Mechanism reduction strategies for multicomponent gasoline surrogate fuels

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Introduction

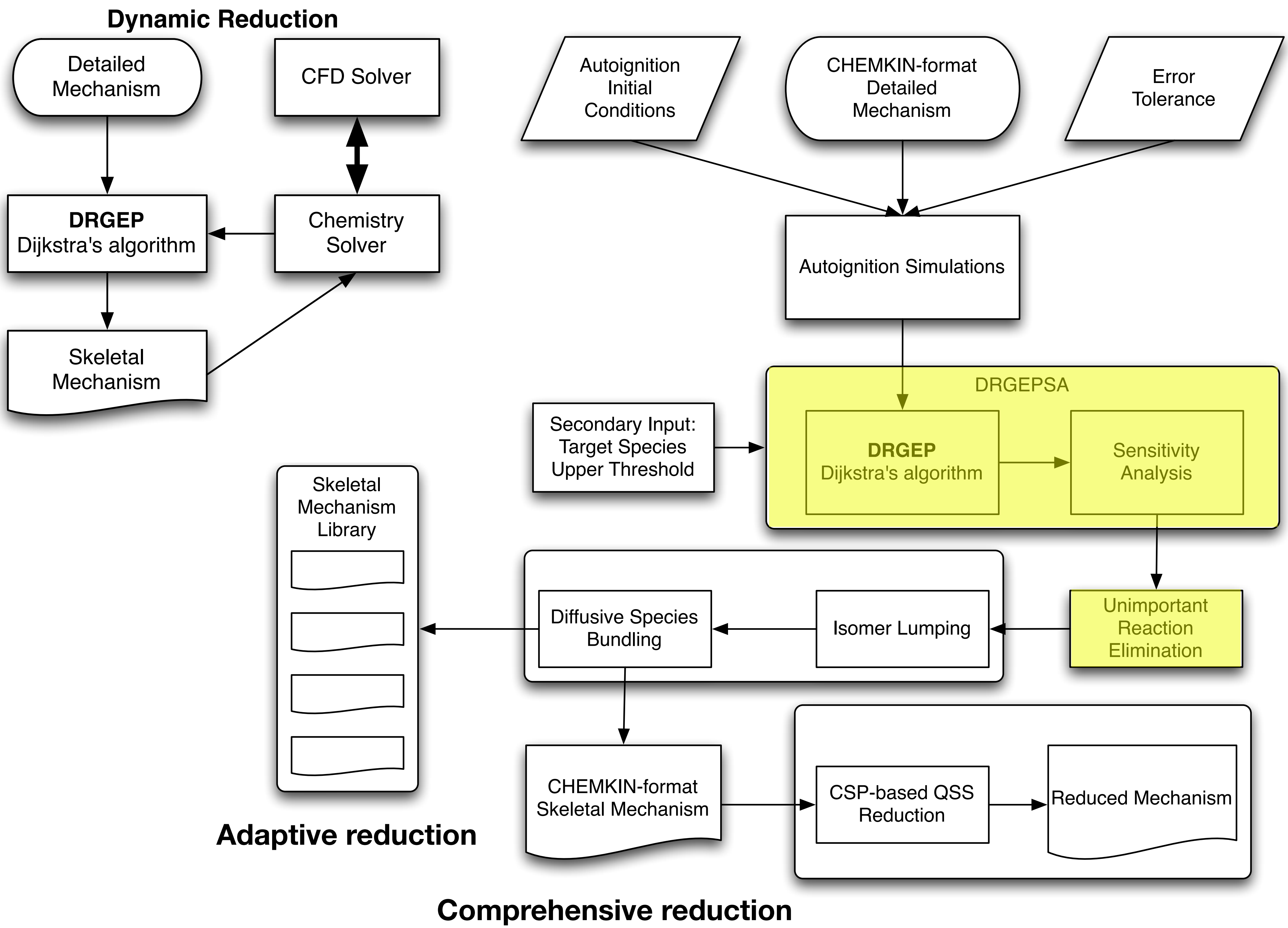
- Why is this research needed?
- Need accurate chemistry model for simulations of engine/burner combustion
- Limited by mechanism size:
  - LLNL gasoline: 1550 species & 6000 reactions
  - LLNL diesel: 2800 species & 11000 reactions
  - LLNL biodiesel: 3300 species & 10800 reactions
  - Jet-A: 2115 species & 8157 reactions (Dooley et al. *CNF* 2010)

Mechanism Reduction

Skeletal reduction: elimination of unimportant species and reactions

- Directed Relation Graph (**DRG**): Lu and Law 2005
  - Graph reaction pathways: Bendtson, Glarborg, Dam-Johansen 2001
- DRG with Error Propagation (**DRGEP**): Pepiot-Desjardins and Pitsch 2005 & 2008
- DRG-aided Sensitivity Analysis (**DRGASA**): Lu and Law 2007
- DRGEP with Sensitivity Analysis (**DRGEPSA**): Niemeyer, Raju, and Sung 2010
- Path Flux Analysis (**PFA**): Sun et al. 2010

Reduction Strategies



Objectives

- Demonstrate reduction capability of DRGEPSA + reaction elim. on large TRF mechanism
  - Accurate & efficient DRGEP search algorithm
- Discuss strategies for reduction of ternary mixture
  - Can a single mixture point produce skeletal mechanisms accurate over other conditions?

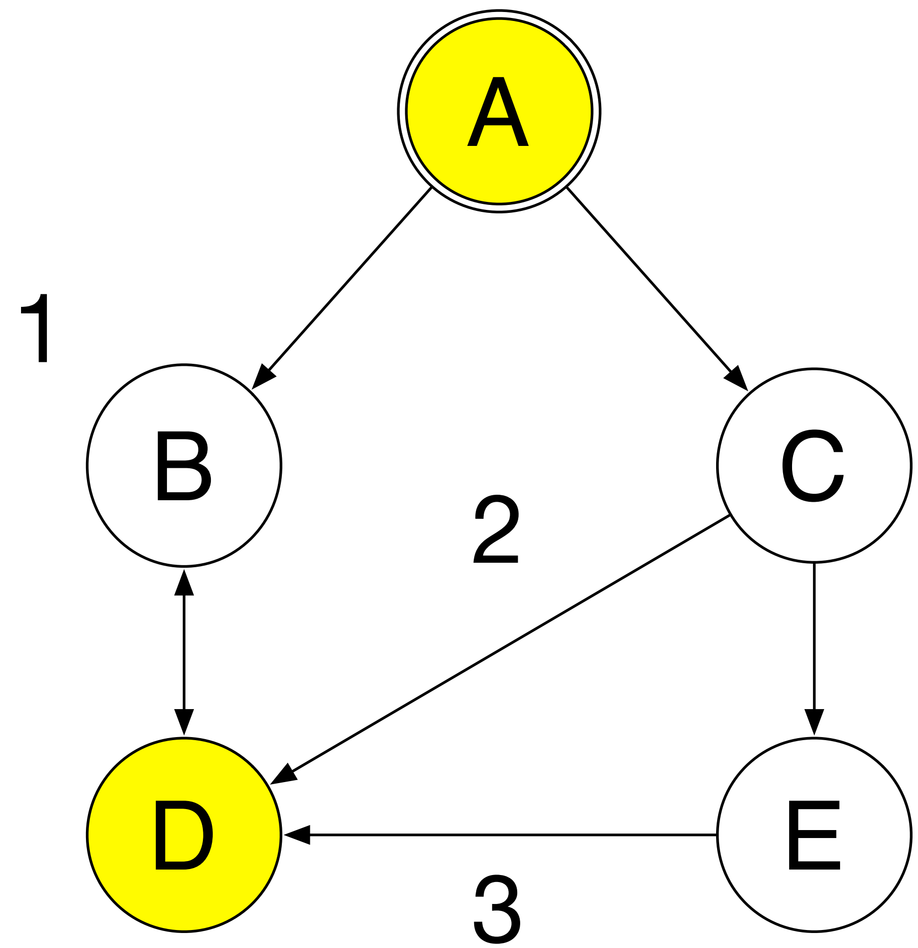
DRG/DRGEP

- Graph-theory-based methods to identify unimportant species for removal
- Species are nodes, connections represent species dependencies
- Target species: fuel, oxidizer, important radicals
- Unimportant connections trimmed using error threshold

DRGEPSA

- DRGEP as presented originally by Pepiot-Desjardins & Pitsch *CNF* 2008
  - Includes coefficient scaling
- DRGEPSA: see Niemeyer, Sung, Raju *CNF* 2010
- See current conference paper as well

