Modeling Dynamical Instability of Homogeneous Charge Compression Ignition (HCCI) in Combustion Engines

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Oak Ridge National Laboratory

Dynamics Days 2008

3-6 January 2008

Knoxville, Tennessee

Sponsor: U.S. DOE, Office of Vehicle Technologies

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Background / Motivation:

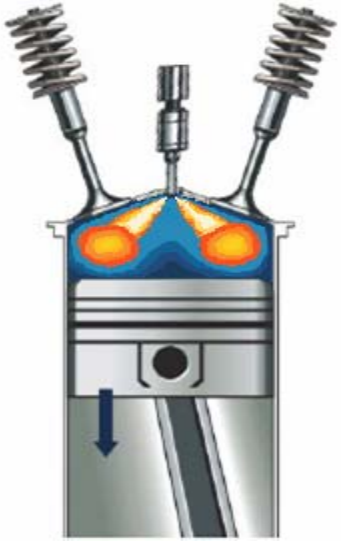
- **There is much interest in utilizing HCCI combustion in transportation engines for reducing nitrogen oxide (NOx) emissions and increasing fuel efficiency**
- **HCCI is fundamentally different from conventional combustion**
  - **Volumetric reaction rather than localized flame front**
  - **Only occurs for limited range of temperature and chemical species concentrations**

Spark-ignition

- **Pre-mixed fuel-air charge**
- **Spark ignition**
- **Flame front propagates through pre-mixed charge**

Diesel

- **Fuel injected into compressed fresh-air charge**
- **Hot air ignites fuel**
- **Relatively stationary diffusion flames**



HCCI

- **Pre-mixed, pre-heated fuel-air charge**
- **Compression ignition**
- **Uniform, spontaneous combustion without flame front**

† Graphics adapted from GM

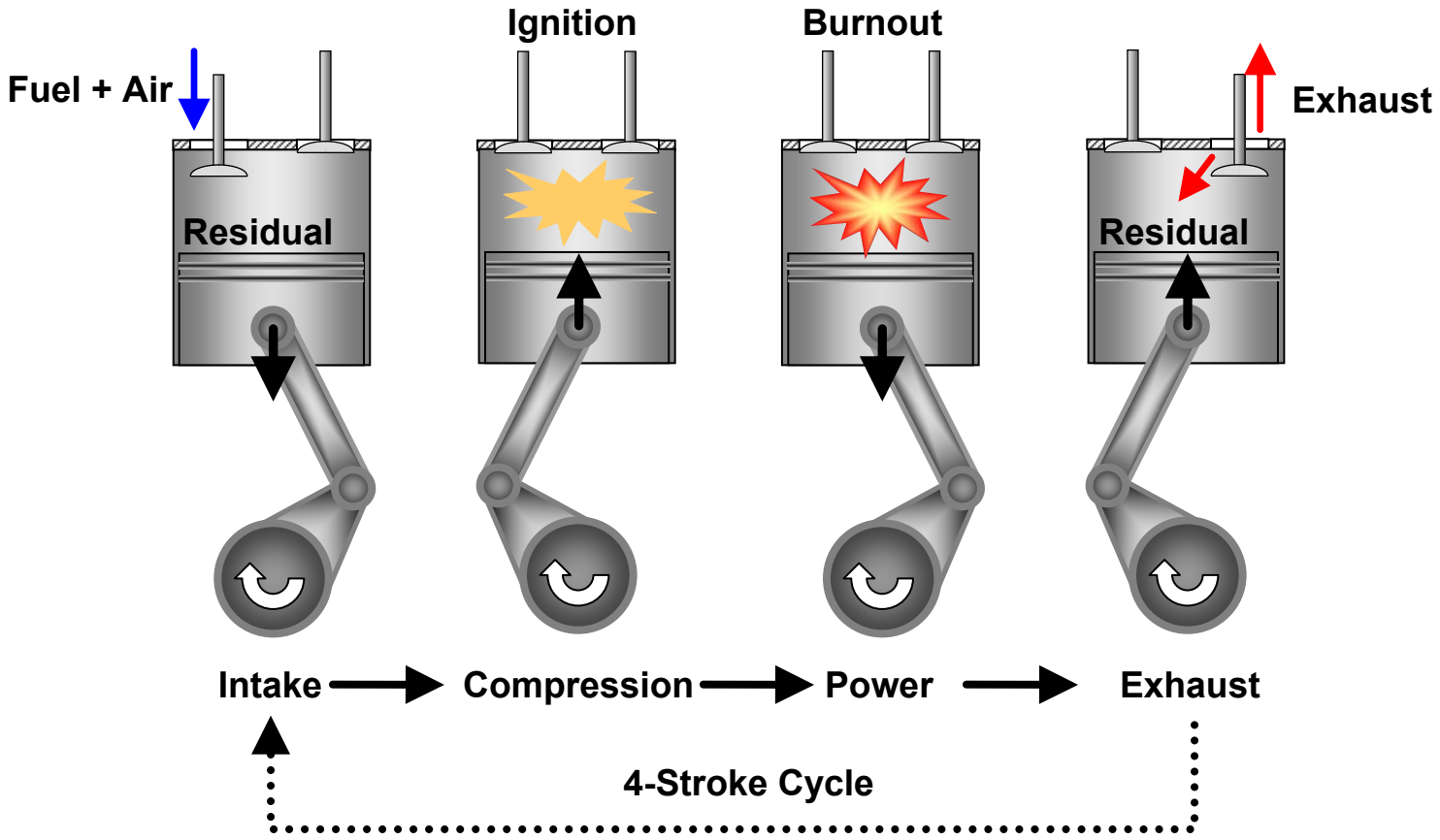
Motivation:

