# Some Future Capabilities Under Development

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CHEMKIN in Combustion Workshop

August 3, 2008

# Several new capabilities are in progress, particularly for automotive applications

- **Fuel analysis tools**
  - Octane Number Calculator
  - Cetane Number Calculator
- **Mechanism Reduction facility**
  - Skeletal vs. severe-reduction methods
  - Reduction to target tolerances
- **More performance improvements**
  - Sparse-matrix solver for large mechanisms

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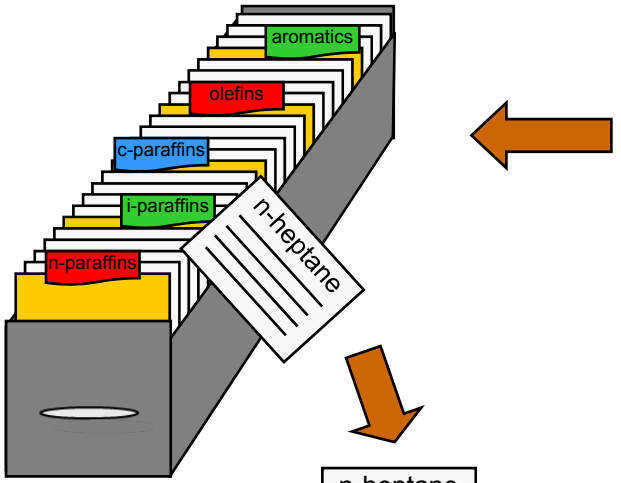
# With a database of mechanisms, we are working toward defining surrogate blends

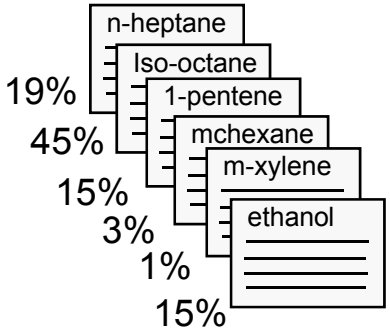
**Real Fuel Characteristics**
- Class composition
- Heat-release rate
- Octane / Cetane #
- H/C ratio, O content

New Real Fuel Blend

**Match Properties**
- Select Molecules
- Set Composition




**Merge Mechanisms**
- Species
- Reactions




**Surrogate Fuel Composition**

Chemical Model for Simulation



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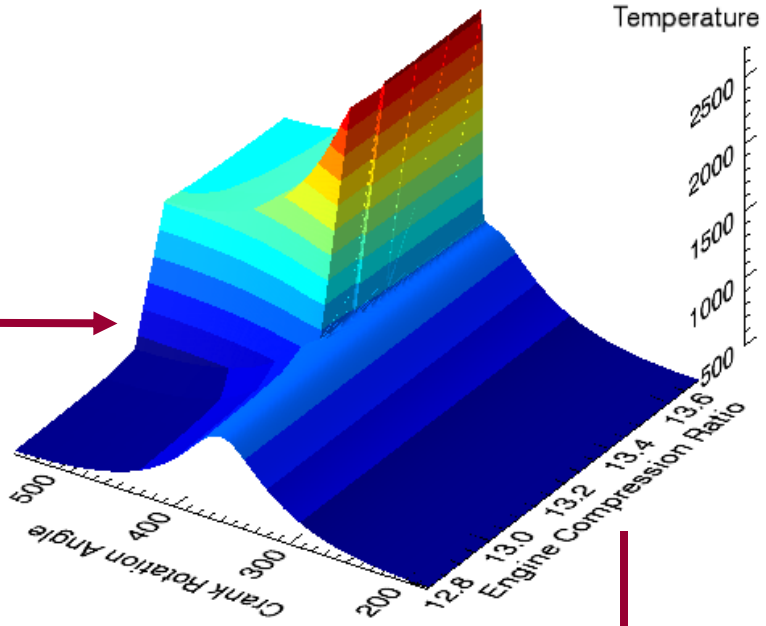
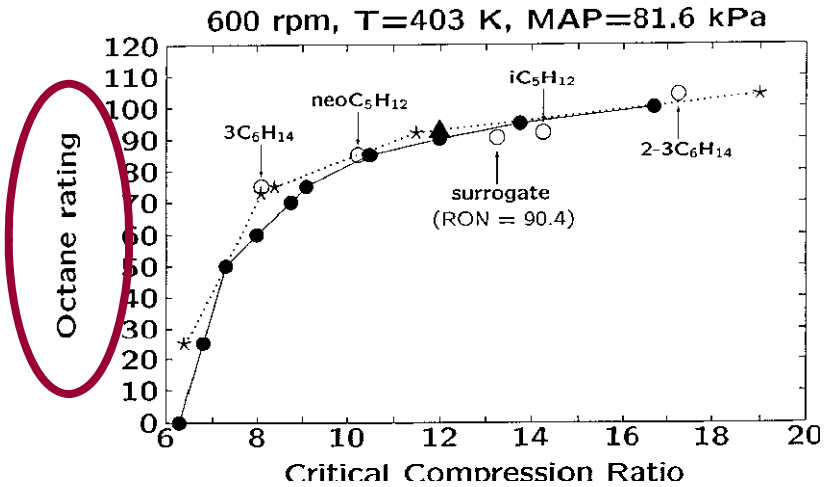
# The Octane Number Calculator allows prediction of RON / MON for arbitrary fuel