DRGEP Method

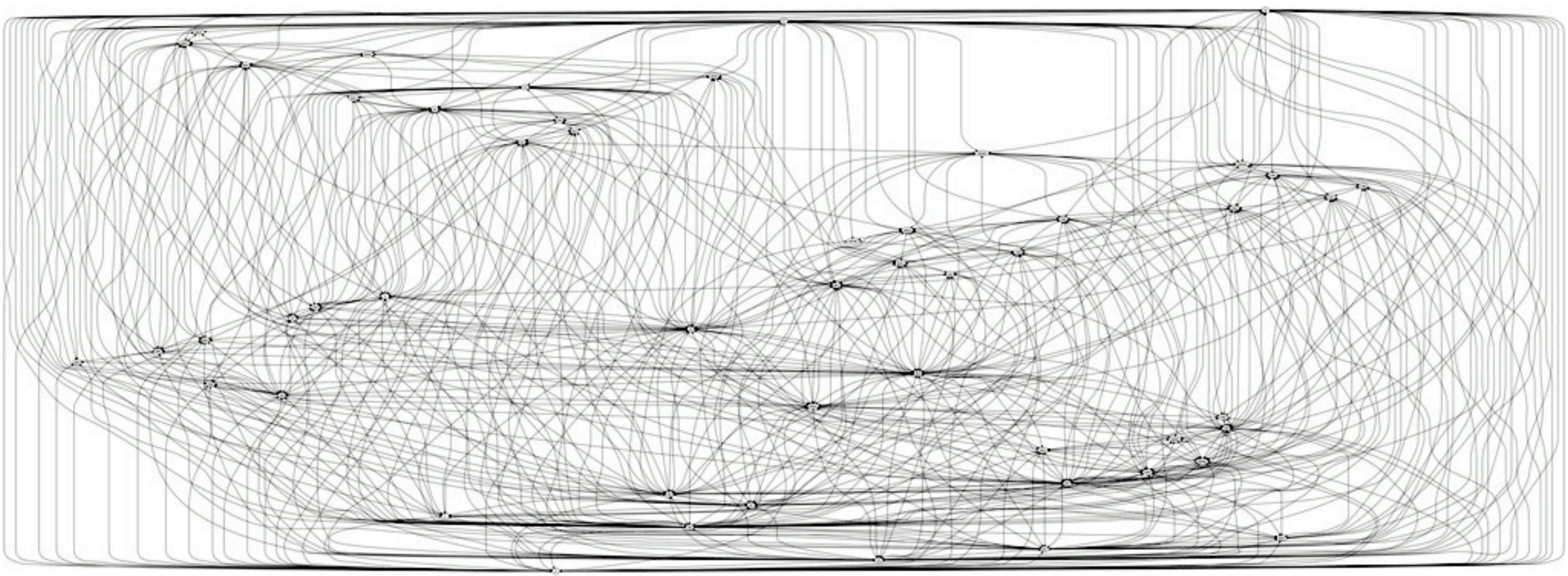


$$R_{AD} = \max\left(r_{AD,1}, r_{AD,2}, r_{AD,3}\right)$$

$$r_{AD,1} = r_{AB} \cdot r_{BD}, \quad r_{AD,2} = r_{AC} \cdot r_{CD}, \quad r_{AD,3} = r_{AC} \cdot r_{CE} \cdot r_{ED}$$

R_{AD} is the overall interaction coefficient of species D to species A

GRI-Mech 3.0 Graph



53 species
1082 connections

Graph Search

- Method used here: **Dijkstra's algorithm**
  - Classical solution to shortest-path problem
  - See Niemeyer & Sung *CNF* in press
    - Correct results, independent of species order
    - Most efficient algorithm
      - with binary heap, ~100x faster
    - compared vs. DFS, mod-DFS, BFS, **RBFS**

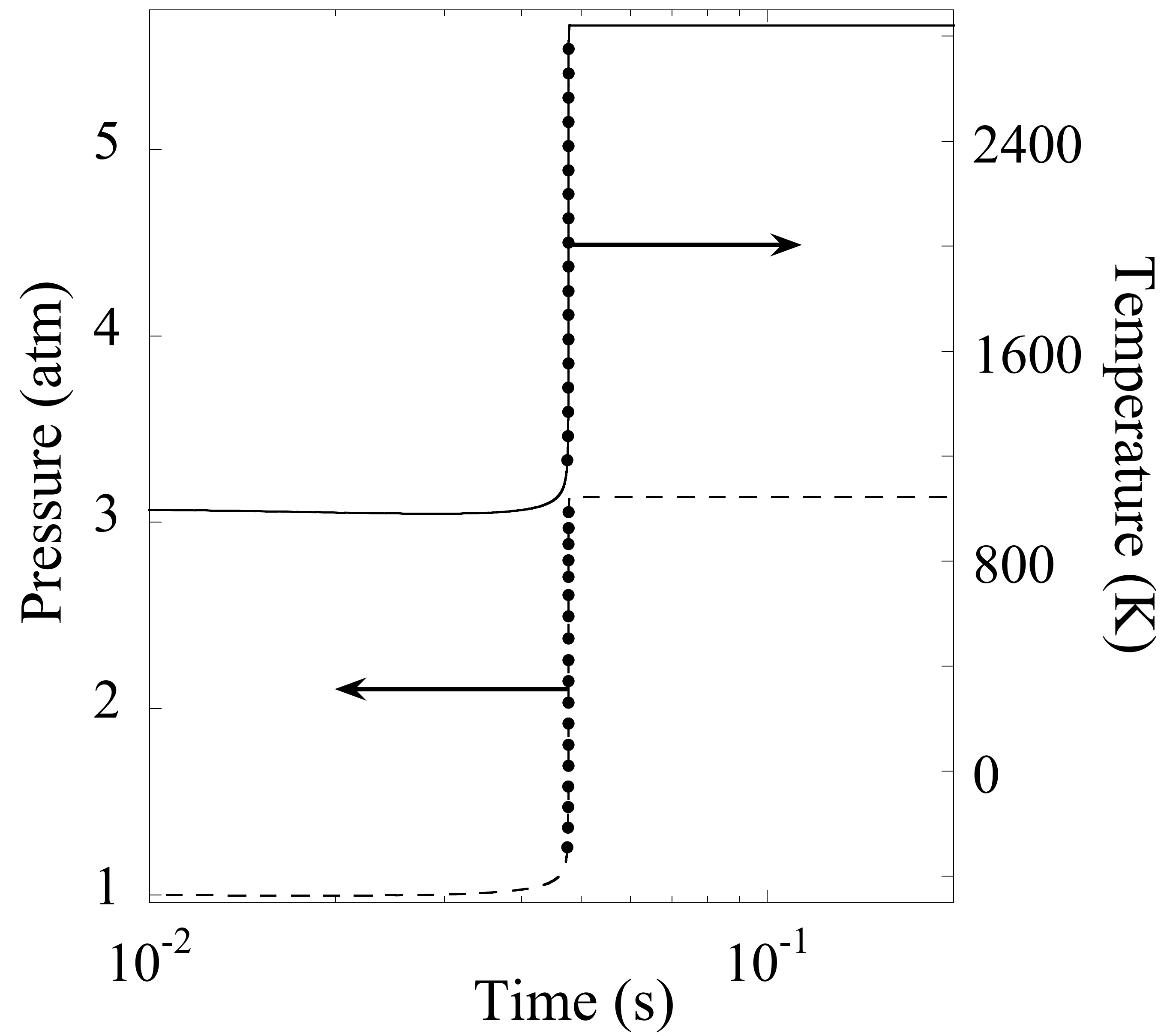
Elimination of Unimportant Reactions

- DRGEP & SA stages: reactions removed when participating species removed
- Further reaction elimination:
  - CSP importance index: $$I_{A,i} = \frac{|\nu_{A,i}\omega_i|}{\sum_{j=1,n_R} |\nu_{A,j}\omega_j|}$$
  - Remove reactions where $$\max_{\text{all species } A} I_{A,i} < \varepsilon_{\text{reac}}$$

* see Lu & Law *CNF* 2008

Sampling Procedure

- Constant volume autoignition simulations (SENKIN)
- Chemical kinetics data sampled during ignition evolution



