n*-Heptane has rapid “cool” combustion chemistry (800 K).
  - Induces “hot” chemistry (ignition) within 1 ms.
- Iso-octane has very slow “cool” combustion chemistry (800 K).
  - 8 ms to induce “hot” chemistry.
- In “hot” combustion regime (T > ~1100 K), both fuels burn equally fast.
- For typical engine timescales -
  - *n*-Heptane: rapid “cool” chemistry causes ignition before mixture can be compressed to 1100 K.
  - Iso-octane: slow “cool” chemistry allows (requires) compressing to ~1100 K.

P = 50 atm.; f = 0.5



Vary Fuel Loading





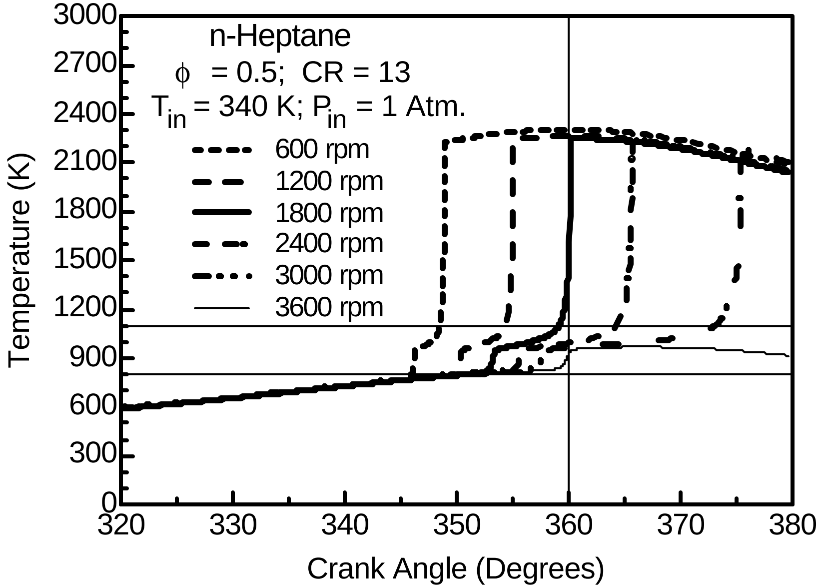
Diesel-fuel surrogate: CN = 56

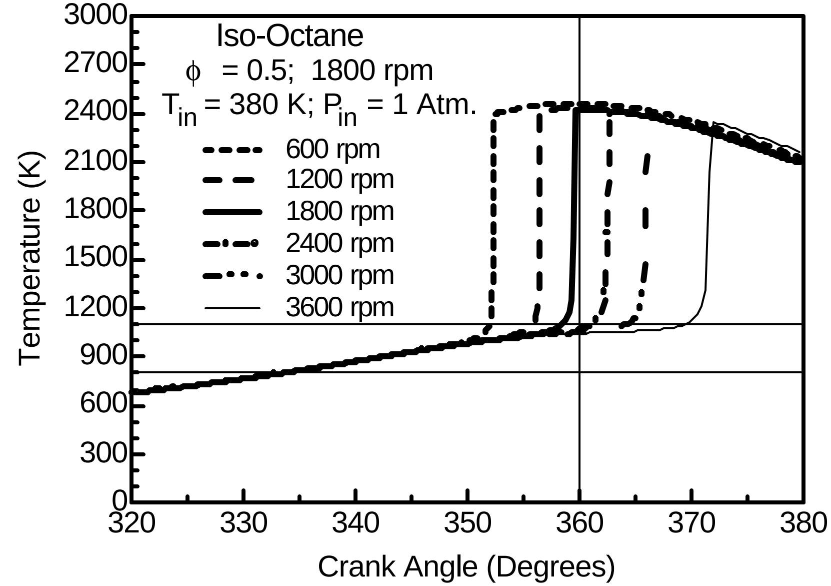
- Ignition timing sensitive to fuel-air mixture due to active cool-combustion chemistry.
  - Competing effects of γ & induction time.
- Low volatility - harder to make a uniform mixture.
- Substantial compensation required to control ignition timing.

Gasoline surrogate: ON = 100

- Ignition timing not as sensitive to fuel-air mixture.
  - Affected mainly by γ alone.
- Higher volatility - easier to make a uniform mixture.
- Simpler ignition-timing control strategies.

