A Comparison of HCCI Engine Performance Data and Kinetic Modeling Results over a Wide Range of Gasoline Range Surrogate Fuel Blends

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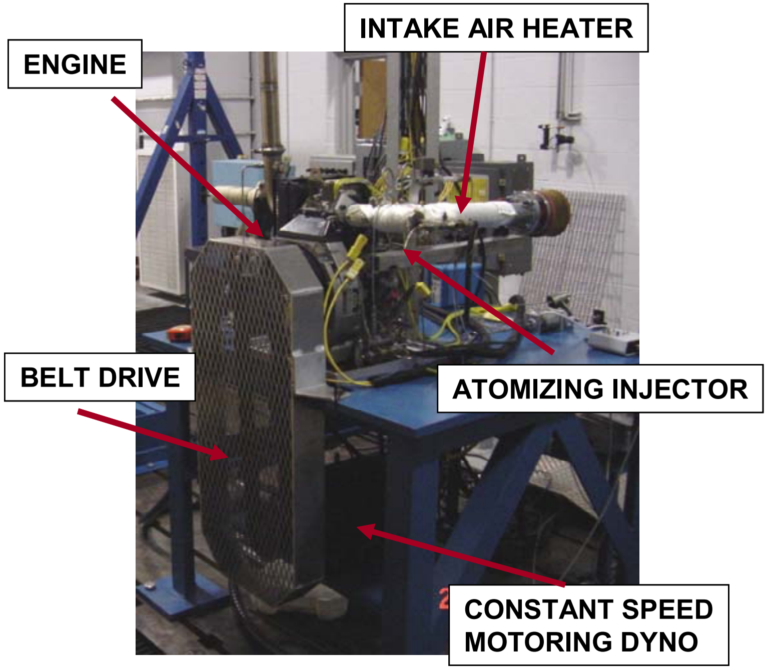
Goal of research

- In general, kinetic models of fuels are needed to allow the simulation of engine performance for research, design, or verification purposes
  - Desire to match a specific fuel to support design work
  - Desire to match a group of fuels for fuel sensitivity studies
  - Desire to accurately reproduce chemistry effects for more open study of future fuel options
- For this research, we wish to gather and develop tools to allow kinetic modeling of an HCCI engine over a wide range of surrogate fuel blends
  - Develop and verify model over a range of experimental data
  - Use model to help plan and estimate results for future studies
  - Learn how to represent a wide range of fuels with surrogate mixtures
  - Develop efficient modeling and mechanisms for rapid calculation of results

Modeling options

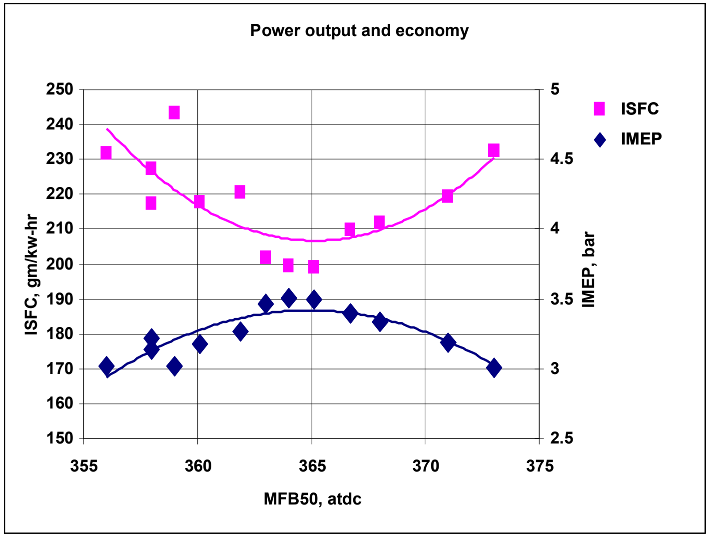
- Single zone kinetic model
  - Can predict ignition
  - SAE 2008-01-2399 (ORNL and RD)
- Multi-zone kinetic model (this talk)
  - Ignition, burning
  - Some emissions capability
- Multi-zone kinetic model with CFD front end
  - CFD front end defines zone conditions at start of combustion
  - Evaluated in SAE 2009-01-0669 (RD and ORNL)
- Multi-zone kinetic model with zone mixing
  - Ignition, burning
  - Better chance to predict emissions
- CFD model
  - Most true to flow, mixing, and heat loss processes

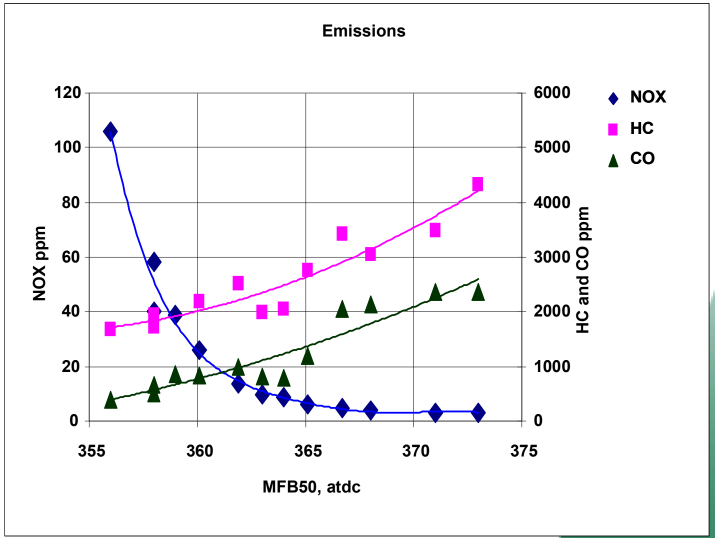
ORNL HCCI engine



- **Modified from Hatz single cylinder diesel**
- **Fully premixed, dilute, with ignition controlled by intake heating**
- **Simple platform for fuels research**
  - **Performance dominated by fuel effects**
- **Recently upgraded with boost, throttle, improved measurements**