* Niemeyer, Sung, Raju *CNF* 2010

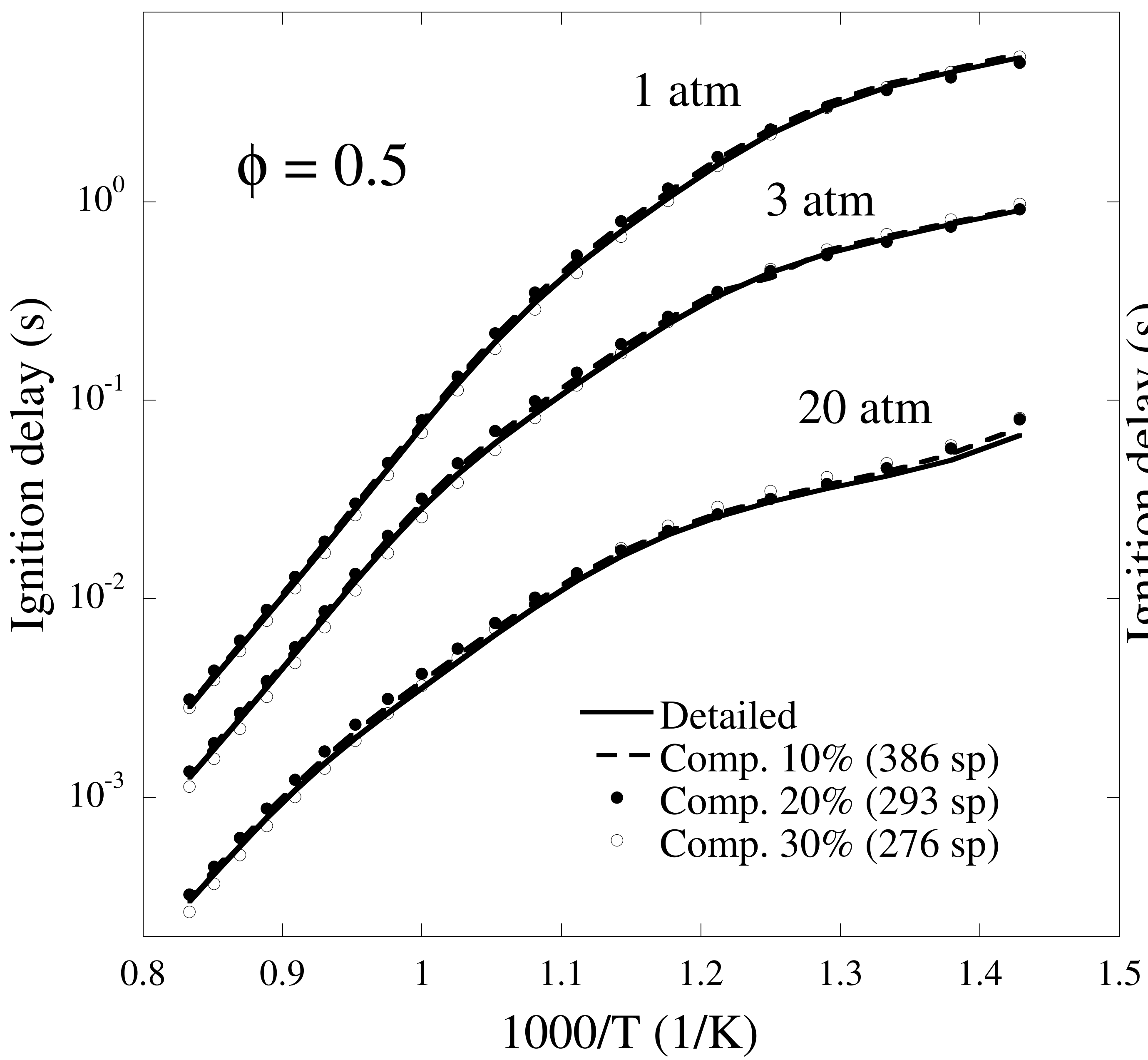
TRF Skeletal Mechanisms

- Ultimate goal: use of multicomponent surrogate mechanisms
- LLNL toluene reference fuel (TRF) mechanism (*n*-heptane + *iso*-octane + toluene): **1389 species and 5935 reactions**
- Generate skeletal mechanisms using DRGEPSA + unimportant reaction elimination
  - Error limits: 10%, 20%, 30%
  - Comprehensive (600-1600 K) and high-temperature (1000-1600 K), 1-20 atm, Φ=0.5-1.5
  - Mixture: 60.54/20.64/18.82% (by liq. volume) tol/ic8/nc7
    - taken from Morgan et al. *CNF* 2010, RON=95 / MON=85

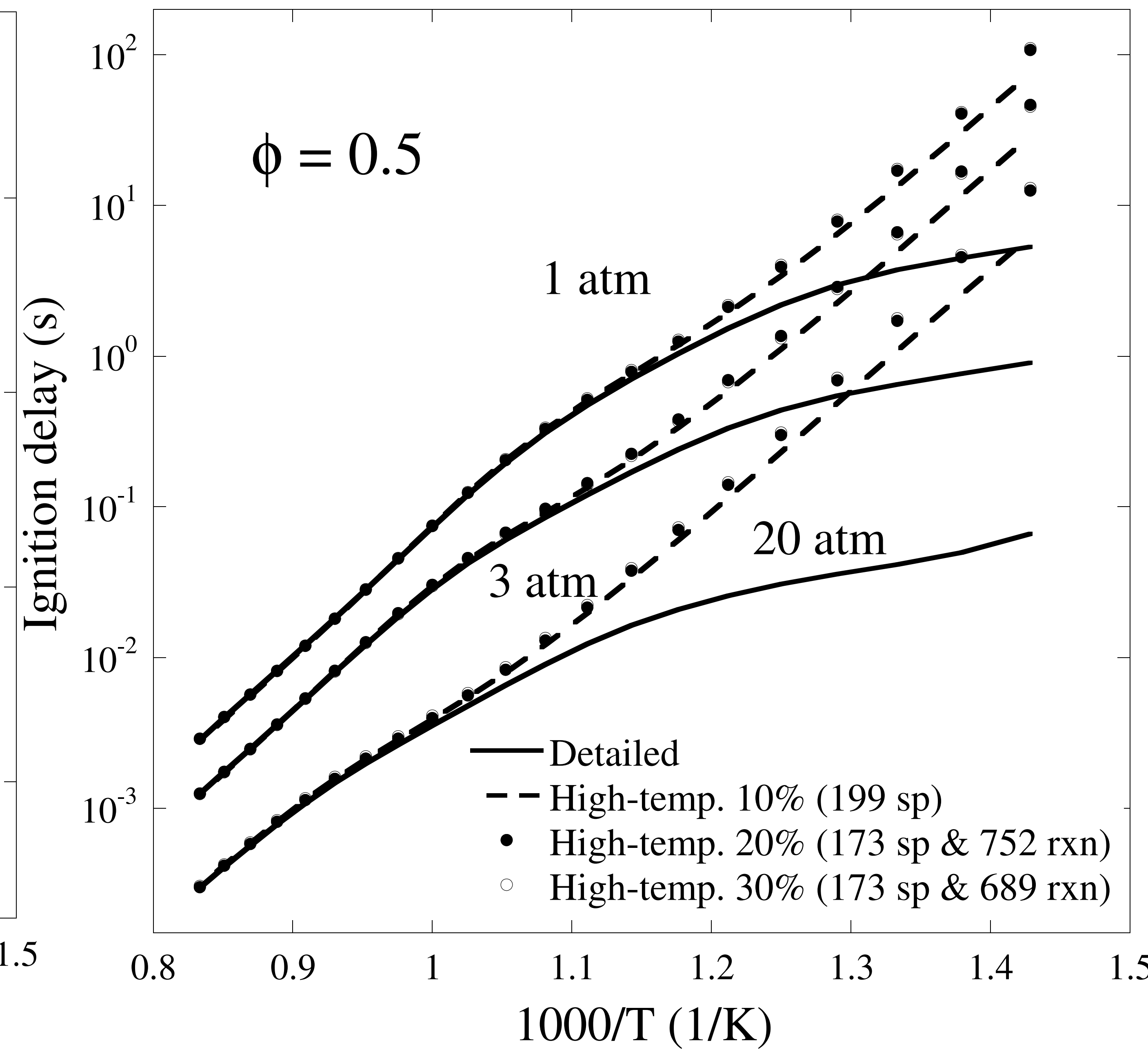
TRF Skeletal Mechanisms

Error limit	Comp-temperature		High-temperature	
	# species	Max. error	# species	Max. error
10%	386	9.2%	199	9.9%
20%	293	19.8%	173	18.4%
30%	276	24.3%	173	23.1%

