

Micro-Homogeneous Charge Compression Ignition (HCCI) Combustion: Investigations Employing Detailed Chemical Kinetic Modeling and Experiments

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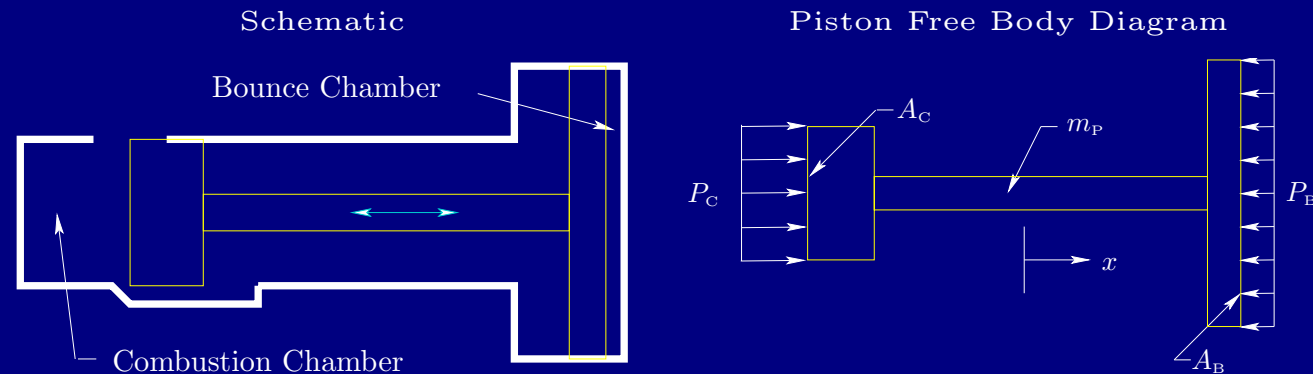
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Micro-Engines

- Goal:
 - Replace batteries with engine-generators.
 - 10 W from 1 cm³ packaged volume.
 - Specific Energy: Hydrocarbon: $40 \frac{\text{MJ}}{\text{kg}}$; Battery: $1 \frac{\text{MJ}}{\text{kg}}$.
- Programs:
 - Micro-Gas Turbine Engine (MIT)
 - MEMS Rotary Engine (University of California Berkeley)
 - MEMS Free-Piston Engine-Generator (Georgia Tech.)
 - MEMS Free-Piston Knock Engine (Honeywell International)

Micro-Engine Concept

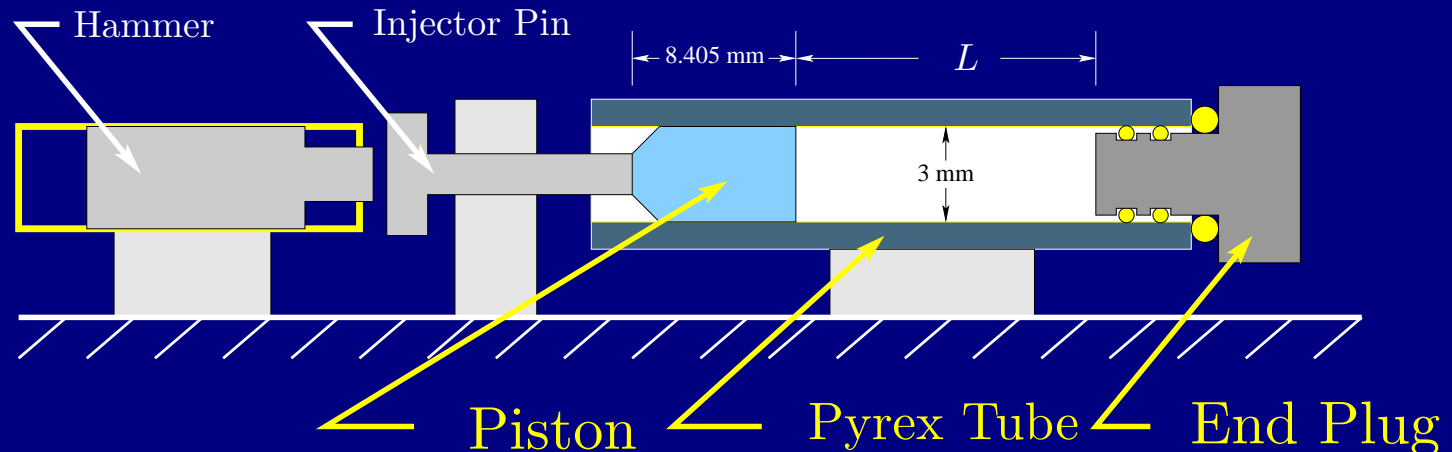
- **Homogeneous Charge Compression Ignition (HCCI):**
 - Homogeneous explosion—no external ignition system—fast.
 - Depends upon compression process and kinetics.
 - Control is a problem.
- **Free-piston configuration:**