- **In today's engines, stable HCCI only possible for limited range of speed and load**
- **Practical application requires two key developments:**
  - **Rapid switching between HCCI and spark-ignition (SI) combustion**
  - **Expansion of HCCI operating envelope via feedback stabilization**

Study Objectives:

- **Improve understanding of dynamic combustion instability associated with HCCI**
- **Develop simplified combustion models for rapid simulation, diagnostics, and controls**

Engineering Context: The 4-Stroke IC Engine



- In conventional gasoline engines, a spark plug ignites combustion
- HCCI requires residual gas for preheating but no spark plug
- For HCCI, typically >50% of gas in cylinder is residual
- High residual creates strong cycle-to-cycle coupling

Explicit modeling of combustion chemistry and kinetics can be extremely complex

No.	Reaction
1f	O2 + H→OH +O
2f	H2 + O→OH +H
3f	H2 + OH→H2O +H
4f	2OH→H2O +O
5f	2H + M →H2 + M
6f	2O + M →O2 + M
7f	H + OH + M →H2O + M
8f	H + O2 + M →HO2 + M
9f	HO2 + H→2OH
10f	HO2 + H→H2 + O2
11f	HO2 + H→H2O +O
12f	HO2 + O→OH + O2
13f	HO2 + OH→H2O + O2
14f	2HO2 →H2O2 + O2
15f	2OH + M →H2O2 + M
16f	H2O2 + OH→H2O + HO2
17f	CO + OH→CO2 +H
18f	CO + HO2 →CO2 + OH
19f	CO + O + M →CO2 + M
20	CH + O2 →HCO +O
21	CH + CO2 →HCO + CO
22f	CH + H2O→CH2OH
23f	HCO + M →CO + H + M
24f	HCO + O2 →CO + HO2
25f	3-CH2 + H→CH + H2
26f	23-CH2 →C2H2 + H2
27f	3-CH2 + CH3 →C2H4 +H
28f	3-CH2 + O2 →CO + OH +H
29f	3-CH2 + O2 →CO2 + H2
30f	1-CH2 + M →3-CH2 + M

No.	Reaction
31f	1-CH2 + O2 →CO + OH +H
32f	1-CH2 + H2 →CH3 +H
33f	CH2O + M →HCO + H + M
34f	CH2O + H→HCO + H2
35f	CH2O + O→HCO + OH
36f	CH2O + OH→HCO + H2O
37f	CH2O + HO2 →HCO + H2O2
38f	CH3 + O→CH2O +H
39f	CH3 + H→CH4
40	CH3 + OH→CH3O +H
41	CH3 + O2 →CH2O + OH
42f	CH3 + HO2 →CH3O + OH
43f	CH3 + HO2 →CH4 + O2
44	2CH3 →C2H4 + H2
45f	2CH3 →C2H6
46f	CH3O + M →CH2O + H + M
47f	CH3O + H→CH2O + H2
48f	CH3O + O2 →CH2O + HO2
49f	CH2OH + M →CH2O + H + M
50f	CH2OH + H→CH2O + H2
51f	CH2OH + O2 →CH2O + HO2
52f	CH4 + H→H2 + CH3
53f	CH4 + OH→H2O + CH3
54f	HCCO + H→3-CH2 + CO
55	HCCO + O→2CO +H
56f	C2H2 + O2 →HCCO + OH
57f	C2H2 + O→3-CH2 + CO
58f	C2H2 + O→HCCO +H
59f	C2H3 →C2H2 + H
60	C2H3 + O2 →CH2O + HCO