TRF Skeletal Mechanisms Validation



Comprehensive

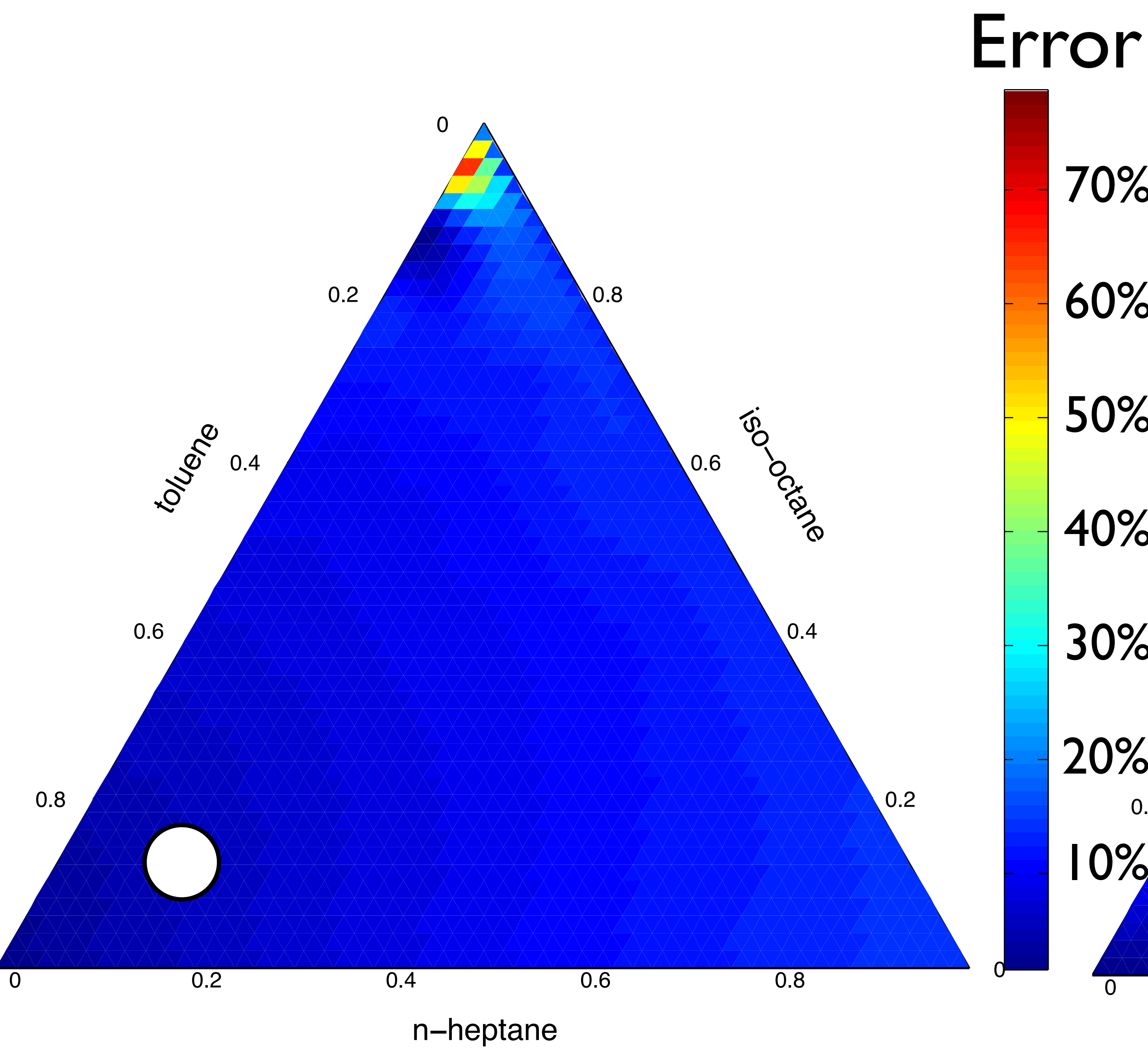


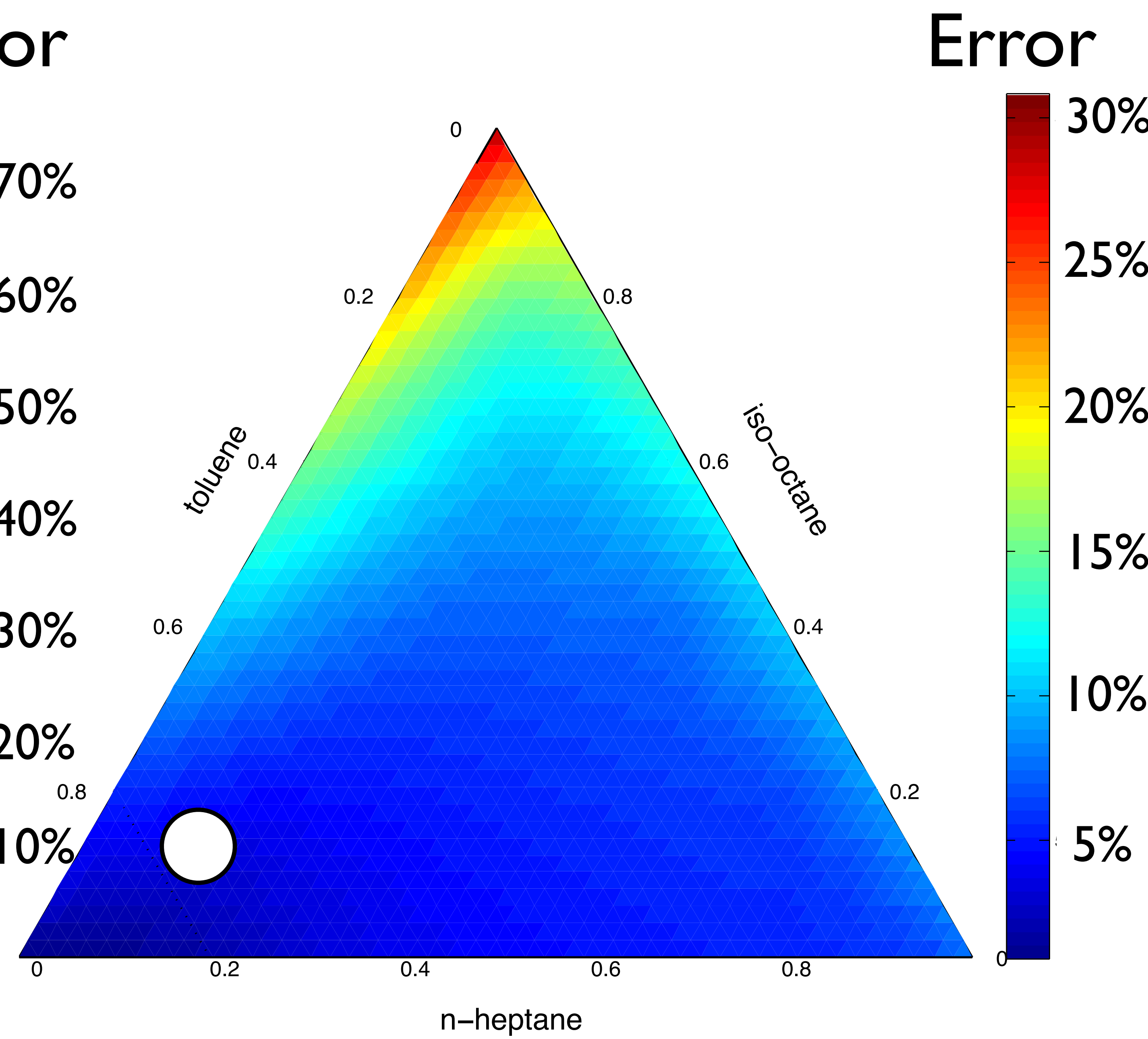
High-temp

RON / MON validation

- Skeletal mechanisms for gasoline surrogates should predict both RON and MON well (capture sensitivity)
- Also determine accurate range of skeletal mechanisms over mixture composition
- Perform SENKIN constant-volume simulations:
  - MON-like: 900 K, 20 bar, $\phi = 1.0$
  - RON-like: 800 K, 23 bar, $\phi = 1.0$
  - Comprehensive skeletal mechanisms only (low T)