- **Special reactor model**
  - RON / MON test conditions
- **Determine critical compression ratio (CCR)**
  - Lowest CR for ignition
- **Correlate CCR with RON or MON**




**Stars: PRF Experimental:**
**Closed Circles & Triangle: Experimental pure component**
**Open Circles: Previously calculated values**

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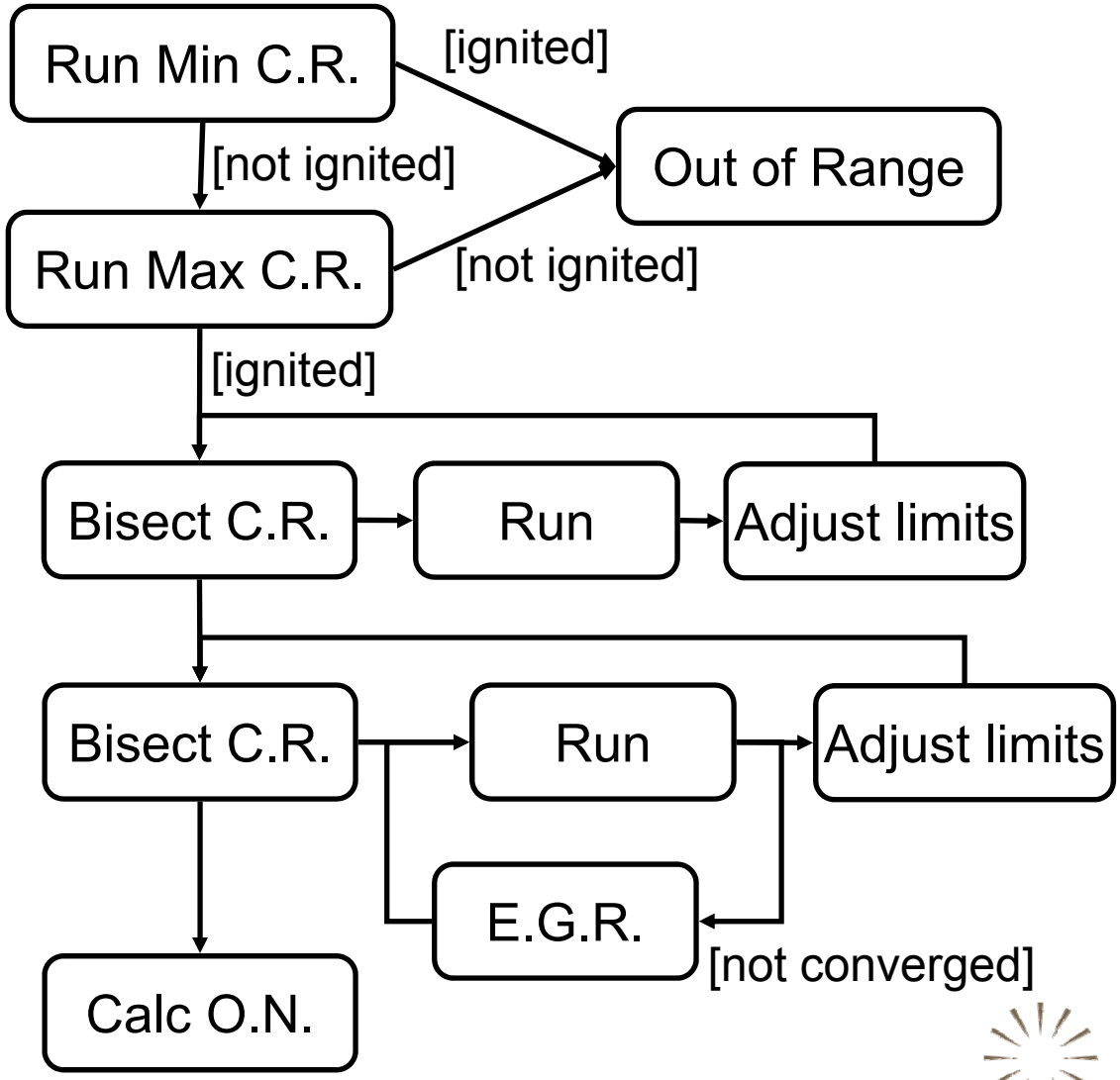
# An iterative method is used to calculate critical compression ratio