No.	Reaction
61f	C2H4 + M →C2H2 + H2 + M
62f	C2H4 + H→C2H3 + H2
63f	C2H4 + OH→C2H3 + H2O
64f	C2H5 →C2H4 + H
65f	C2H5 + H→2CH3
66f	C2H5 + O2 →C2H4 + HO2
67	C2H6 + H→C2H5 + H2
68	C2H6 + OH→C2H5 + H2O
69	C2H6 + CH3 →C2H5 + CH4
70	C3H4 + OH→CH2O + C2H3
71	C3H4 + OH→HCO + C2H4
72f	C3H5 →C3H4 +H
73f	C3H5 + H→C3H4 + H2
74f	C3H5 + O2 →C3H4 + HO2
75f	C3H6 →C2H3 + CH3
76f	C3H6 + H→C3H5 + H2
77f	C3H6 + OH→C2H5 + CH2O
78f	C3H6 + OH→C3H5 + H2O
79	C3H6 + CH3 →C3H5 + CH4
80f	N-C3H7 →CH3 + C2H4
81f	N-C3H7 →H + C3H6
82f	N-C3H7 + O2 →C3H6 + HO2
83f	1-C4H8 →C3H5 + CH3
84f	1-C4H8 + OH→N-C3H7 + CH2O
85	P-C4H9 →C2H5 + C2H4
86	1-C5H11 →C2H4 + N-C3H7
87	C6H11 →C3H5 + C3H6
88	1-C6H12 →N-C3H7 + C3H5
89	1-C6H12 + H→C6H11 + H2
90	1-C6H12 + OH→C6H11 + H2O

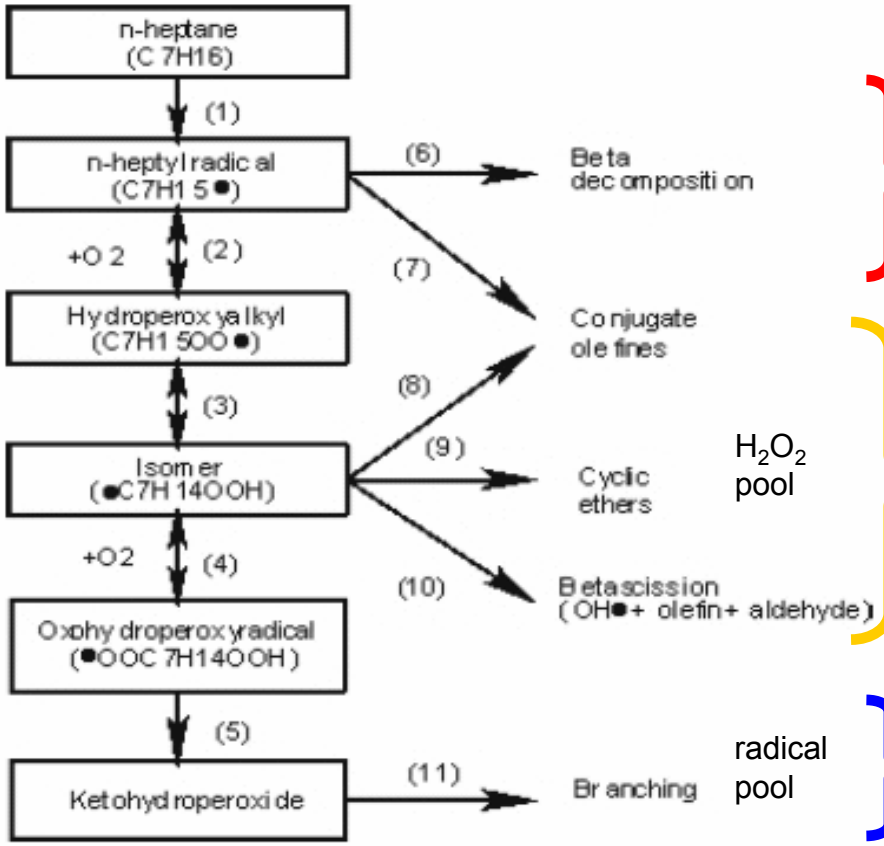
No.	Reaction
91	1-C7H15 →1-C5H11 + C2H4
92	2-C7H15 →P-C4H9 + C3H6
93	2-C7H15 →1-C6H12 + CH3
94	1-C7H15 →2-C7H15
95	2-C7H15 →1-C7H15
96	N-C7H16 →P-C4H9 + N-C3H7
97	N-C7H16 + H→1-C7H15 + H2
98	N-C7H16 + H→2-C7H15 + H2
99	N-C7H16 + OH→1-C7H15 + H2O
100	N-C7H16 + OH→2-C7H15 + H2O
101	N-C7H16 + HO2 →1-C7H15 + H2O2
102	N-C7H16 + HO2 →2-C7H15 + H2O2
103	N-C7H16 + O2 →1-C7H15 + HO2
104	N-C7H16 + O2 →2-C7H15 + HO2
105f	1-C7H15 + O2 →RO2
105b	RO2 →1-C7H15 + O2
106f	2-C7H15 + O2 →RO2
106b	RO2 →2-C7H15 + O2
107	RO2 →RO'2H
108	R'O2H + O2 →O2R'O2H
109	O2R'O2H→HO2R"O2H
110	HO2R"O2H→OR"O2H + OH
111	OR"O2H→OR"O + OH
112	OR"O→CH2O + 1-C5H11 + CO

+ Selected reverse reactions

'Skeletal' *n*-heptane mechanism by Liu *et al.* (2004)[†]: 43 species, 185 reactions

[†] ***Combustion and Flame*, 137, pp 320-329.**

Chemical Context: Parallel reaction pathways depend strongly on temperature and species