RON/MON: 10%

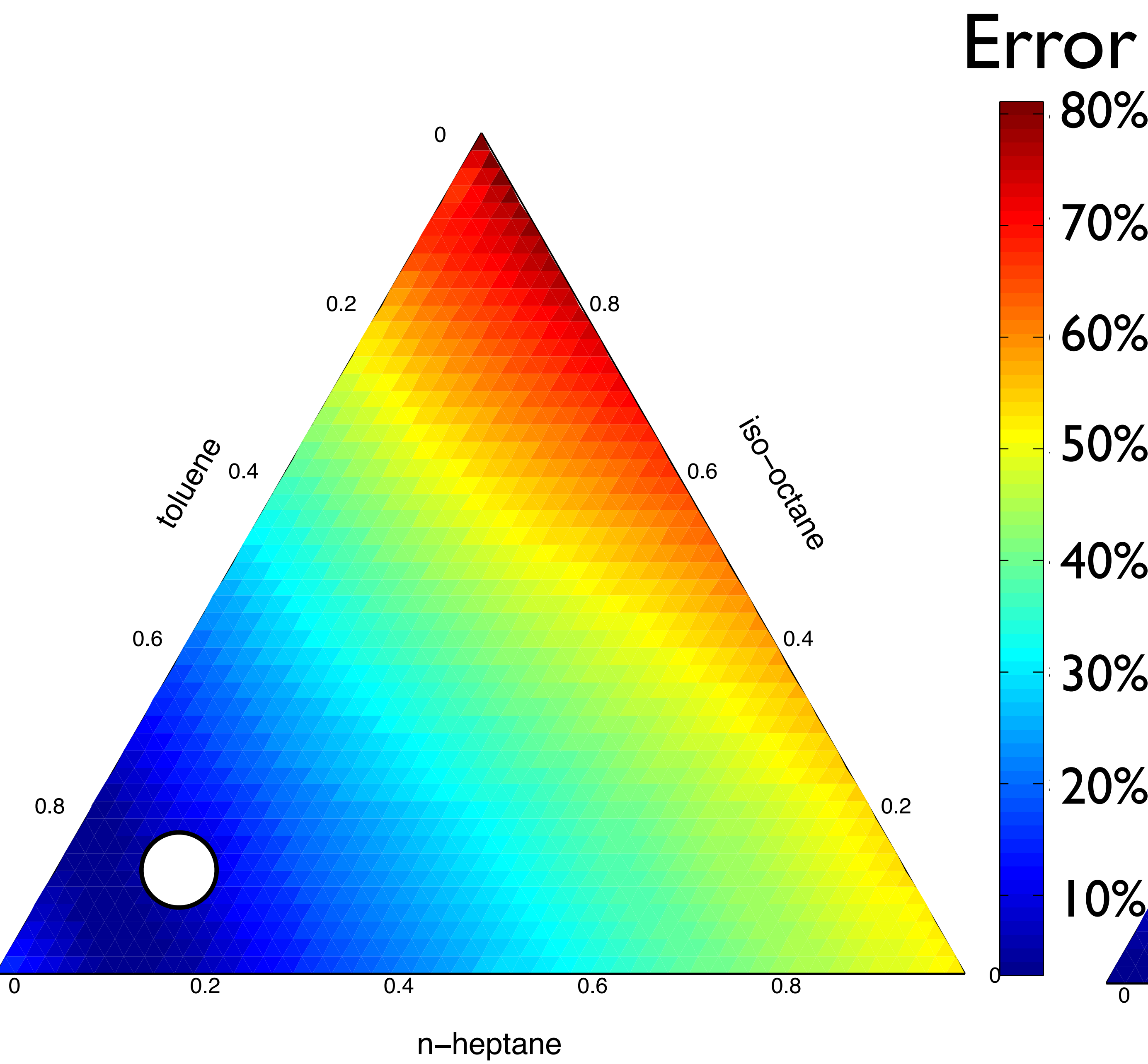




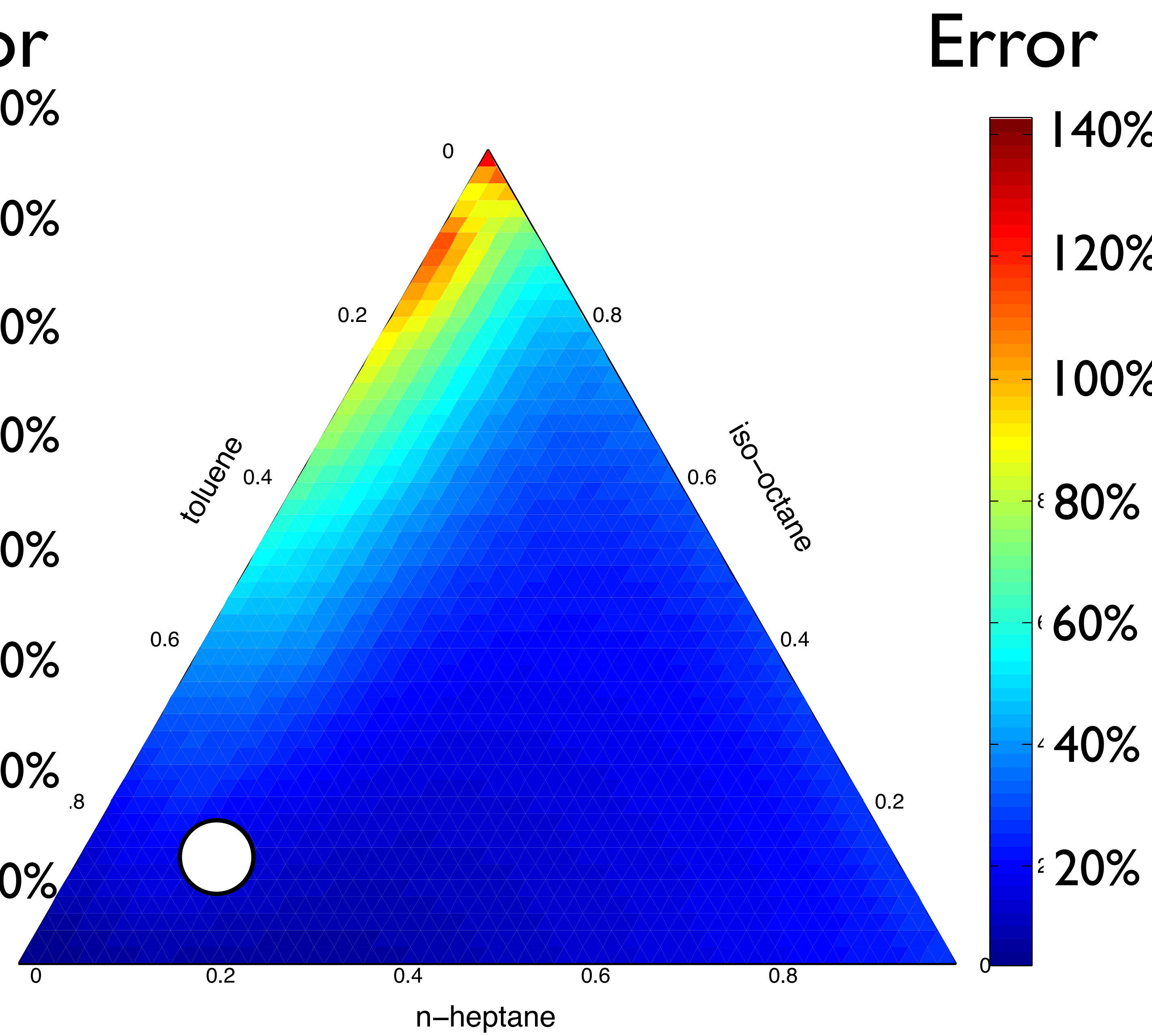
MON ignition delay error

RON ignition delay error

RON/MON: 30%



MON ignition delay error



RON ignition delay error

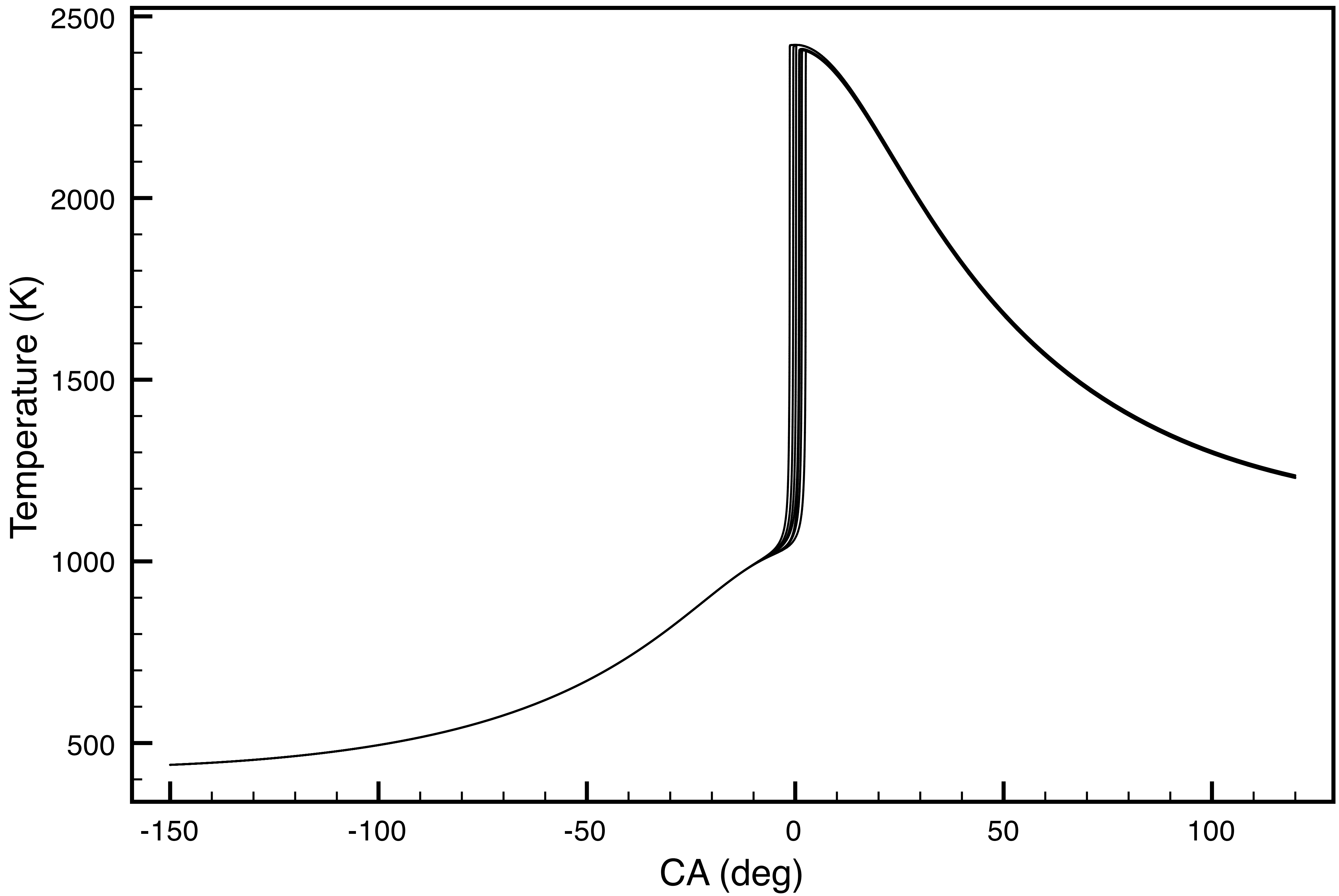
HCCI Simulations

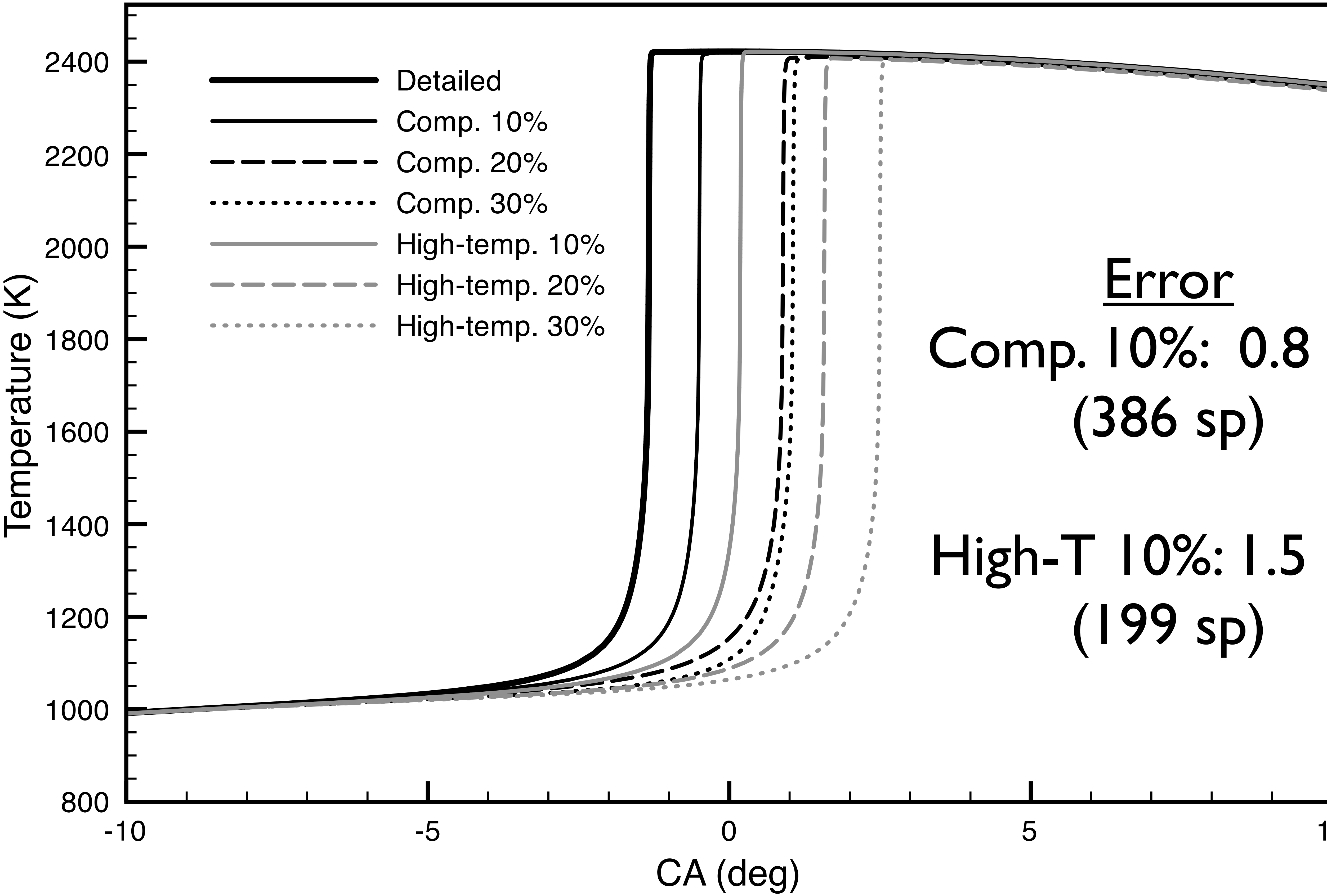
- Engine specs taken from Sjöberg, Dec, Hwang (Sandia)

Compression ratio	14