EMISSIONS AND ECONOMY TRADEOFFS VS. COMBUSTION PHASING





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Experimental data

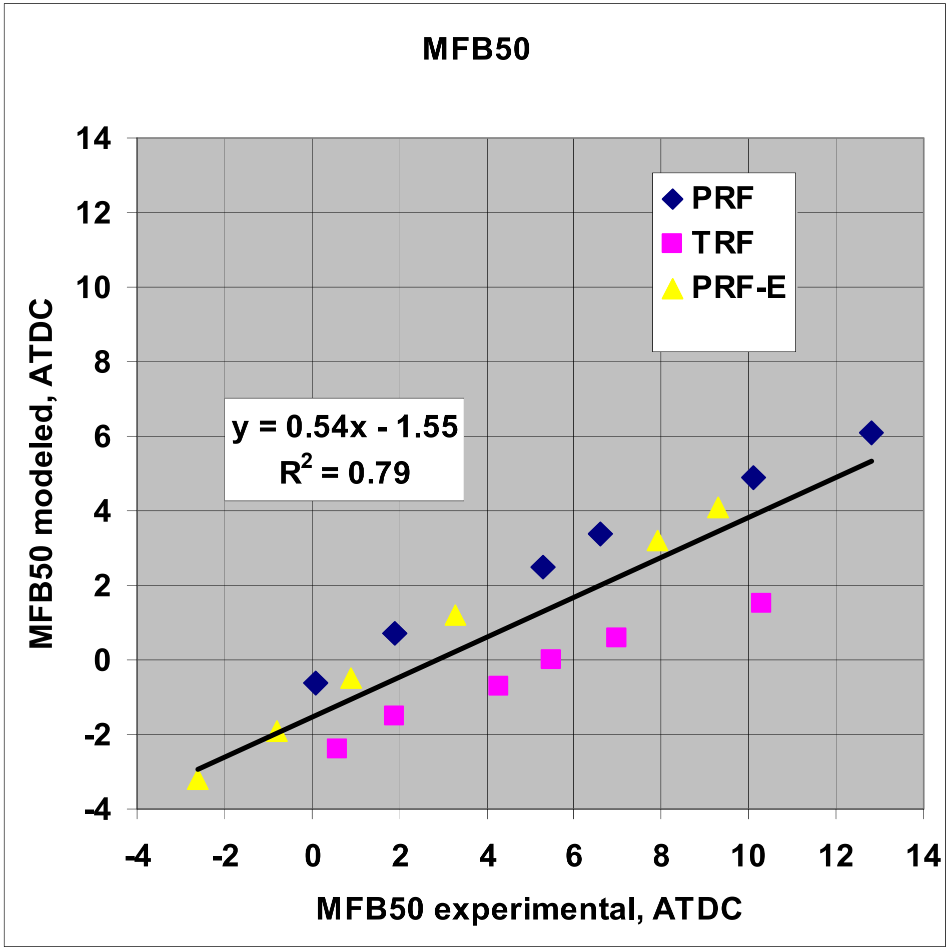
- This research encompassed 18 experimental HCCI engine runs
  - 3 gasoline surrogate blends
  - 6 combustion timings (intake temperatures) per fuel
  - One fuel rate (≈9.1 grams per minute)
  - 1800 rpm
  - 2.4 to 3.2 bar IMEP
- Fuels are
  - PRF, 87 RON
  - TRF, 87 RON
  - PRF + 30% ethanol, 105 RON
- We have much more data, including diesel and bio-diesel, and plan further analysis based on the results of this preliminary study

Multi-zone model used for this presentation

- Chemkin MFC, by Reaction Design
- Combined gasoline ethanol mechanisms, by Reaction Design
  - 1747 species, 8487 reactions
  - Primarily derived from open literature sources
  - Merged, reconciled, and verified by Reaction Design
- Using 5 zone model with heat loss
  - Woschni correlations
    - Coefficients same as SAE 2009-01-0669
  - Details of zones:

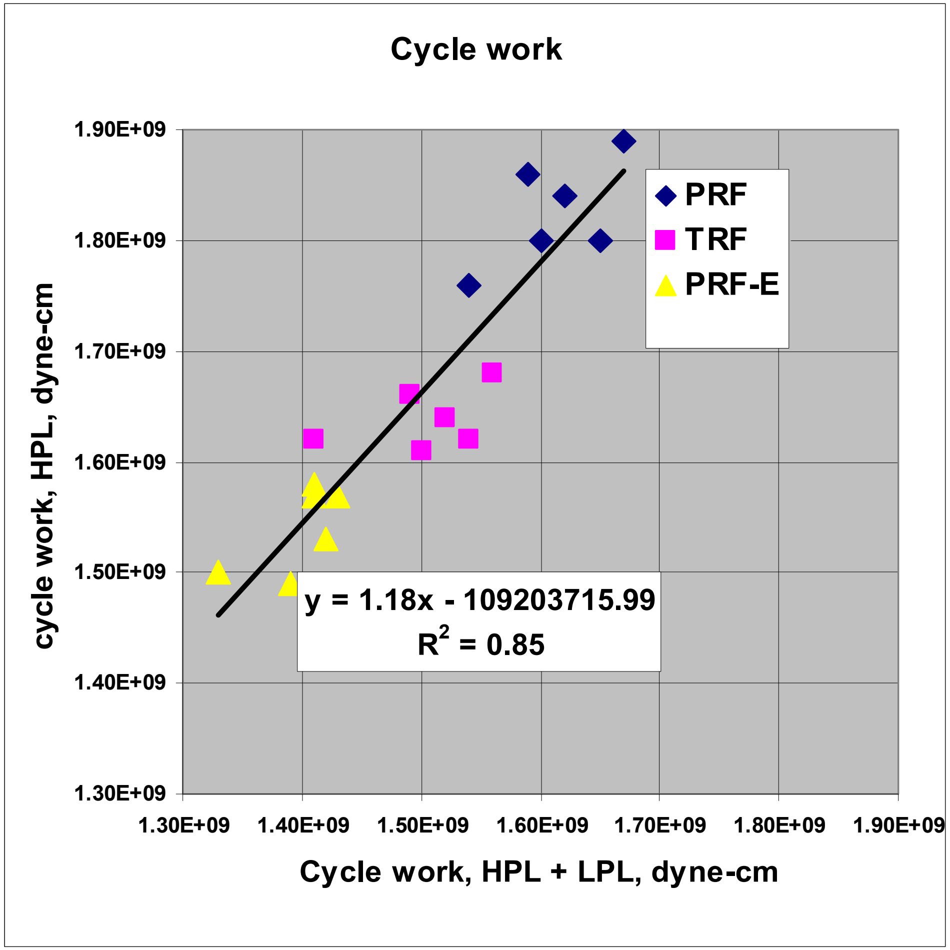
ZONE	% MASS	% SURFACE AREA	S.A./MASS
1	5	45	9.0
2	15	25	1.7
3	20	15	0.8
4	25	10	0.4
5	35	5	0.1

MFB50 match, model to experiment



- Plots show agreement for variables between model and experiment
- Fuels differentiated by symbols
- Single trend line shows good R^2 for all fuels fuels
- Slope not 1:1