High T (T>900K)

Branching chains (higher rate)

Ex: $H_2O_2+M \rightarrow OH^*+OH^*+M$

Intermediate T (800K<T<900K)

Propagating chains (lower rate)

Ex: $^*C_7H_{14}OOH \rightarrow C_7H_{14}+HO_2^*$

$Alkane+HO_2^* \rightarrow Alkyl^*+H_2O_2$

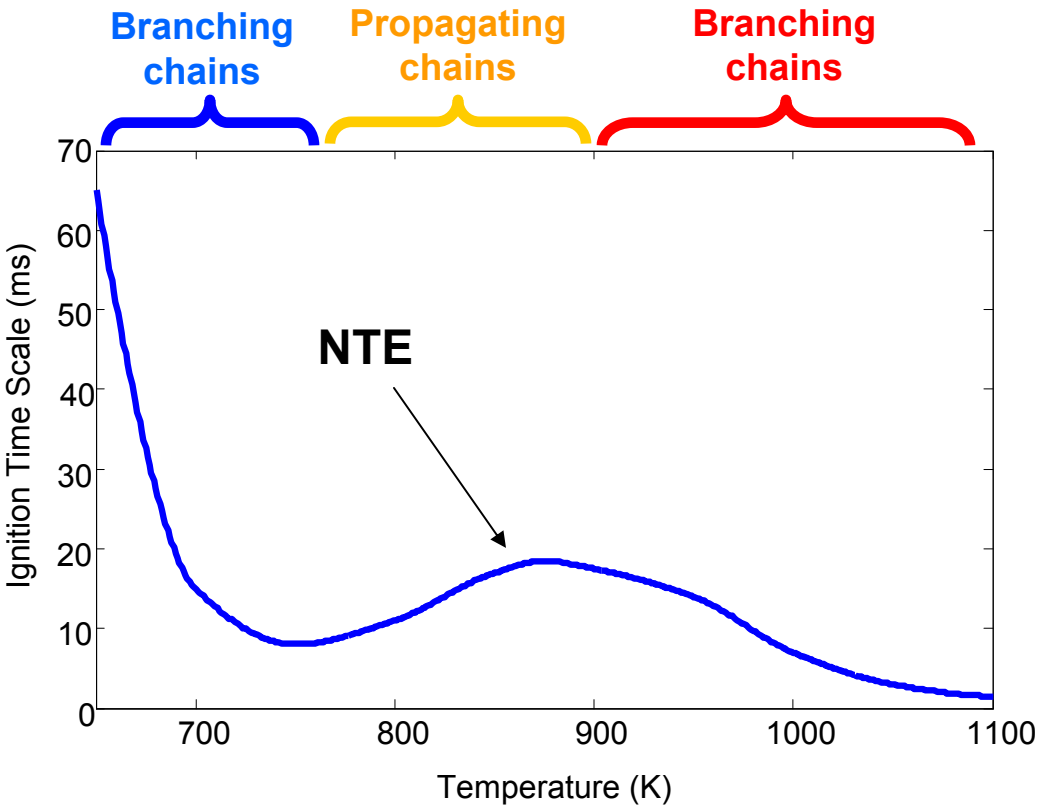
Low T (700K<T<800K)

Branching chains (higher rate)

Ex: Ketohydroperoxide → R1*+R2*

As T increases, reaction rate rises, falls, and rises again as available pathways change. This creates the Negative Temperature Effect (NTE).

However, numerical studies of HCCI mechanisms reveal relatively simple global behavior



***n*-heptane mechanism from previous slide. Stoichiometric mixture, 8 atm and an inert to oxygen mole ratio of 5. Curve shifts with pressure and dilution, but basic features are preserved over wide range of conditions.**

'Low-Order' Modeling of HCCI Dynamics

- **Objective: Capture main features of cyclic variation in combustion (*i.e.*, HCCI instability associated with cycle-by-cycle residual coupling)**
- **Assumptions:**
  - **Global mass and/or heat balances used to generate mapping functions**
  - **Combustion kinetics approximated as global reaction rates that depend on temperature and gas composition at key points in the compression and/or combustion strokes**
  - **Iterating map over a range of residual (EGR) reveals regions of stability/instability**

Proposed HCCI Mapping Function

$$z(i+1) = r\left(1-\eta_1(i)\right)\left(1-\eta_2(i)\right)\left(1+z(i)\right)$$

- **Based on fuel-air mass balance**
- ***z(i)* = residual unburned fuel-air returning to cycle *i* (normalized by the fresh air-fuel mass)**
- ***r* = fraction of the exhaust being recycled in the EGR**
- **$\eta_1(i)$, $\eta_2(i)$ = fractional conversions of combined fuel-air mixture in compression and power strokes in cycle *i*, respectively**

Additional constraints/assumptions:

- **Stoichiometric fueling (equivalent amounts of air and fuel fed)**
- **Throttle adjusted for constant feed rate for fuel and air as EGR varies**
- **Combustion split between compression and power strokes**
- **Compression stroke heating is dominant factor controlling temperature at start of power stroke**