$$\Sigma F_x = m_P \frac{d^2 x}{dt^2} = P_C A_C - P_B A_B$$

- **Variable compression ratio**—HCCI control strategy.
- Few moving parts, but difficult to design.

Single-Shot Experiments

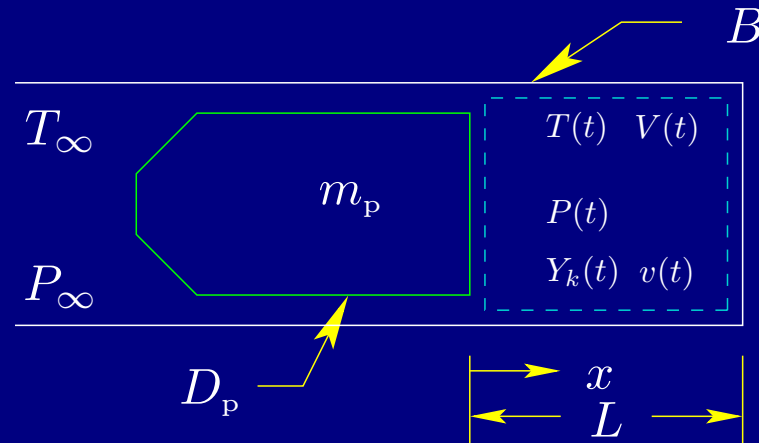


- Objective:
 - Demonstrate micro-HCCI combustion.
 - Understand free-piston and HCCI combustion coupling.
- Setup:
 - Piston: 3 mm Diameter \times 8.4 mm; mass 0.435 g.
 - Precision Pyrex tubes, $32 \text{ mm} \leq L \leq 57 \text{ mm}$.
 - $5 \mu\text{m}$ Piston cylinder gap—no seal.

Single-Shot Experiments

- **Measurements:**
 - Digital movies with Phantom v4.0 Digital camera.
 - Position and velocity from movies: Resolution: $16\ \mu\text{s}$ and $0.1\ \text{mm}$ – $0.4\ \text{mm}$.
- **Results (Heptane-air):**
 - HCCI combustion is demonstrated with $\Phi=0.69$ and $\Phi=0.25$.
 - Charge initially at ambient conditions; no external ignition system, catalysts, or heating used.
 - Lean case suggests combustion occurs through a series of explosions.

Single-shot Experiment Model



- Assumptions:

- Homogeneous—Detailed Chemical Kinetics.
- Leakage modeled with 1-D quasi-steady compressible flow.
- Conduction is the dominant heat transfer mode.

- Formulation:

- Mass, species, and energy balances on the gas.
- Force balance on the piston.

Single-Shot Model

Energy:
$$\frac{dT}{dt} = \frac{\dot{q}}{c_v} - \frac{P}{c_v} \frac{dv}{dt} - \frac{v}{c_v} \sum_{k=1}^{N_s} u_k \dot{\omega}_k W_k$$

Species:
$$\frac{dY_k}{dt} = v \dot{\omega}_k W_k$$

Mass:
$$\frac{dv}{dt} = \frac{v^2}{V} \dot{m} + \frac{v}{V} V_1$$

Force:
$$\frac{dV_1}{dt} = - \frac{A_c A_p (P_\infty - P)}{m_p}$$

Velocity:
$$\frac{dV}{dt} = V_1$$

Heat Loss:
$$\dot{q} = \frac{v}{V} \left(\frac{\pi B^2}{2} + \pi B (L - x) \right) \bar{q}'';$$