Cycle work

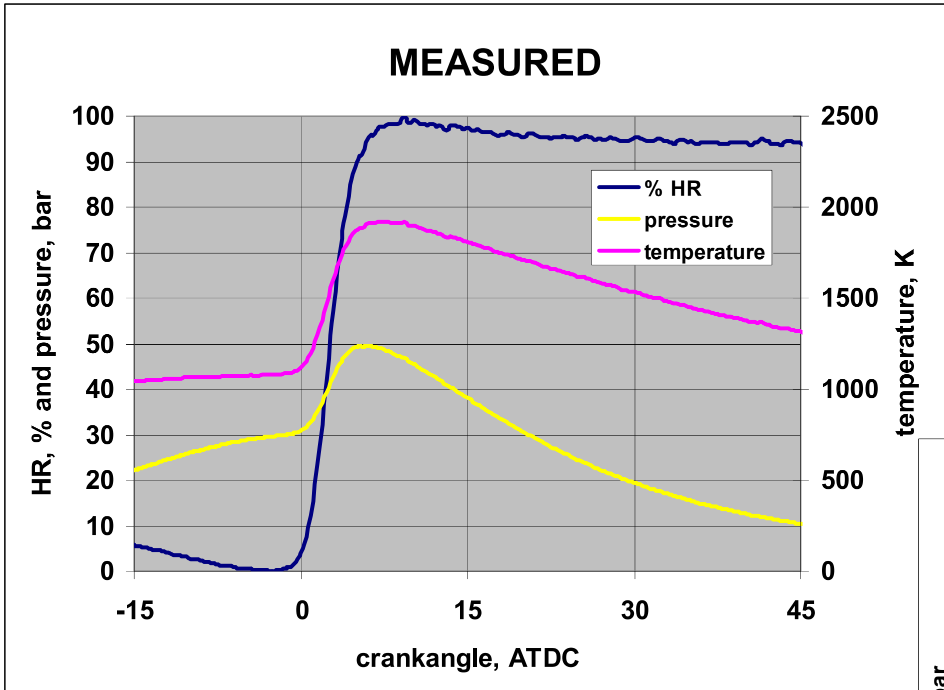


MODELED PRESSURE WORK

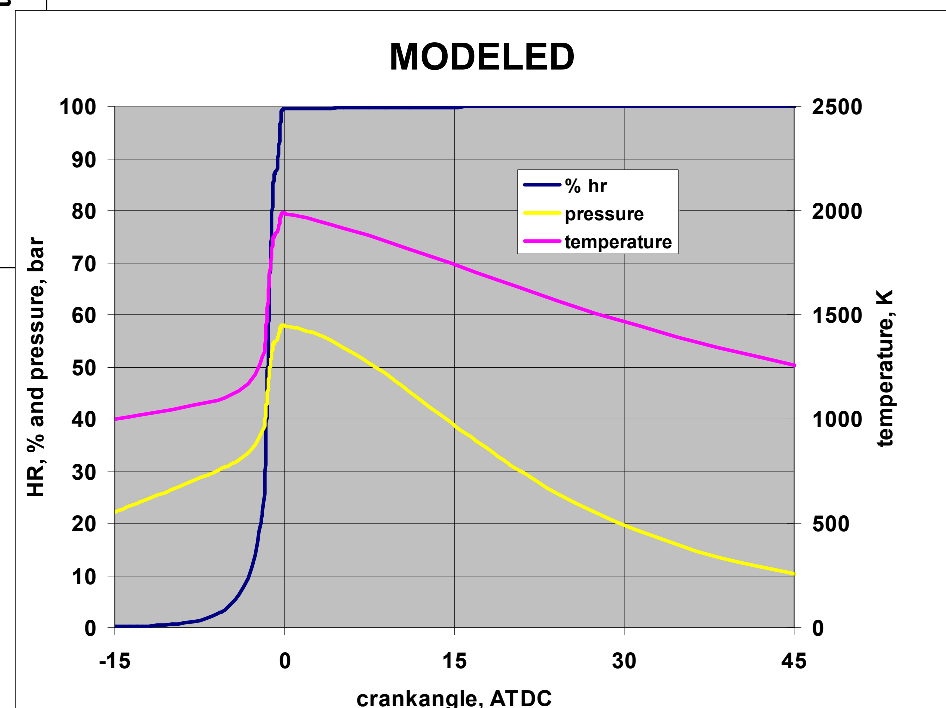
EXPERIMENTAL PRESSURE ANALYSIS

- **Work shows good agreement, need wider range of data**
- **Need to differentiate HPL and LPL work in future experiments**

HR, P, T comparisons, TRF run 2



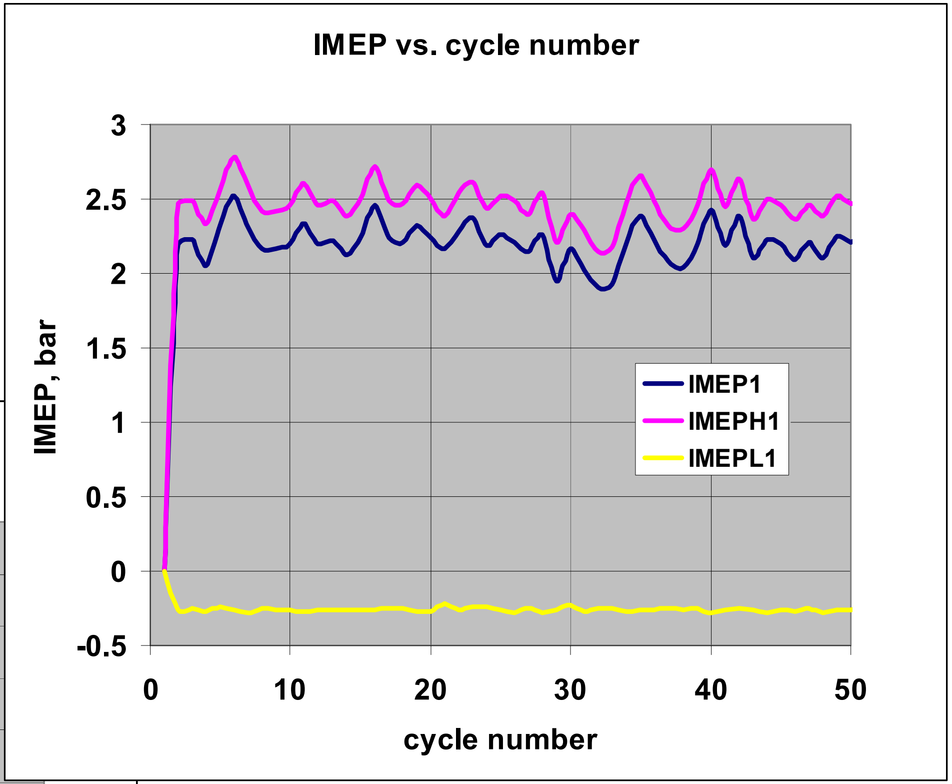
- Model has faster HR
- Temperatures about same
- Model peak pressure higher