HCCI Mapping Function Details (1)

Burn fraction during stage 1:

$$\eta_1(i) = k_1 \frac{z(i)}{1+z(i)}$$

- k_1 = compression stroke (stage 1) burn rate constant (0-1), fixed for given engine and speed
- Stage 1 burning proportional to fraction of residual unburned fuel

Mixture temperature at start of stage 1 (prior to compression):

$$T_m = (1-r)T_a + rT_e$$

- T_a = air-fuel feed temperature
- T_e = exhaust temperature

Temperature at beginning of stage 2 (after compression and stage 1 combustion):

$$T^*(i) = T_m\, R^{\gamma-1} - h_1\left(T_m - T_a\right) + \eta_1(i)\left(1+z(i)\right)\left(1-r\right)\Delta T$$

- R = compression ratio
- γ = ratio of constant pressure and constant volume heat capacities
- h_1 = wall heat transfer coefficient
- ΔT = adiabatic heating from combustion reaction

HCCI Mapping Function Details (2)

Burn fraction during stage 2:

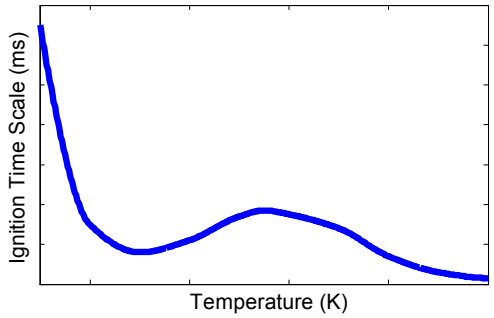
$$\eta_2(i) = 1 - \exp\left[\frac{\ln(0.9)}{(t_2/\tau)^{m+1}}\right]$$

- t_2 = time interval for power stroke burn (stage 2)
- τ = kinetic reaction time scale
- m = Wiebe profile constant
- Stage 2 burning follows Wiebe reaction profile

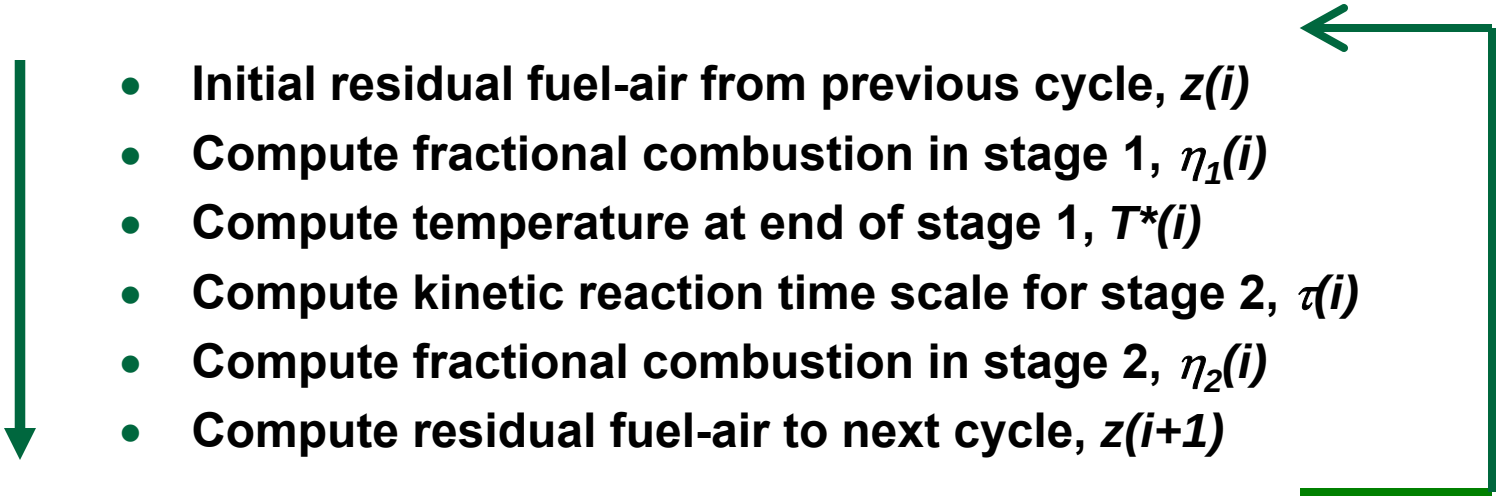
$$\ln(\tau) = aT^{*3} + bT^{*2} + cT^{*} + d + \frac{e}{T^{*}}; \qquad T^{*} < 1100K$$

$$\ln(\tau) = p + q\ln(T^{*}); \qquad T^{*} \geq 1100\,K$$

- a, b, c, d, e, p, q = constants determined by fitting results from numerical simulations of skeletal mechanism at average pressure of power stroke for a range of T^{*}