Engine speed	1200 rpm
Disp. volume	981 cm^3
Connect. rod : Crank radius	3.2

- Performed using CHEMKIN-PRO
  - Mixture: 69/14/17% (by liq. volume) ic8/tol/nc7
    - Gauthier et al. *CNF* 2004, ON 87 gasoline
  - Normal operation: P_i = 1 atm, ϕ = 0.5
  - Low-load (idle) operation: P_i = 1.3 atm, ϕ = 0.12

HCCI - Normal operation



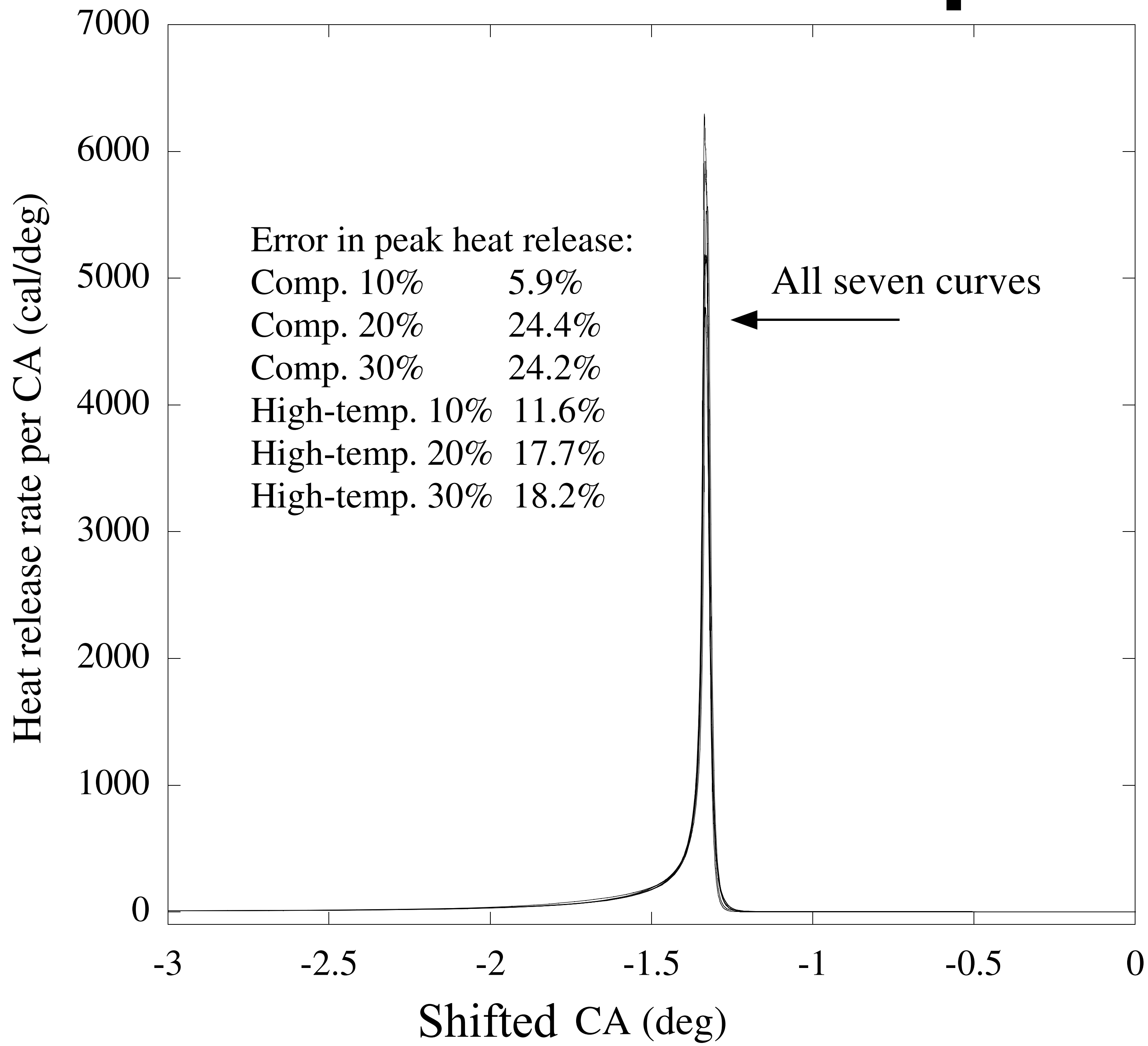


<u>Error</u>

Comp. 10%: 0.8 CA
(386 sp)