- **Work flow:**
  - Use IC Engine model
  - Same process for Research and Motor engines
    - Different engine specs
  - Search for critical compression ratio
    - Use bisection to search
  - Recycle residuals for several iterations
    - Assure convergence in case of non-ignition



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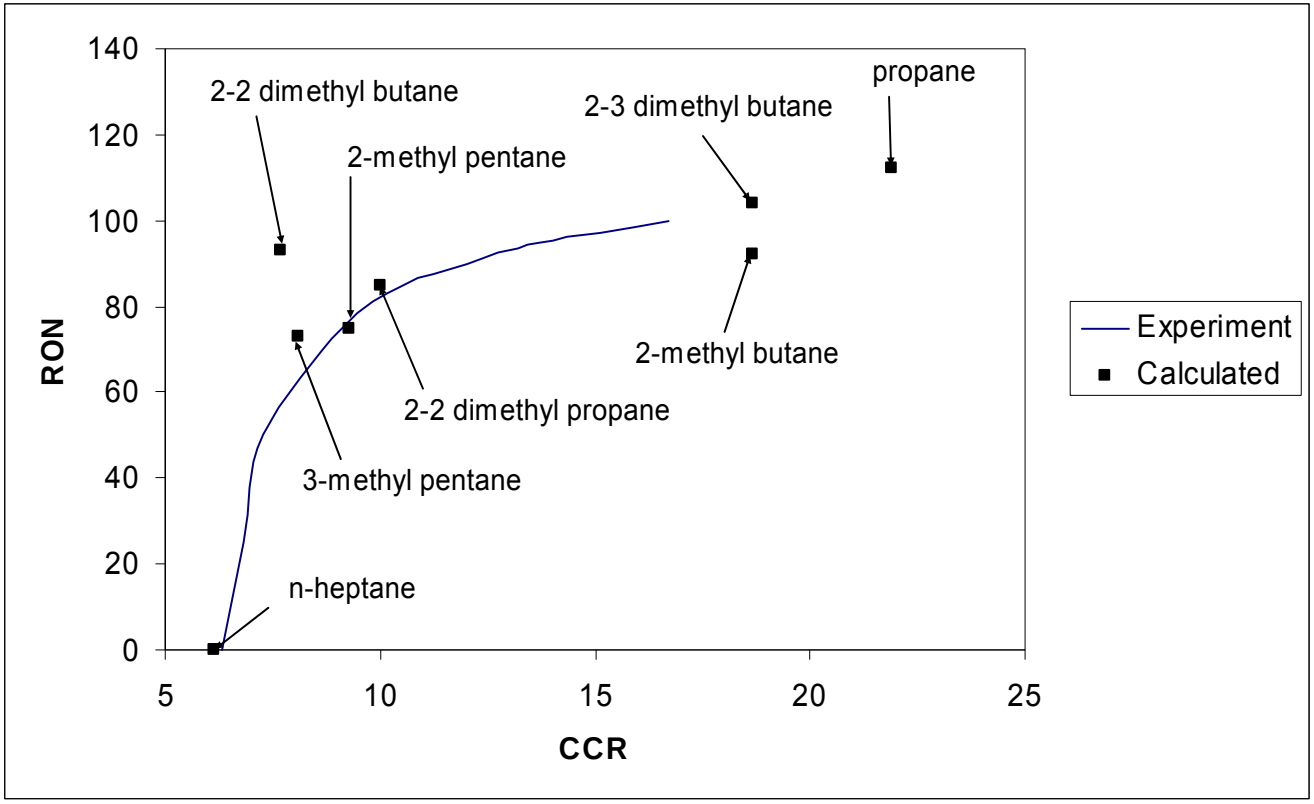
# Preliminary results show reasonable predictive capability for RON and MON