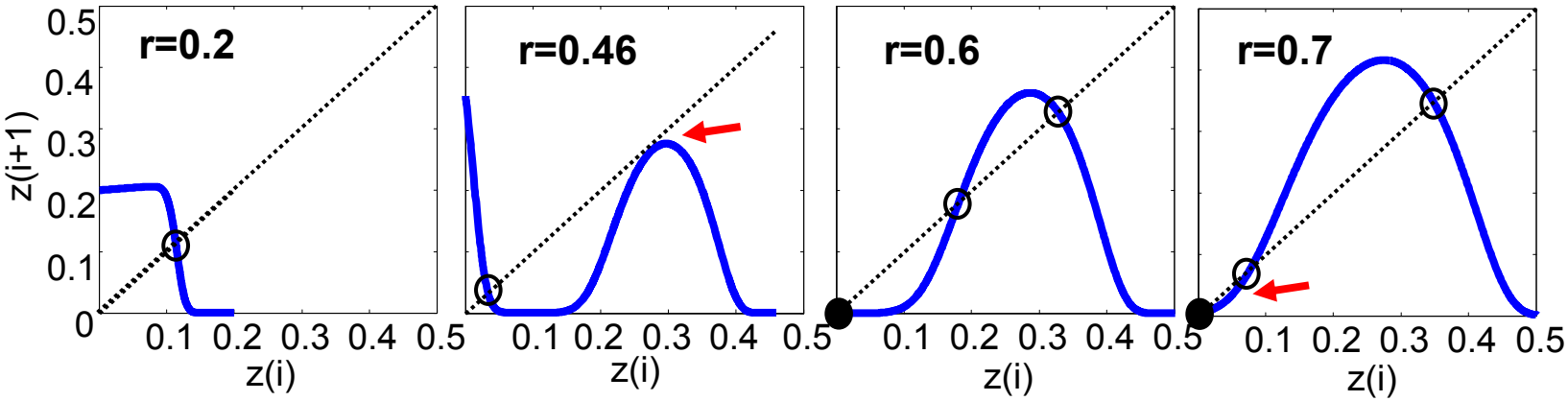
Iterating the HCCI Mapping Function



- **Initial residual fuel-air from previous cycle, *z(i)***
- **Compute fractional combustion in stage 1, $\eta_1(i)$**
- **Compute temperature at end of stage 1, *T*(i)***
- **Compute kinetic reaction time scale for stage 2, $\tau(i)$**
- **Compute fractional combustion in stage 2, $\eta_2(i)$**
- **Compute residual fuel-air to next cycle, *z(i+1)***

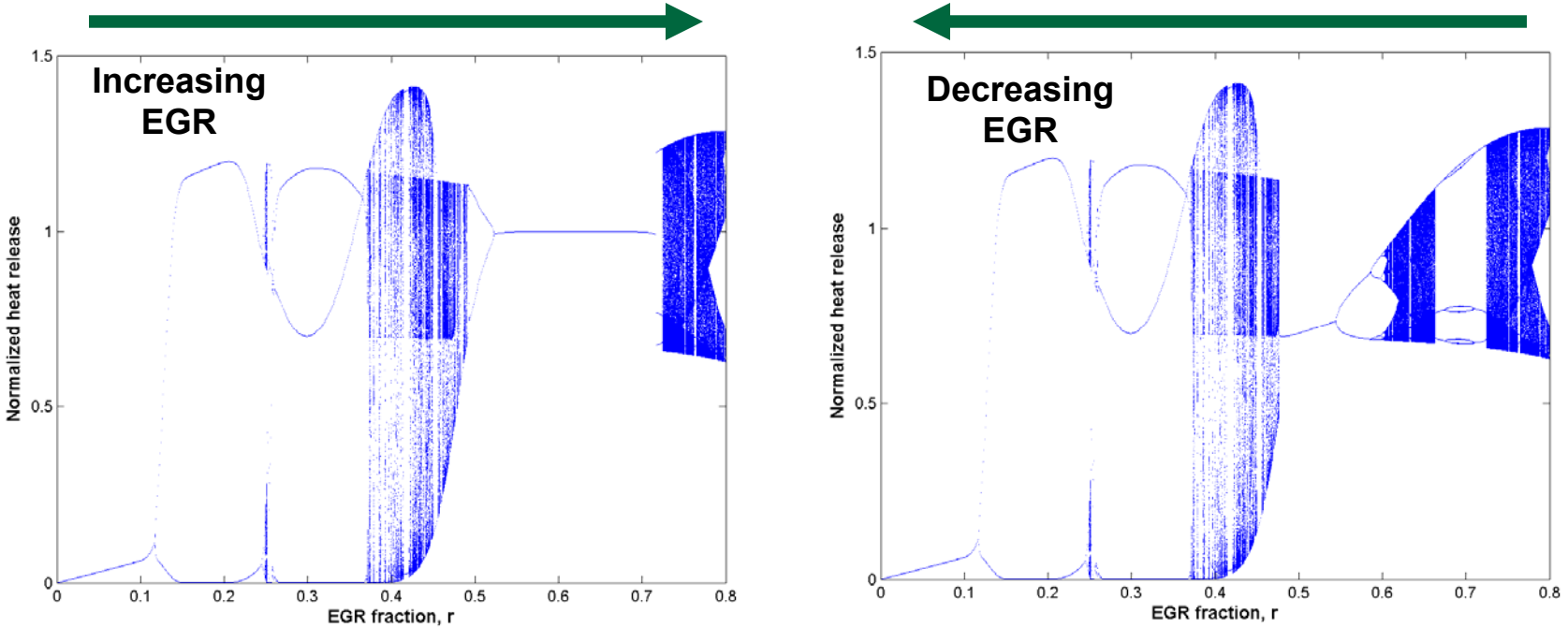
Note: All parameters except k_1 from engine specs, engineering correlations, or chemical kinetics.