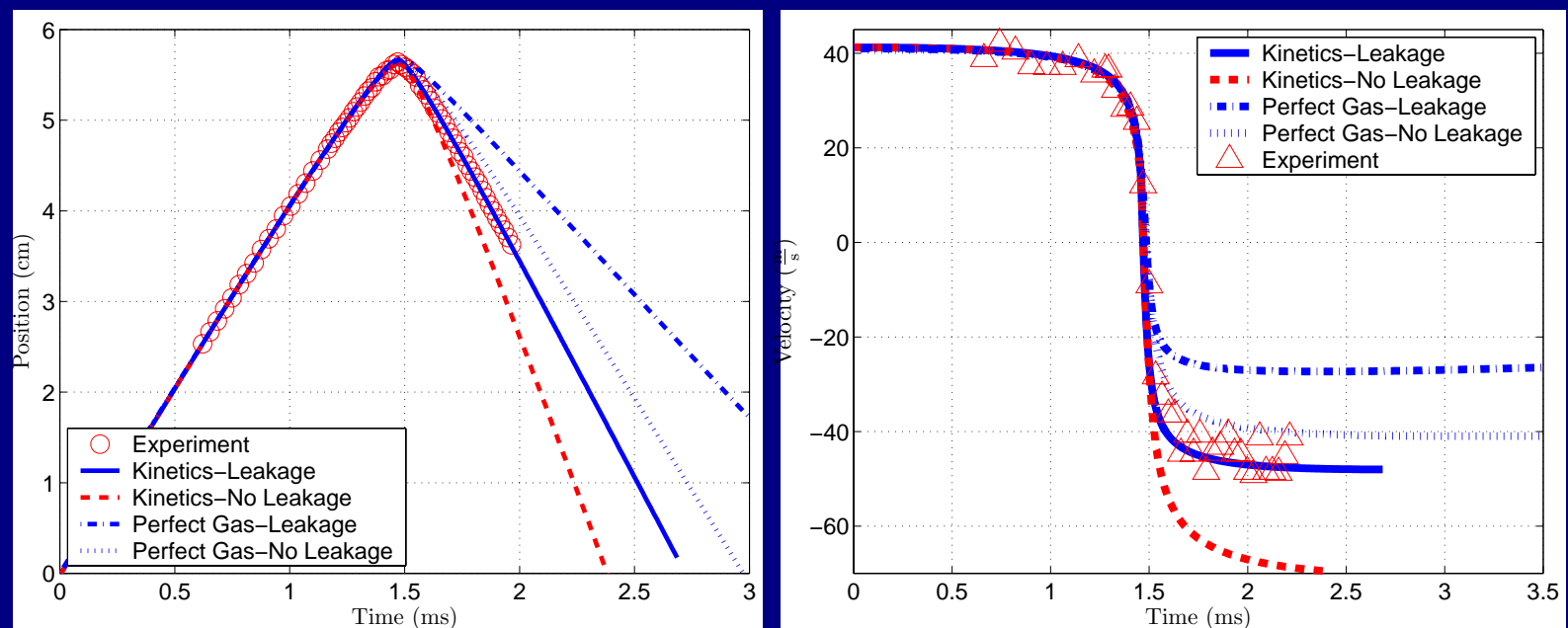
$$\bar{q}'' = \frac{2k_T(T_0 - T_w)}{(L-x)} \left[\frac{0.440332\pi^2 + 5.09296 \left(\frac{L-x}{B} \right)^2}{\pi + 2\pi \left(\frac{L-x}{B} \right)} \right]$$

Leakage:
$$\dot{m} = \frac{C_d A_t P}{(R_m T)^{\frac{1}{2}}} M(P, P_\infty, \gamma);$$

$$M(P, P_\infty, \gamma) = \begin{cases} \left(\frac{P_\infty}{P} \right)^{\frac{1}{\gamma}} \left\{ \frac{2\gamma}{\gamma-1} \left[1 - \left(\frac{P_\infty}{P} \right)^{\frac{\gamma-1}{\gamma}} \right] \right\}^{\frac{1}{2}} & \frac{P_\infty}{P} > \left(\frac{2}{\gamma+1} \right)^{\frac{\gamma}{\gamma-1}} \\ \gamma^{\frac{1}{2}} \left(\frac{2}{\gamma+1} \right)^{\frac{\gamma+1}{2(\gamma-1)}} & \frac{P_\infty}{P} \leq \left(\frac{2}{\gamma+1} \right)^{\frac{\gamma}{\gamma-1}} \end{cases}$$