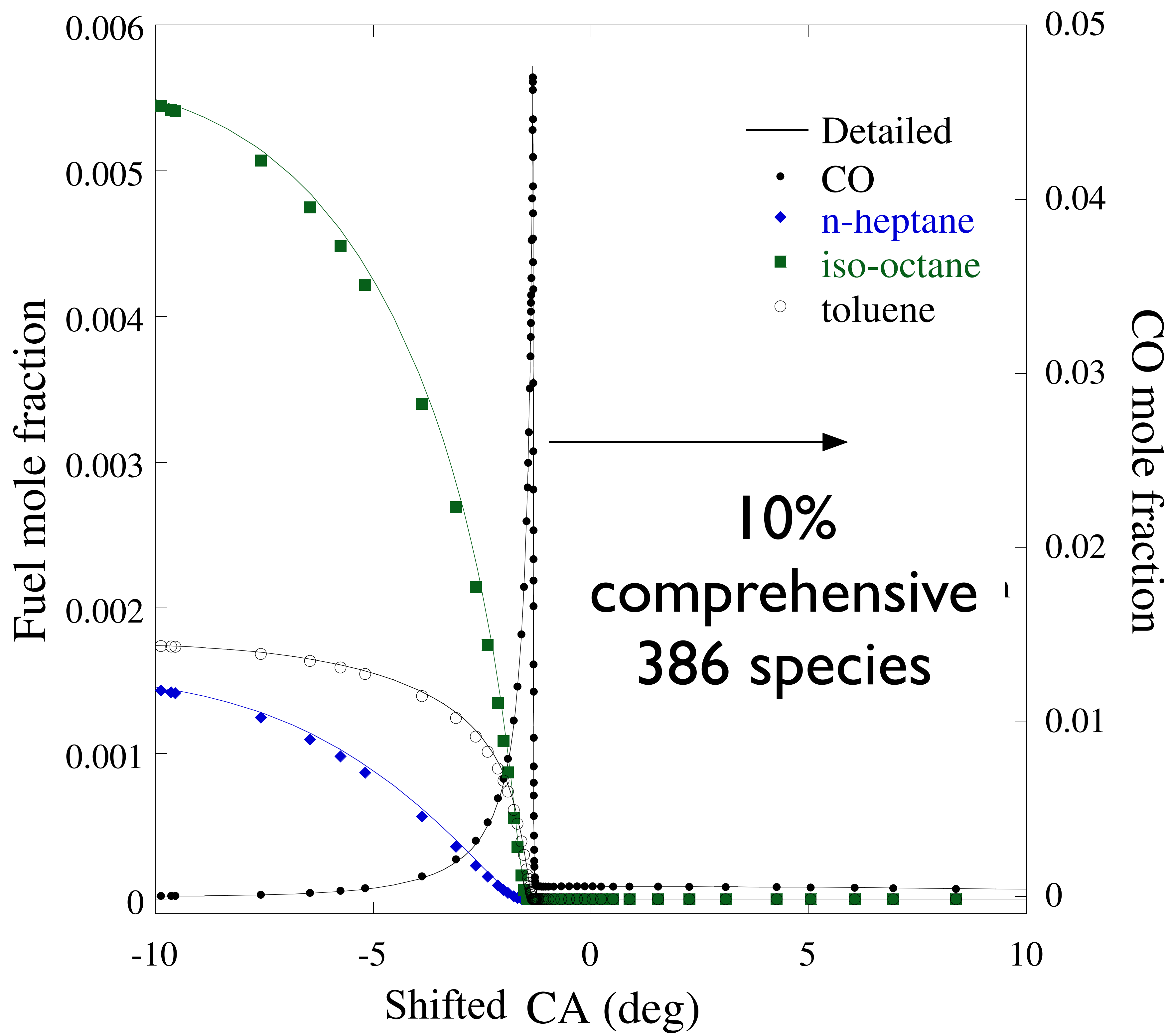
High-T 10%: 1.5 CA
(199 sp)