- **Comparison with measured RON vs. CCR for a range of fuels**



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# We are also developing a Cetane Number Calculator for diesel surrogates

- **Two standards for evaluation were considered:**
  - ASTM D 613
    - Cooperative Fuel Research (CFR) Engine 10 BTDC
    - Difficult to reproduce
  - ASTM 6890 Ignition Quality Test
    - Heated, constant volume combustion chamber
    - Correlation between auto-ignition time and cetane number
    - Measure time between injection and pressure recovery point
      - Pressure and Temperature quenching due to fuel evaporation

# A calculation based on the ASTMD-6890 method has been selected

## ASTM D 613

- Need to simulate engine
- Need accurate mechanisms for PRF*
  - Correlation between CR and CN not available (similar to that for ON)
- Spray and mixing effects
- Simulations can be very time consuming

## ASTM D 6890 (IQT)

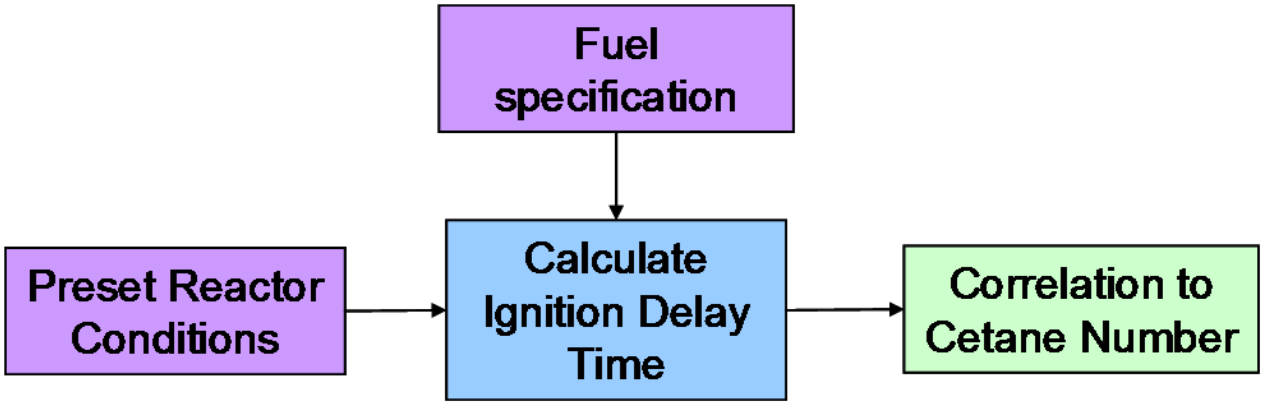
- ✓ Simple setup
- ✓ No need to calibrate based on diesel PRF*
  - Correlation between ignition time and CN available
- Spray and mixing effects
- ✓ Fast simulations