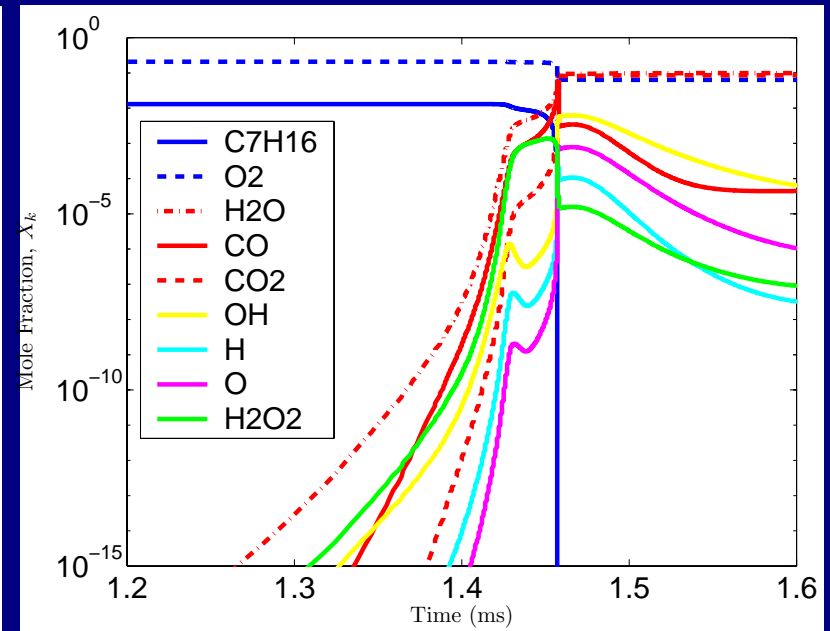
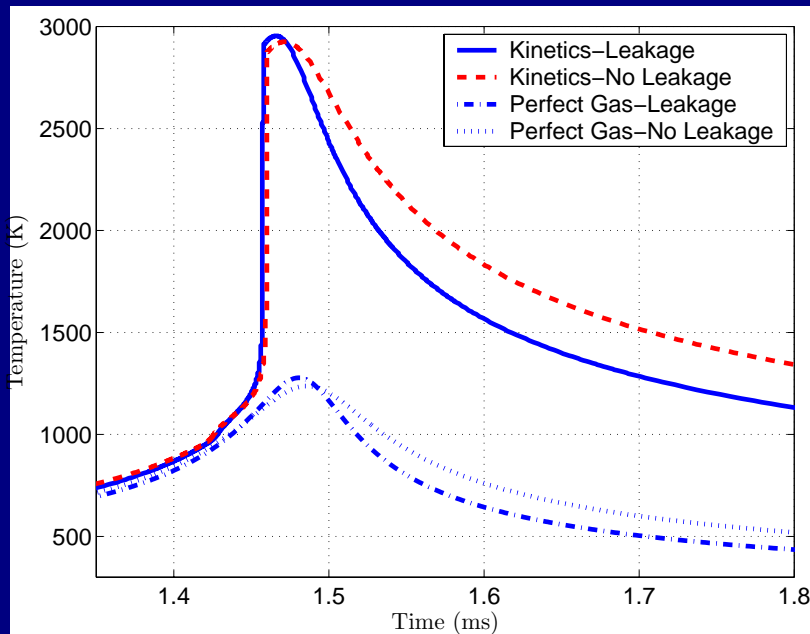
Model Validation

- Replicated heptane-air experiment with $\Phi=0.69$:
 - Also considered perfect gas model.
 - Model predicts position and velocity very well.
 - Infer consequences of leakage and combustion.