Vary Engine Speed





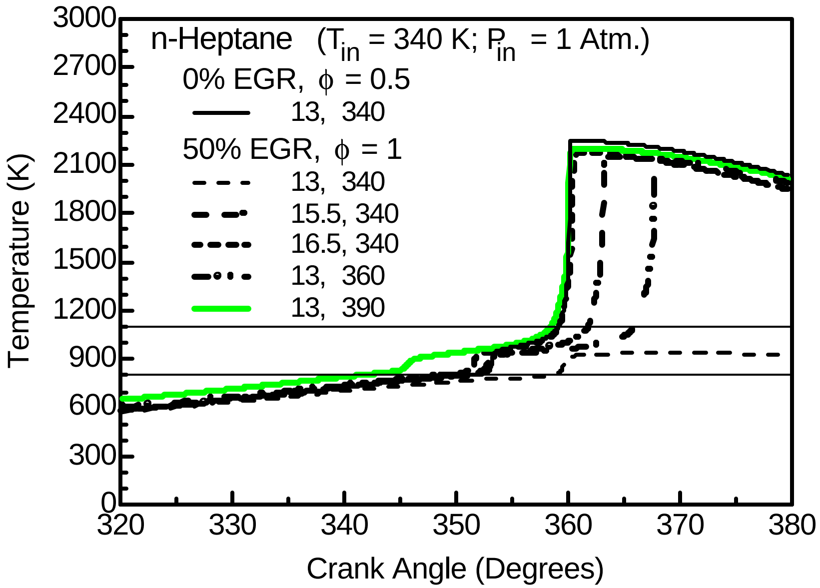
Diesel-fuel surrogate: CN = 56

- Temperature-time history affects timing of the first stage.
- Induction time (1st to 2nd stage) varies with compression or expansion.
- 600 - 3000 rpm: t_{ig} varies 27 CAD.
  - 3600 rpm does not ignite.
- Significant compensation required for changes in speed.

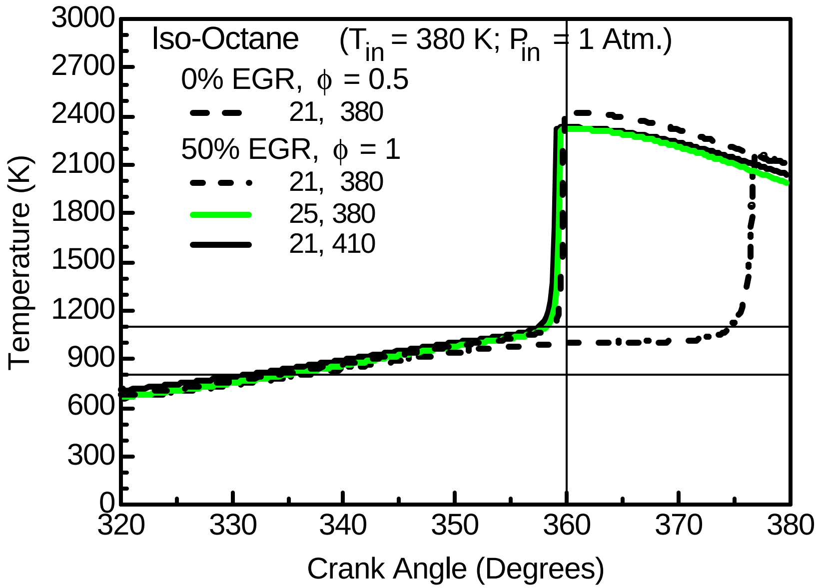
Gasoline surrogate: ON = 100

- Temperature-time history affects t_{ig}.
  - "Cool" chemistry has a small effect.
- 600 - 3000 rpm: t_{ig} varies 14 CAD.
- 3600 rpm ignites.
  - 600 - 3600 rpm: t_{ig} varies 20 CAD.
- Less compensation required for changes in speed.

Effects of EGR/Residual Gases



Diesel-fuel surrogate: CN = 56



Gasoline surrogate: ON = 100

- Adding hot EGR gases is a potential control mechanism for HCCI.
  - External recirculation, or internally by increasing residuals.
- EGR decreases γ (c_p/c_v) reducing compressed-gas temperature.
  - CR or T_{in} must be increased to compensate - affects both fuel types.
- EGR increases the specific heat of the charge.
  - Increases induction time for n-heptane (more energy required to raise gas temp.).
  - Little effect on iso-octane (induction chemistry is not very important).

Conclusions: Ignition-Timing Computations

- Mixing hot EGR into the charge is a viable control mechanism.
  - Complicated by concomitant changes in γ (c_p/c_v) and specific heat.

- Significant differences in the behavior of fuels with two-stage ignition (*e.g.* diesel fuel) and single-stage ignition (*e.g.* gasoline).
  - Two-stage fuel: CR limited to ~13:1, less efficiency
More sensitive to variation in speed and load.
  - Single-stage fuel: High, diesel-like CR, higher efficiency
Less sensitive to variation in speed and load.

- Gasoline-like, single-stage fuels offer advantages, both in efficiency and for controlling ignition timing across the load-speed map.
  - Required CR is high for maximum efficiency and NO_X control.
    - > 87 octane PRF mixture (not shown) lowers CR requirement.
  - Additional research is required.

Concluding Remarks

- CHEMKIN calculations have provided significant insight into the controlling parameters, sensitivity, and tradeoffs of HCCI operation.
  - A paper reporting this investigation has been presented the 2000 International Combustion Symposium.
  - Results will guide the design of our HCCI research engines (*e.g.* selection of compression-ratio ranges).
  - Also guide selection of operating conditions for initial experiments.

- Substantial progress has been made on the design and construction of the HCCI engine laboratory.
  - Expect all-metal engine to become operational in 2001 and optical engine in 2002.