HCCI Map Dynamics (1)



- **Solid circles (●) are stable fixed points**
- **Open circles (○) are unstable fixed points**
- **Red arrows (←) indicate tangent bifurcations**
- **At *r* = 0.6, chaos and a stable fixed point co-exist**

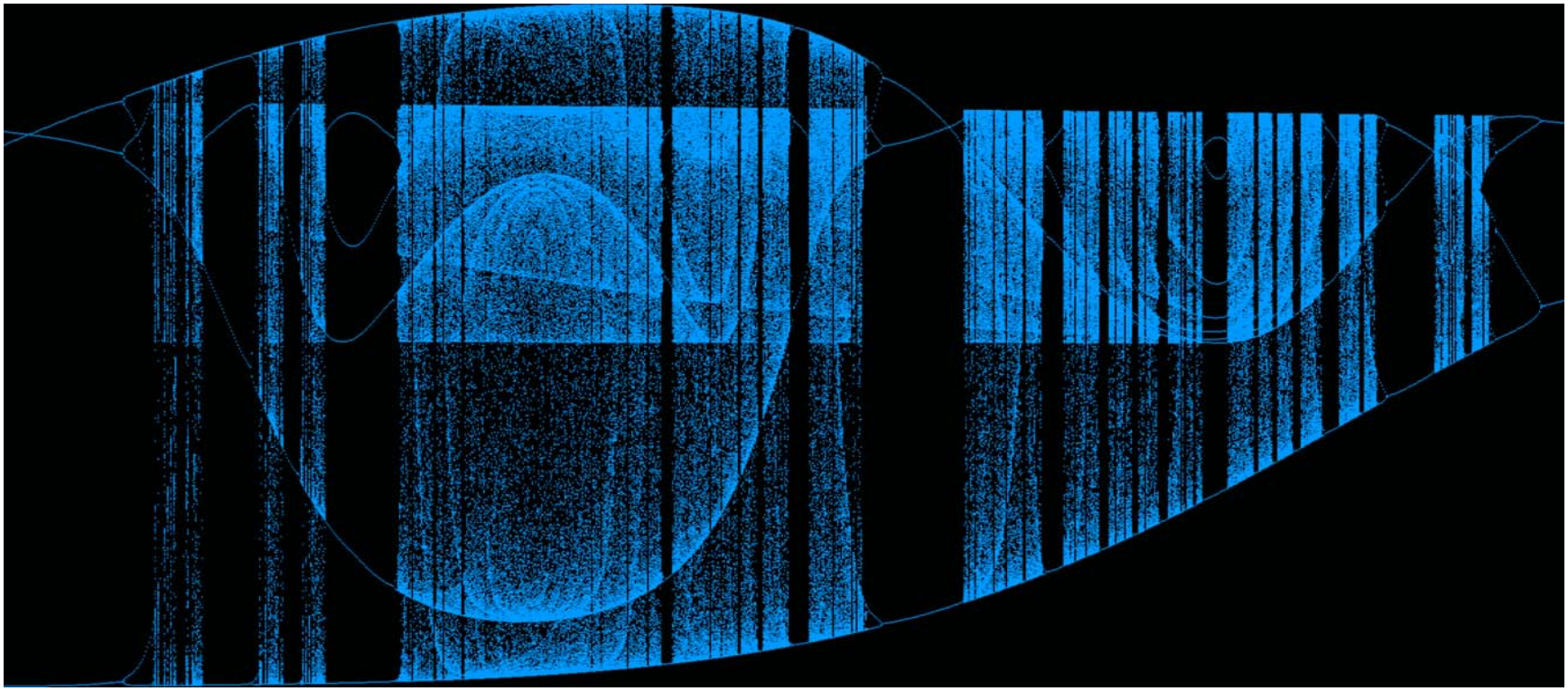
HCCI Map Dynamics (2)



Experiments actually measure heat release, *HR(i)*, which is related to *z(i)* by:

$$HR(i) = \left[\eta_1(i) + \eta_2(i) - \eta_1(i)\,\eta_2(i)\right]\left[1 + z(i)\right]$$

HCCI Map Dynamics (2)