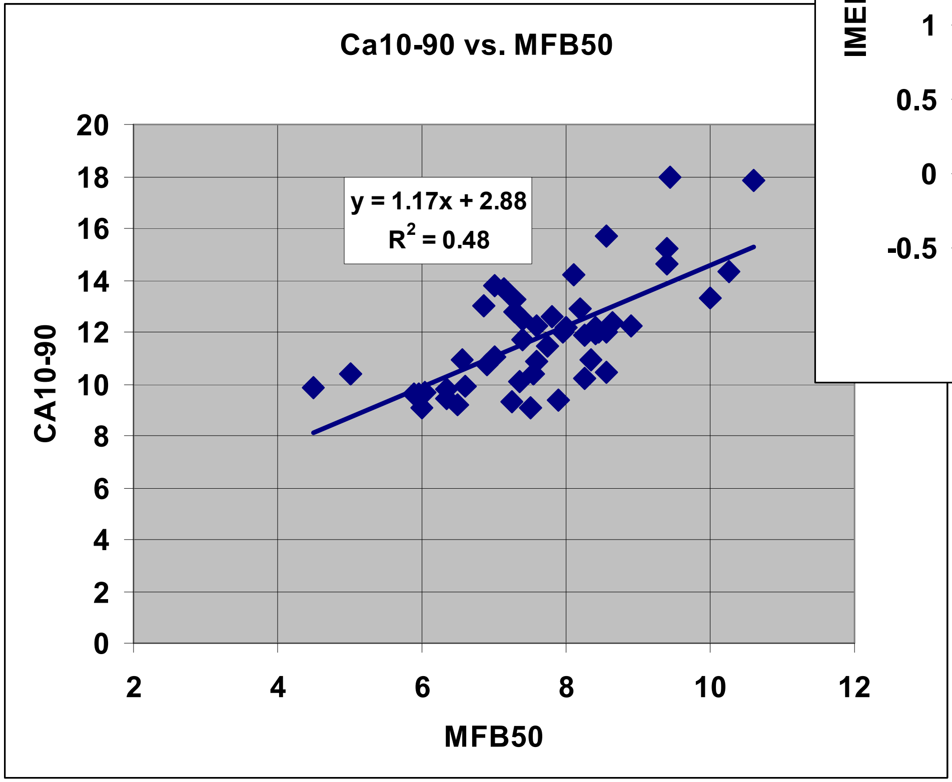


- At this moment, we are also resolving issues related to our experimental heat release
  - More on this topic later

IMEP and combustion data shows cycle to cycle variation

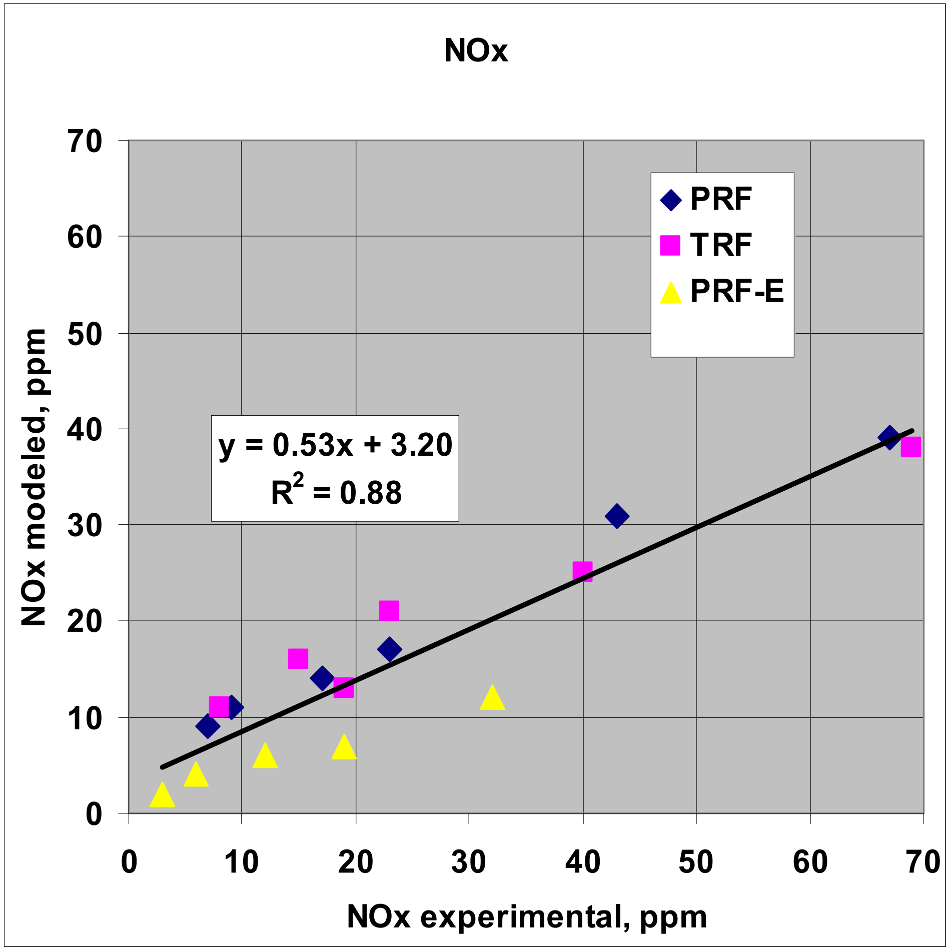
- Cycle variation probably due to fuel flow or gas exchange variations