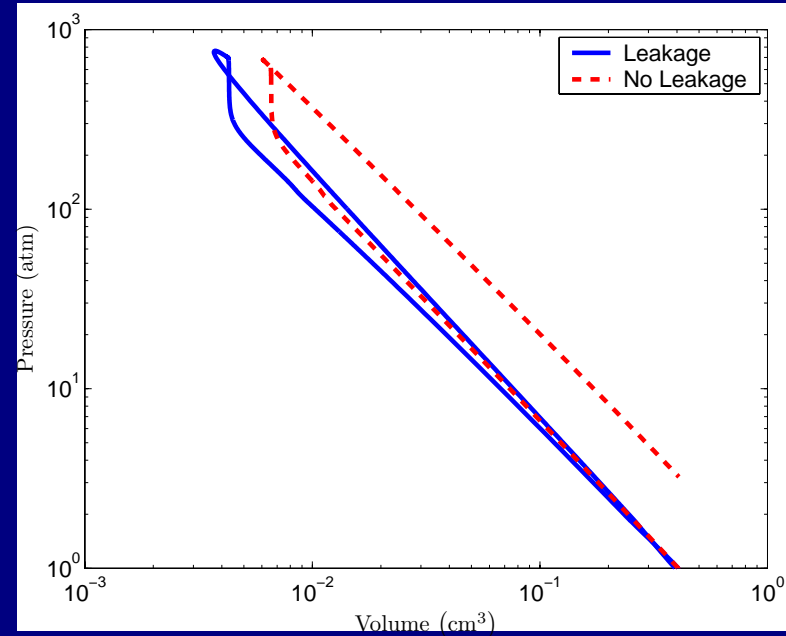
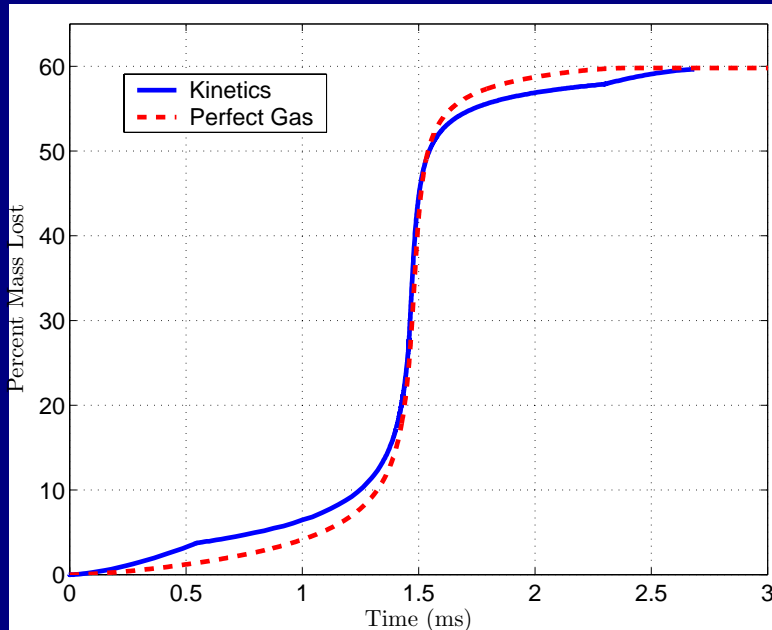
Model Results

- Temperature and Mole Fractions:



Model Results

- Percent Mass Lost and P-V Diagrams:
- Leakage causes the compression ratio to increase.



Parametric Study

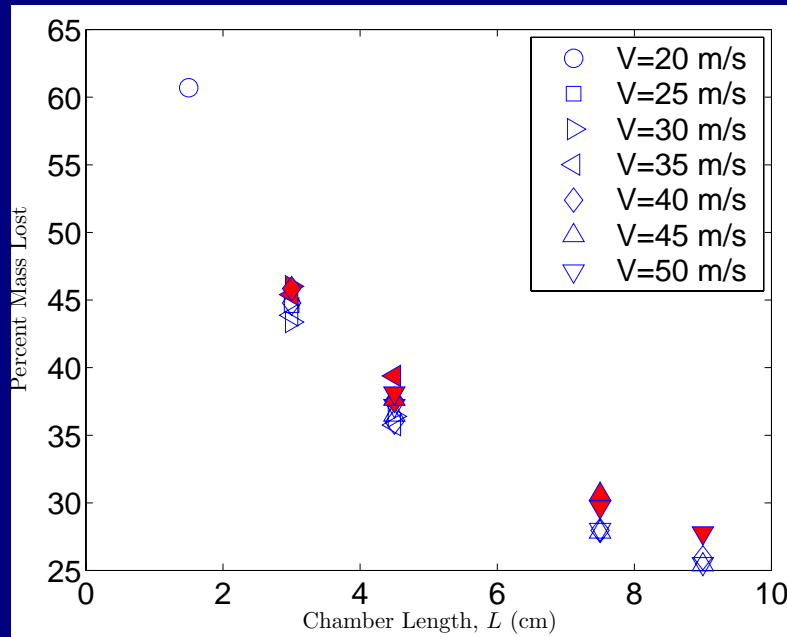
- **Objective:**
 - Explore relationship between initial conditions and compression ratio, leakage, and efficiency.
 - Investigate fuel and equivalence ratio effects.
- **Parameter Values:**