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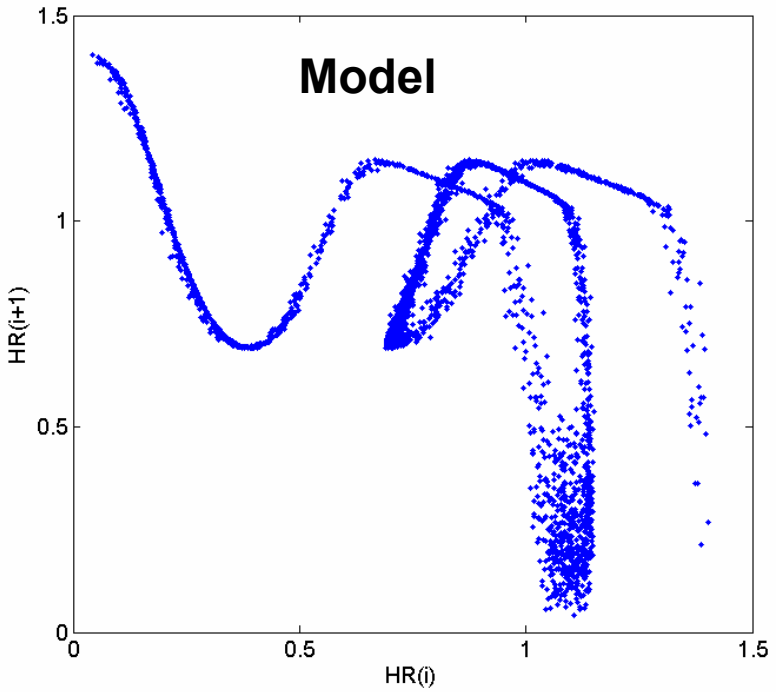
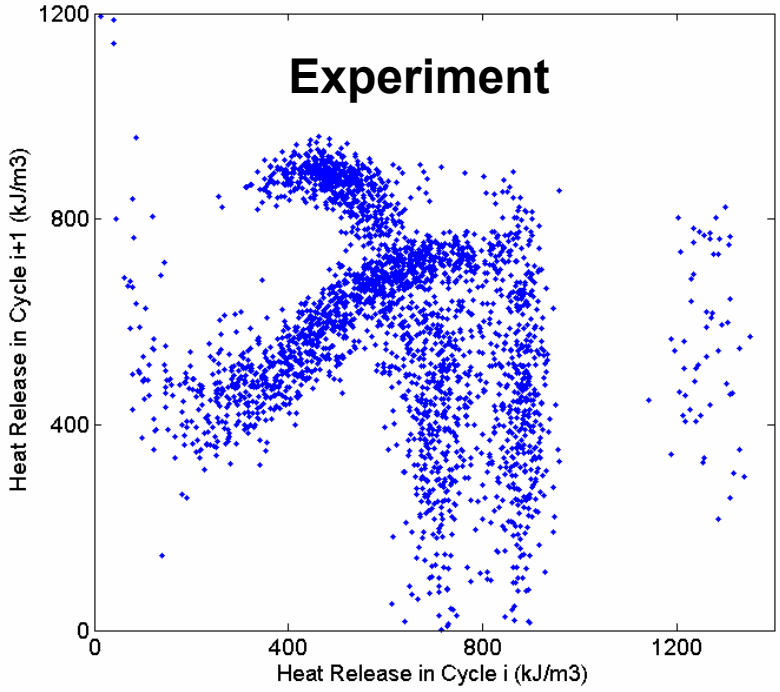
Comparison of HCCI Map with Experiment

***r* = ~46%**



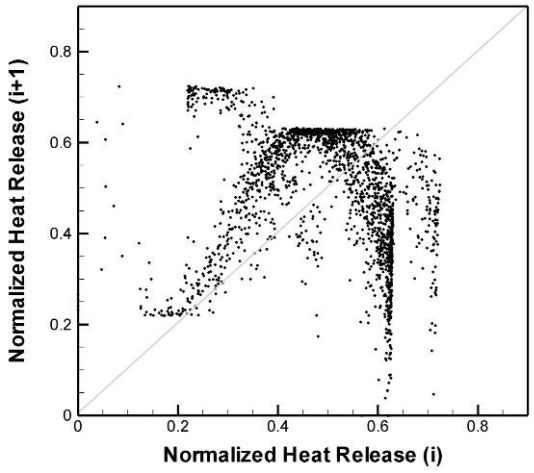


For model, dynamic noise added via $r = r_o + \mathcal{N}(0,\sigma)$, σ = 0.01. Reflects perturbations from background (*e.g.*, flow turbulence, valve chatter).

Future Work

- **Add spark-ignition mechanism for SI-HCCI transition**
- **Improve approximations for detailed kinetics**
- **Systematically explore SI-HCCI transition with experimental engines**
  - **Alternative fuel effects**
  - **Potential control parameters**
  - **Data-derived kinetics**
- **Develop and test on-line diagnostics and controls**

Map from empirical kinetics



Experiment