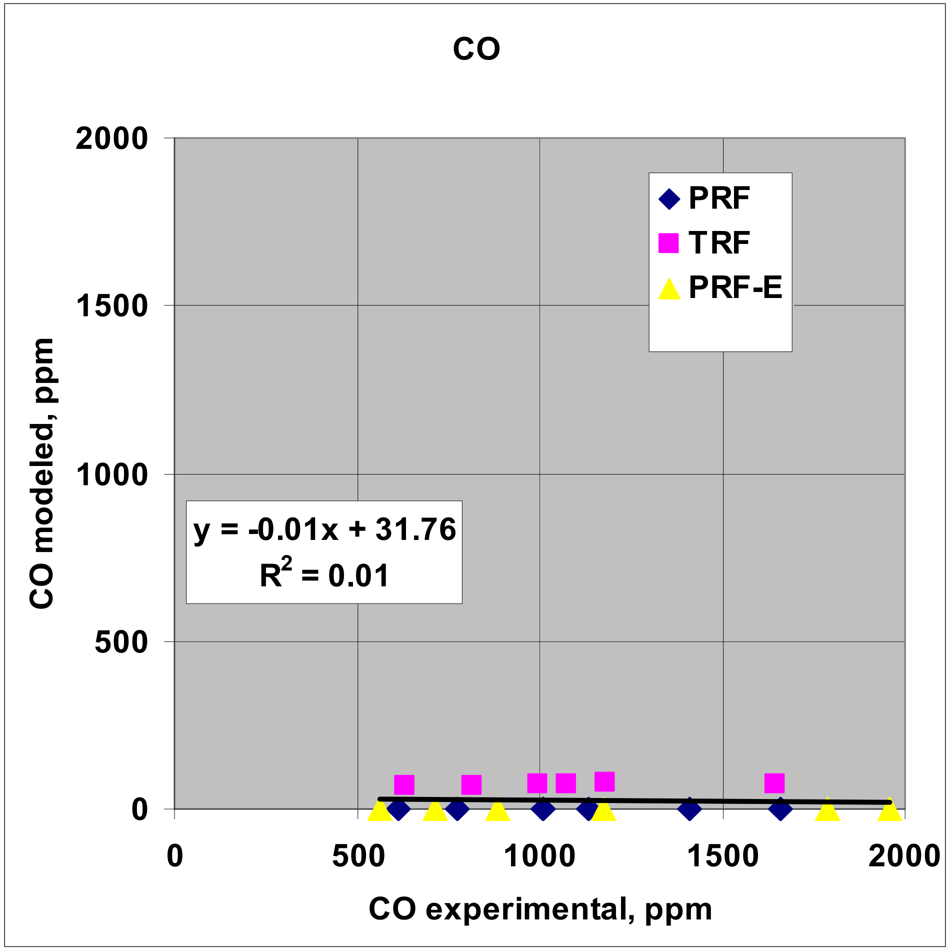
- Shown at 5.7% COV
- Is it more representative to model individual cycles or cycle average?

NOx emissions



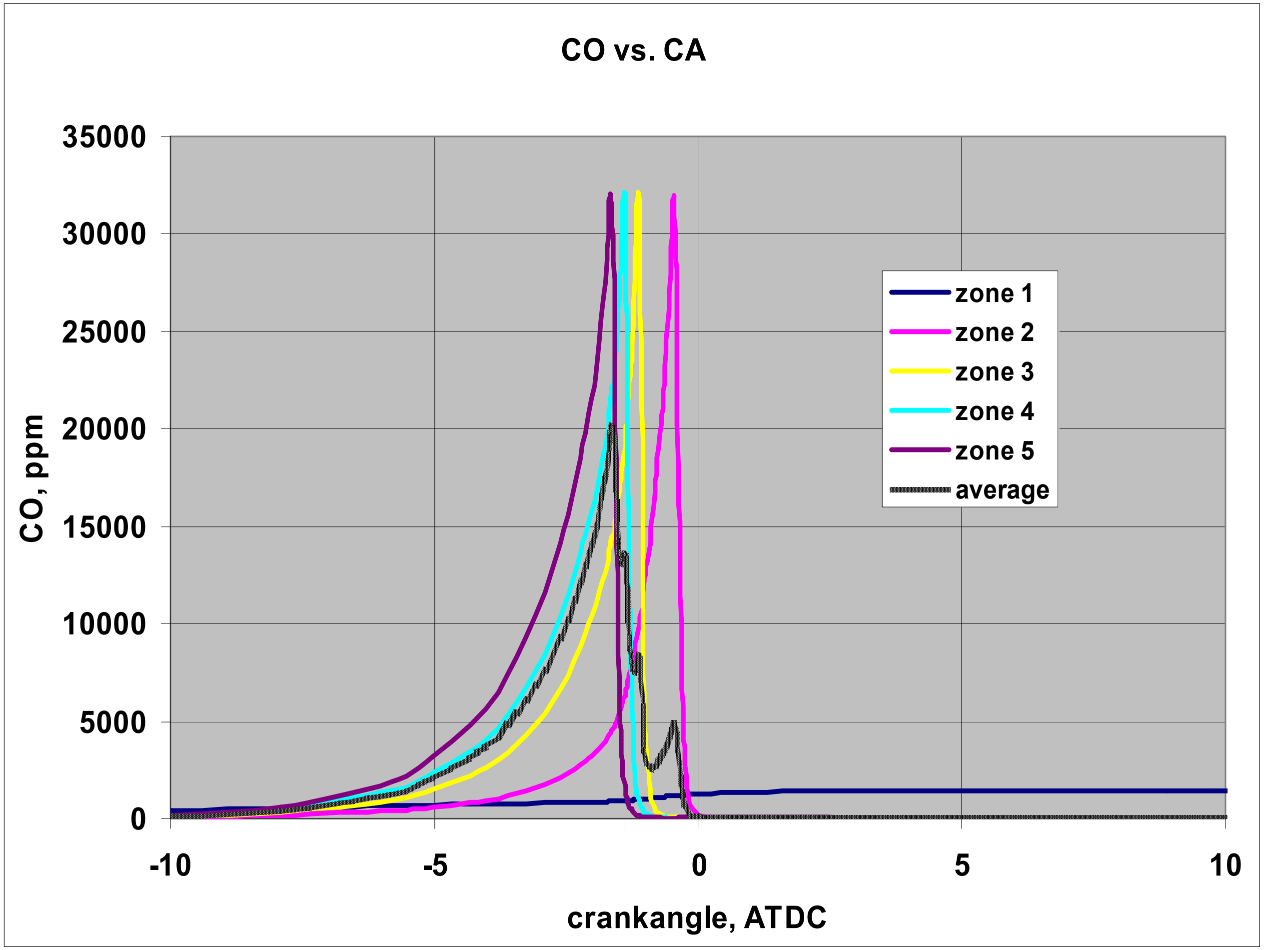
- **NOx emissions follow a definite trend line**
- **Model under-predicts NOx emissions**