Parameter	Values	Unit
Initial Velocity	5, 10, 15, 20, 25, 30, 35, 40, 45, 50	$\frac{m}{s}$
Chamber Length (L)	0.6, 1.5, 3.0, 4.5, 7.5, 9.0	cm
Equivalence ratio (Φ)	0.25, 0.47, 0.69, 0.95, 1.5, 2.9	NA
Fuel (Kinetic Mechanism)	Heptane and Propane	NA

Parametric Study Results—Leakage

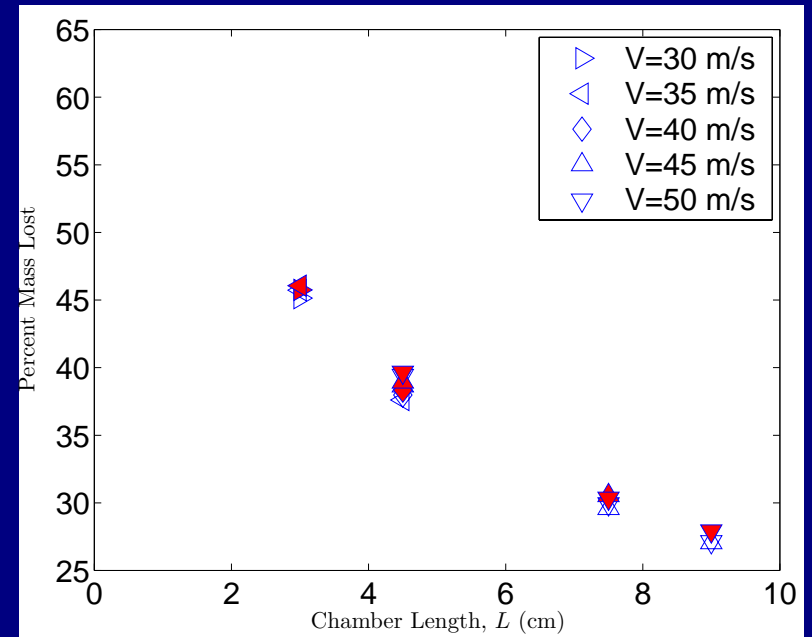
- Leakage depends upon the chamber length.
- Leakage has a weak dependence on fuel, initial velocity, and γ .