HCCI - Normal operation

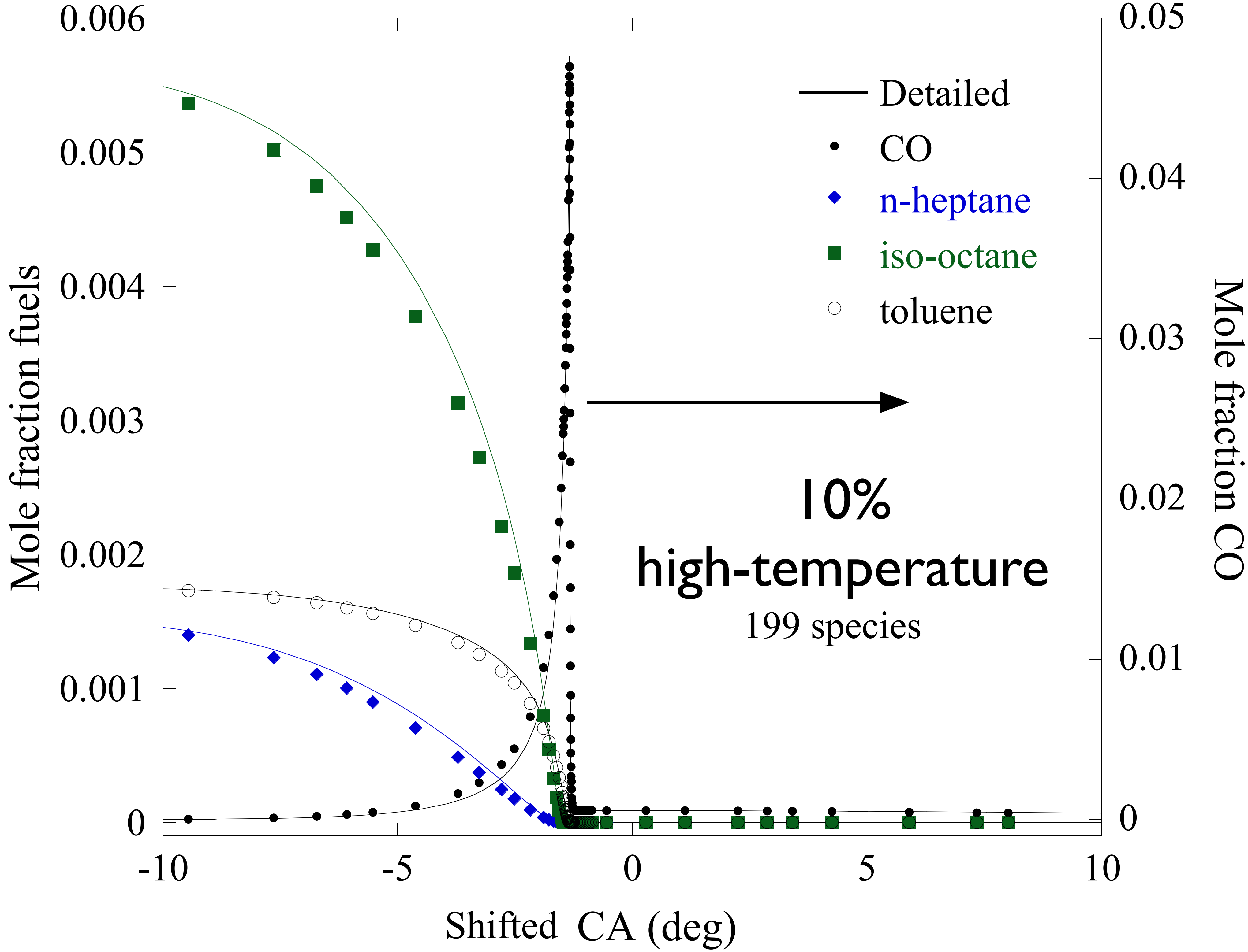


Heat release profile

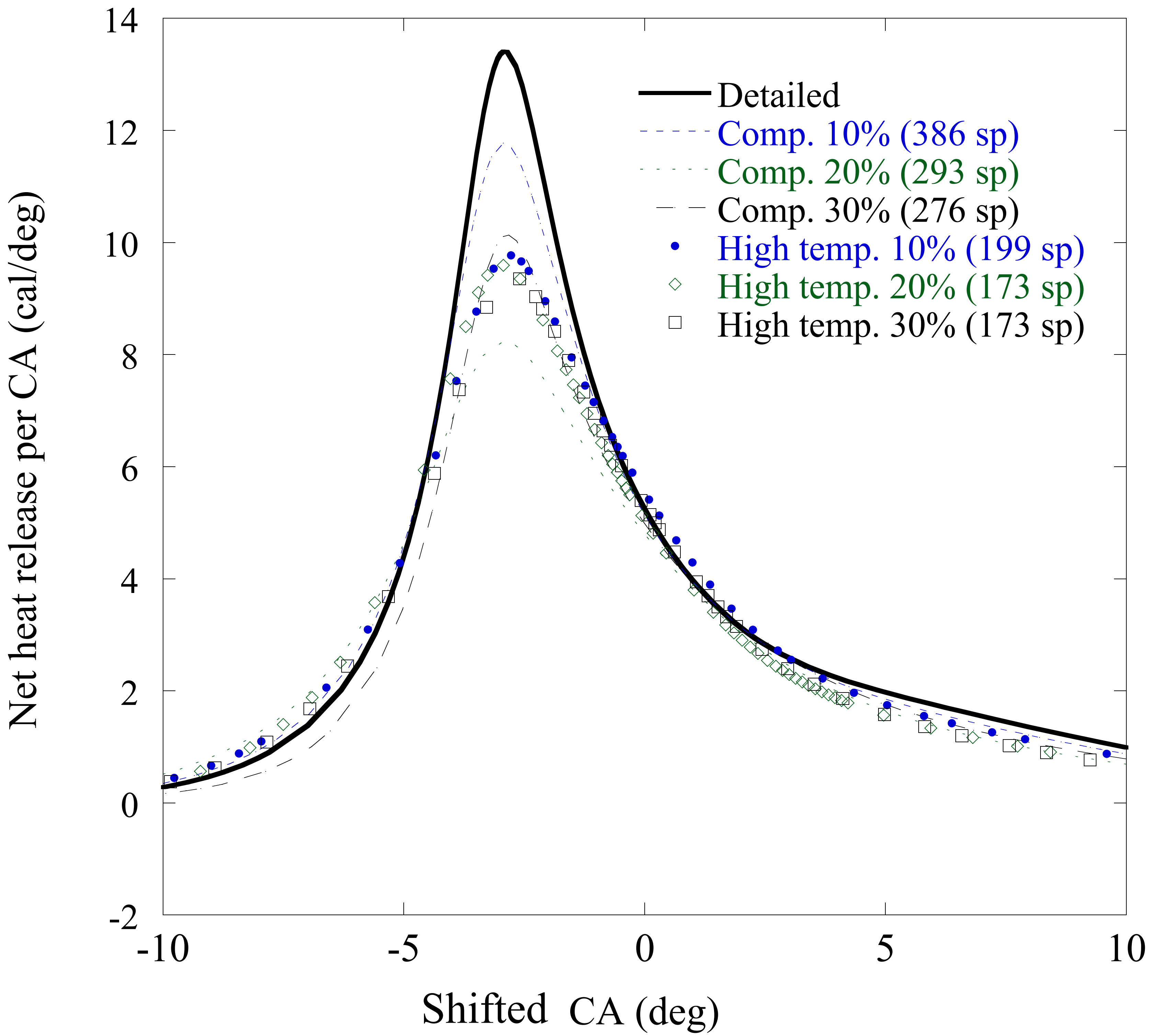
HCCI - Normal operation



HCCI - Normal operation

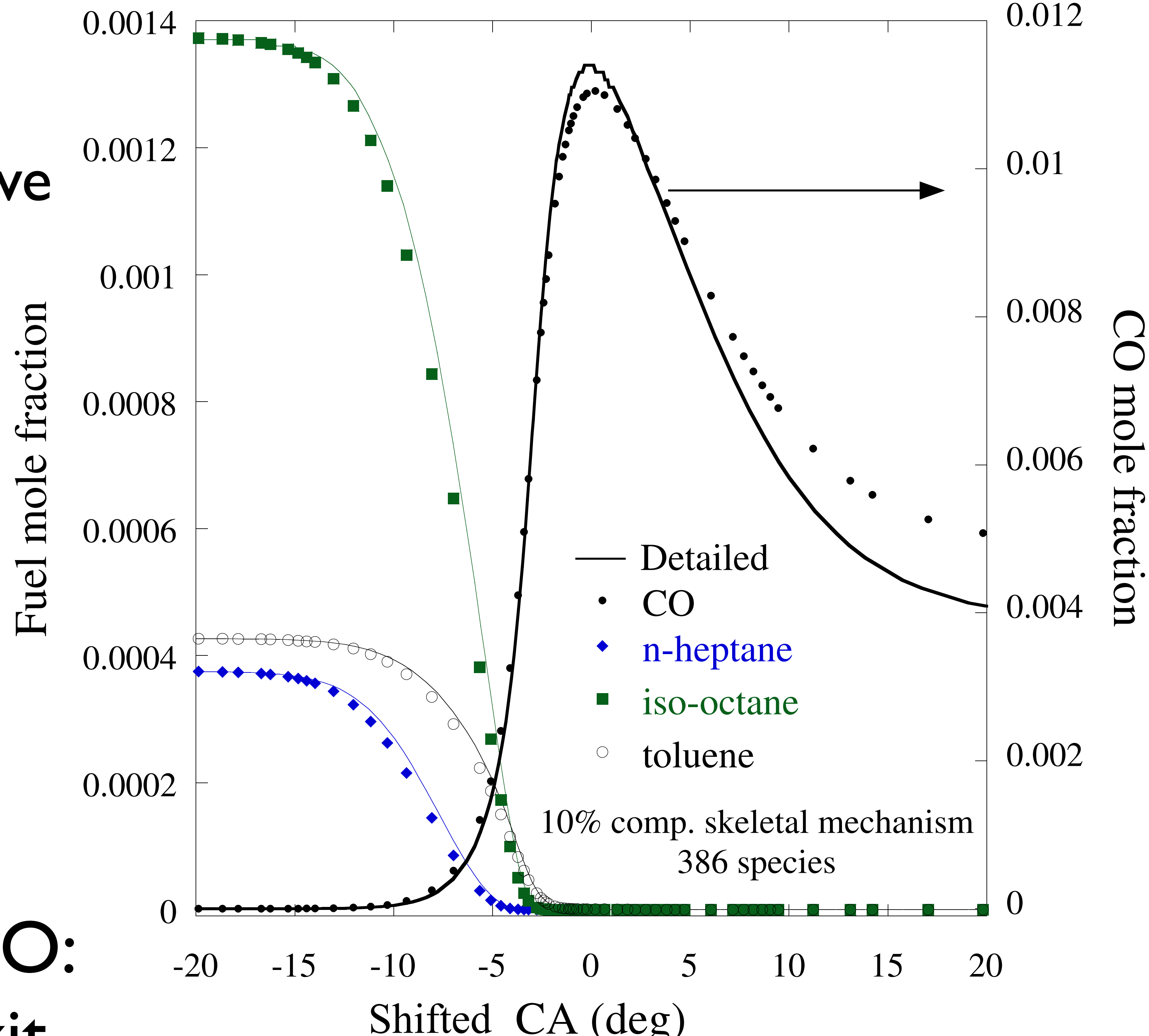


HCCI - Low-load operation



HCCI - Low-load operation

10%
comprehensive



Error in CO:
26% at exit

TRF Skeletal Mechanisms: Discussion

- Cover entire range of mixture for RON and MON, but care at higher error limit (30%)
  - Consistent error: high iso-octane, small amount toluene
- Tight error limit (10%) needed to capture HCCI ignition & heat release rate within ~1 CA degree
  - Fuel and CO profile well captured for normal operation
- Error in exit CO prediction for extremely lean HCCI (idle)

Conclusions

- Applied mechanism reduction using DRGEP with accurate & efficient search algorithm, SA, & unimportant reaction elimination
- TRF skeletal mechanisms at various levels of detail
  - Validated using autoignition, RON/MON-like, and HCCI
  - Tight error limit needed for wide-ranging accuracy
- Skeletal mechanisms still large (~200+)
  - Significant reduction (~85%), but not enough
- **Future work:** adaptive/dynamic reduction using DRGEP

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Questions?

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