CO emissions



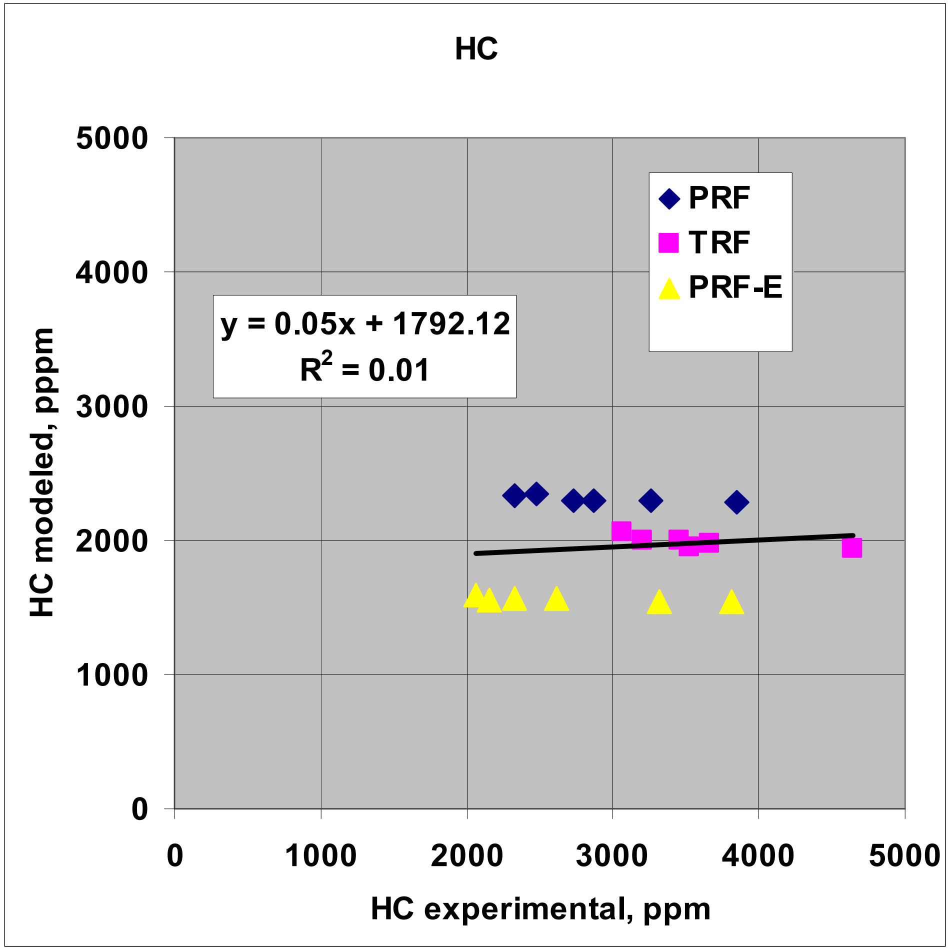
- **Model predicts almost no CO emissions**
- **CO destruction is exothermic and hard to regulate once it starts**
- **5 zone model does not mimic in-cylinder conditions well enough**

Zone CO vs. CA, TRF run 2



- **CO forms as combustion intermediate, destruction is very rapid**
- **In this case, some CO is formed in zone 1 (wall quench zone), which does not undergo combustion**

HC emissions



- It is possible to leave ball park levels of HC in wall quench zone
  - but
- This HC does not follow any trend