$\Phi=0.95$



Open symbols: Heptane-air

$\Phi=0.25$

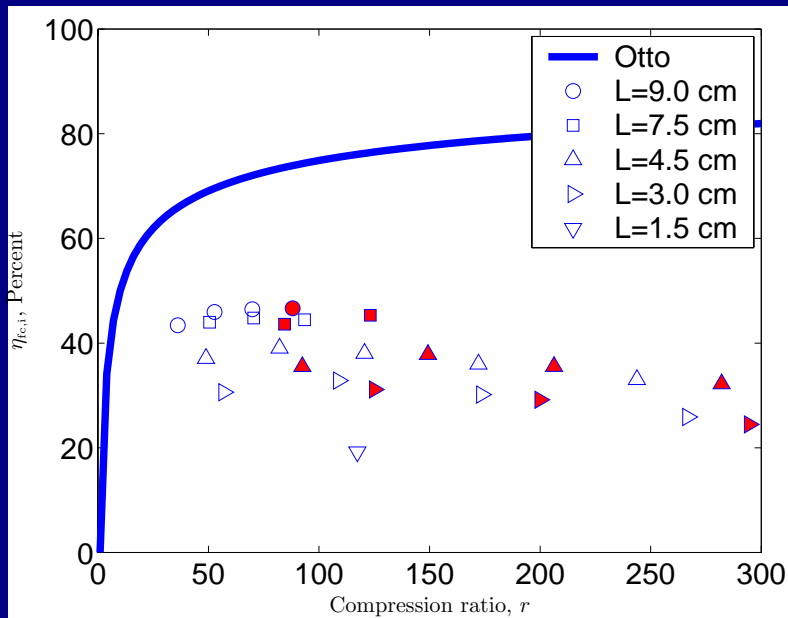


Dark symbols: Propane-air

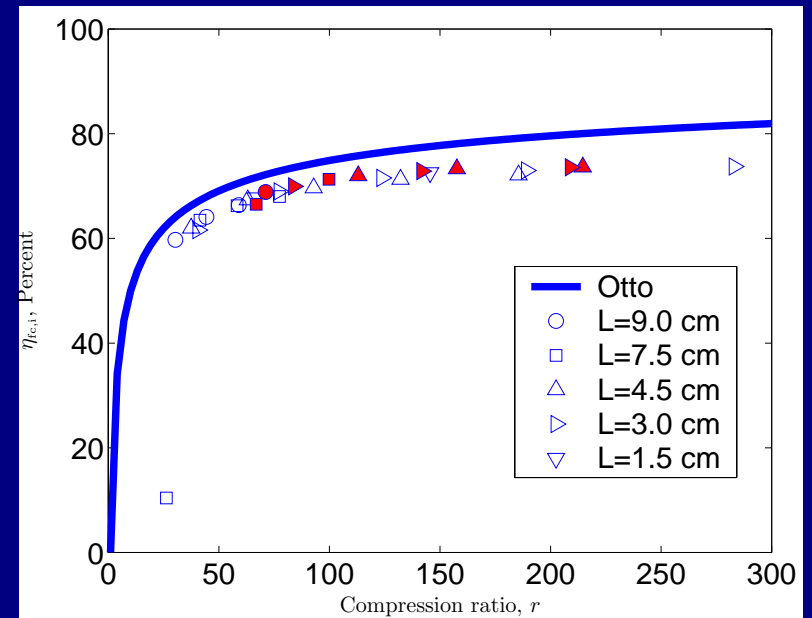
Parametric Study Results—Efficiency

- Leakage constrains efficiency.
- Efficiency depends weakly on fuel.

With Leakage



Without Leakage



Open symbols: Heptane-air

Dark symbols: Propane-air

$$\Phi=0.95$$

Non-Dimensional Analysis

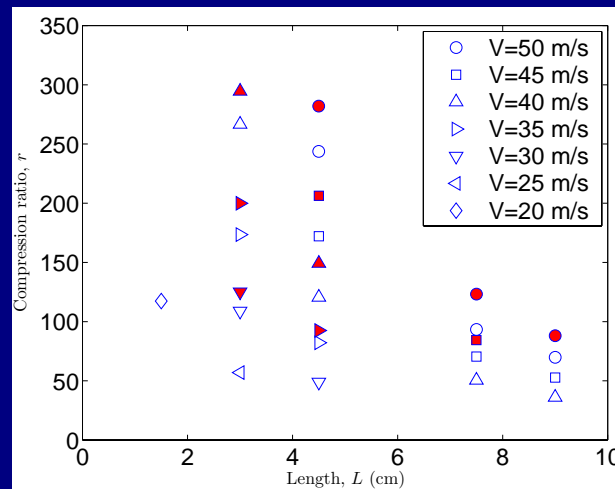
- Non-dimensional leakage parameter:

$$\frac{\tau v_0 \dot{m}}{V_0} \approx 4 \left(\frac{t_G}{D_p} \right) \left\{ \frac{\tau v_0 P_0 C_d M(P_0 P^*, P_0, \gamma)}{L (R_m T_0)^{\frac{1}{2}} R_{\max}} \right\} \left(\frac{P^*}{T^* \frac{1}{2}} \right)$$

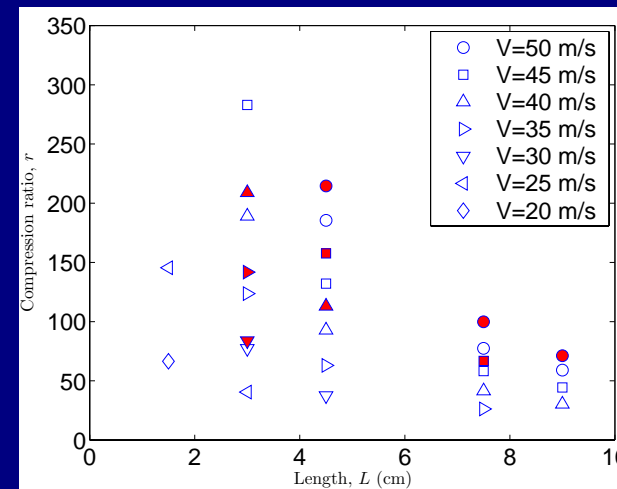
- Can reduce leakage by decreasing $\frac{t_G}{D_p}$ or increasing L .

- Compression Ratio: Complicated Dependence

$\Phi=0.95$, Dark symbols indicate propane.



With leakage

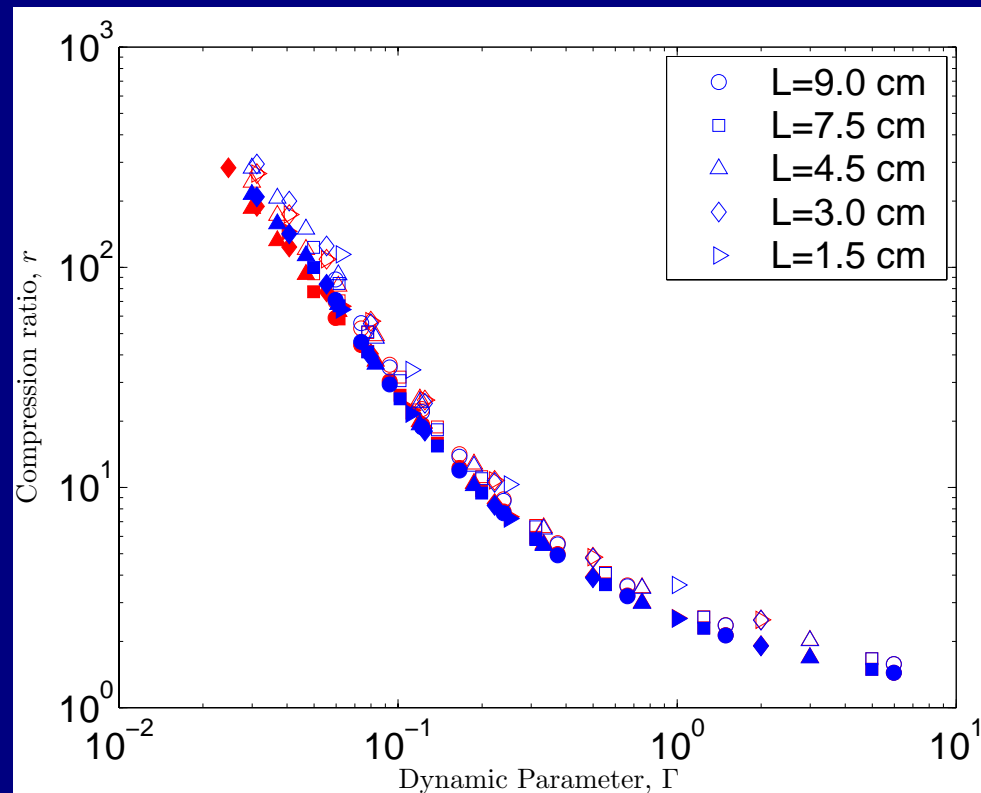


Without leakage

A Proposed Non-Dimensional Parameter

$$\Gamma = \frac{LR_{\max}P_{\infty}}{\dot{x}_0^2 \left(\frac{m_p}{A_p} \right)}$$

- Collapses parametric results from leakage and non-leakage cases and different fuels.



$\Phi=0.95$. Closed symbols indicate non-leakage cases.

A Non-Dimensional Parameter

- Physical Interpretation:

- Rearrange: $\Gamma = \frac{LA_p P_\infty R_{\max}}{m_p \dot{x}_0^2}$; $R_{\max} \approx 1$.
- LA_p : Volume swept by the piston.
- $\Gamma = \frac{\text{Work required to displace the volume swept by the piston}}{2 \times \text{Kinetic energy of the piston}}$.
- Kinetic energy of the piston is also compression work.

- Optimal Initial Conditions:

- Desire $50 \leq r \leq 100$ to maximize efficiency.
- Then $0.45 \leq \Gamma \leq 0.7$ is optimal.
- Hence,

$$1.1 \geq \frac{\text{Kinetic energy of the piston}}{\text{Work required to displace the volume swept by the piston}} \geq 0.7$$

is necessary.

Conclusions

- HCCI in small dimensions has been demonstrated.
- Single-shot experiments have been modeled with **detailed chemical kinetics**.
- The model and single-shot experiments correspond well.
- **Leakage is a “show-stopper”** and accounts for:
 - Changes in the piston path during the expansion stroke.
 - An observed increase in the compression ratio.
 - A decrease in the fuel conversion efficiency.
- **Leakage may be reduced by increasing L or decreasing $\frac{t_G}{D_p}$.**
- A non-dimensional parameter that relates the initial conditions to the compression ratio is introduced.

Future Work

- Further comparisons between model and experiments.
- Further explore the parameter space with the model.
- Explore strategies to reduce leakage.

Acknowledgement

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For More Information:

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