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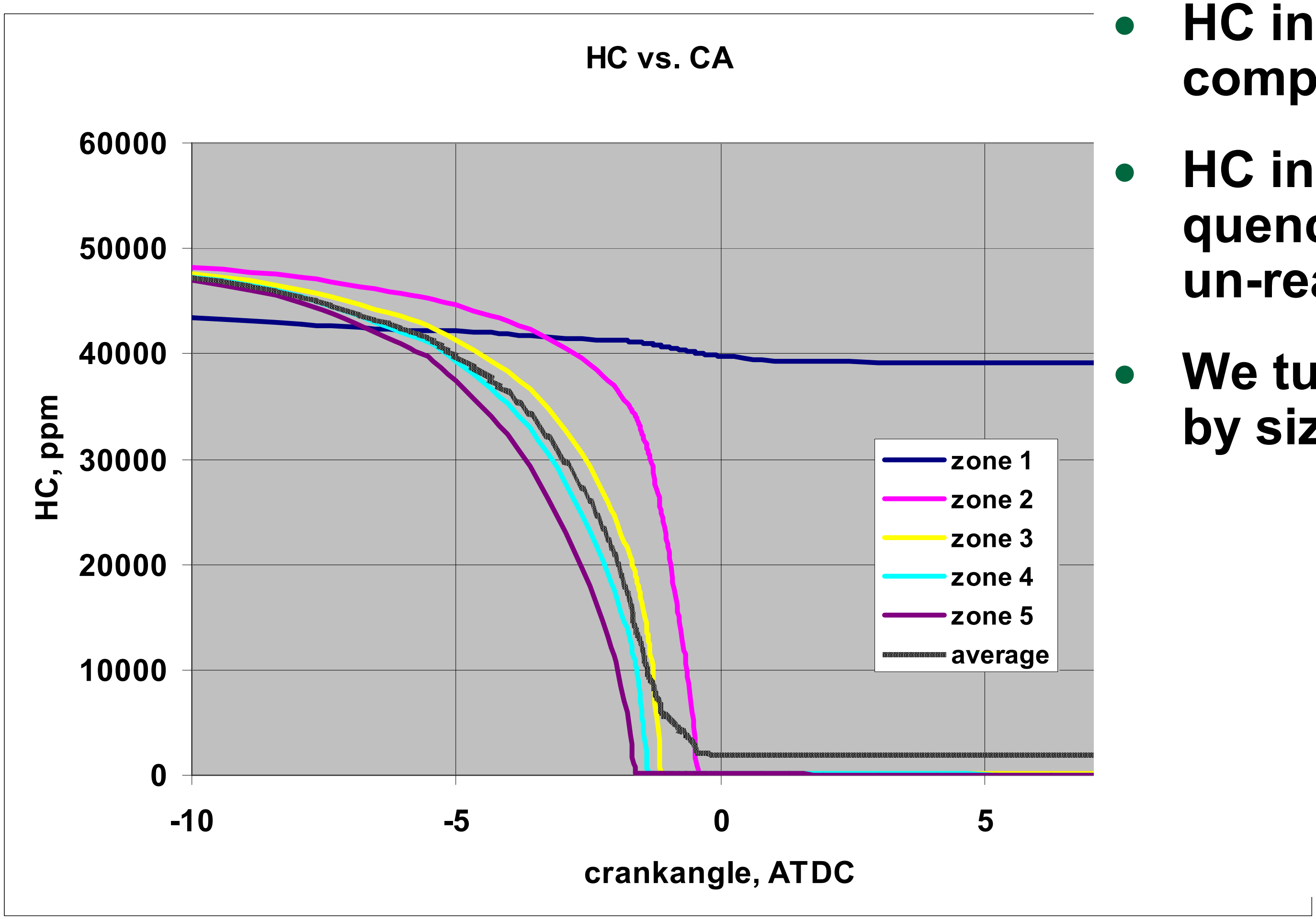
Zone HC vs. CA, TRF run 2



- **HC in hot zones is completely burned**
- **HC in zone 1 (wall quench) is largely un-reacted**
- **We tuned total HC by size of zone 1**

How did we do overall?

VARIABLE	SLOPE	R^2	NOTES
Our goal	1.0	1.0	Perfection!
MFB50, deg. CA	0.54	0.79	
CA10-90, deg. CA	0.12	0.40	
Peak pressure, bar	0.21	0.33	
Peak temperature, K	0.37	0.50	
Work, dyne-cm	1.18	0.85	HPL vs. HPL+LPL
Charge mass, gm.	0.80	0.80	
Oxygen, %	0.81	0.78	Wet vs. dry (≈3.5% corr.)
Carbon dioxide, %	0.82	0.88	Wet vs. dry (≈3.5% corr.)
Nitrogen oxides, ppm	0.53	0.88	Wet vs. wet
Carbon monoxide, ppm	-0.01	0.01	Wet vs. wet
Hydrocarbons, ppm	0.05	0.01	Wet vs. wet
Formalydehyde, ppm	-0.28	0.38	
Acetaldehyde, ppm	-0.16	0.37	

Conclusions

- **The use of a simple, 5 zone engine model for kinetic modeling of fuel effects is not practical**
- **A simple 5 zone model gave fairly good results for work, charge mass, O2, CO_2, NO_x, and MFB50**
- **CO is very difficult to reproduce with a simple model, it's destruction is too rapid**
- **HC can be left behind in a wall quench zone, but this does not represent actual in-cylinder processes**
- **Performing detailed comparisons between experimental data and modeling points out the need for:**
  - **Improving experimental measurements**
  - **Better definition of experimental conditions**
  - **More complex, more realistic engine models**
  - **And probably, better mechanisms**

Experimental improvements underway

- Definition of engine conditions
  - Adding fire-deck temperature and heat flux probes
  - Direct measurement of C/R and TDC
  - Working to improve emissions and flow measurement
  - Reconcile charge mass between measurements and model
  - Cycle resolved gas exchange capability
- Improved heat release
  - Shielded pressure transducers
  - Recording both individual cycle HR and cycle average
  - Reconcile fuel energy per cycle to HR, heat loss, and combustion efficiency