* PRF for diesel: n-hexadecane and heptamethylnonane

- **Spray and mixing effects in ASTM D 6890 method can be compensated by reducing the initial temperature of the bomb**
  - No immediate need for a spray model

# Ignition delay is calculated using a CHEMKIN Closed Homogeneous Batch Reactor

- **Simulate Ignition Quality Tester (IQT) method**
  - Model with closed homogeneous reactor
  - Reactor conditions estimated
    - Sensitive to approximations of quenching



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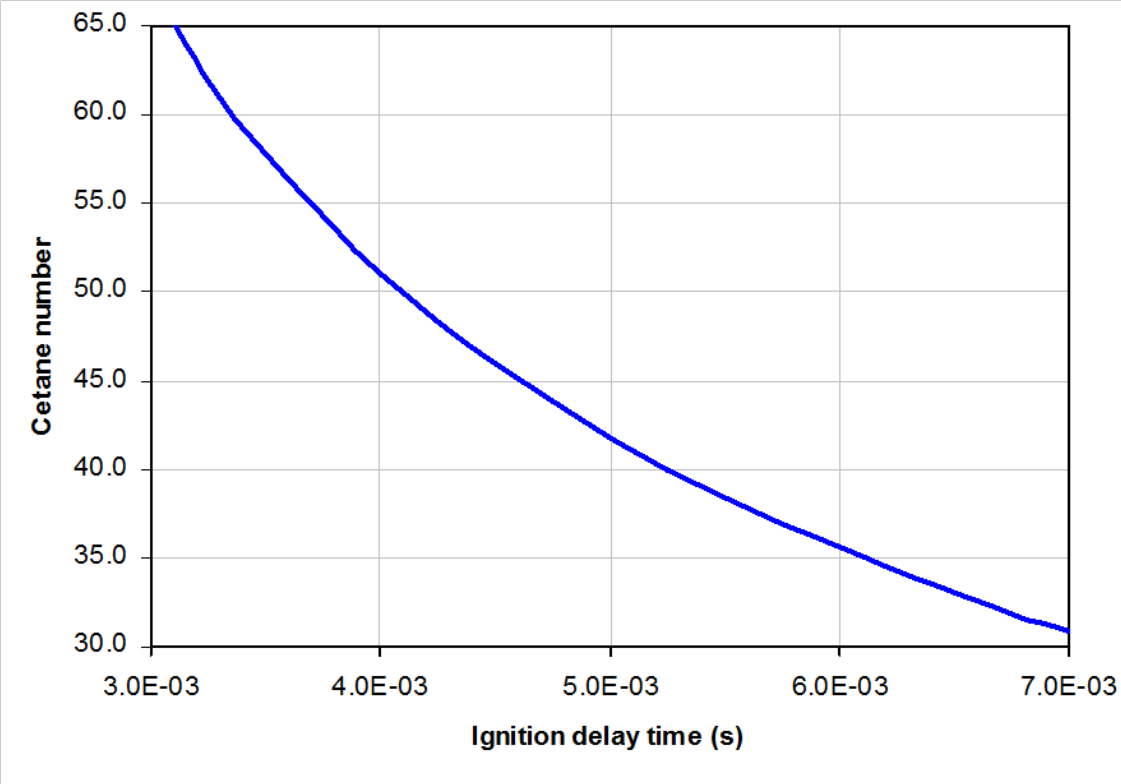
# A correlation is used to get Cetane Number from the ignition-delay time

- Outside limits, the ASTM correlation does not apply
- Second correlation developed outside of given range



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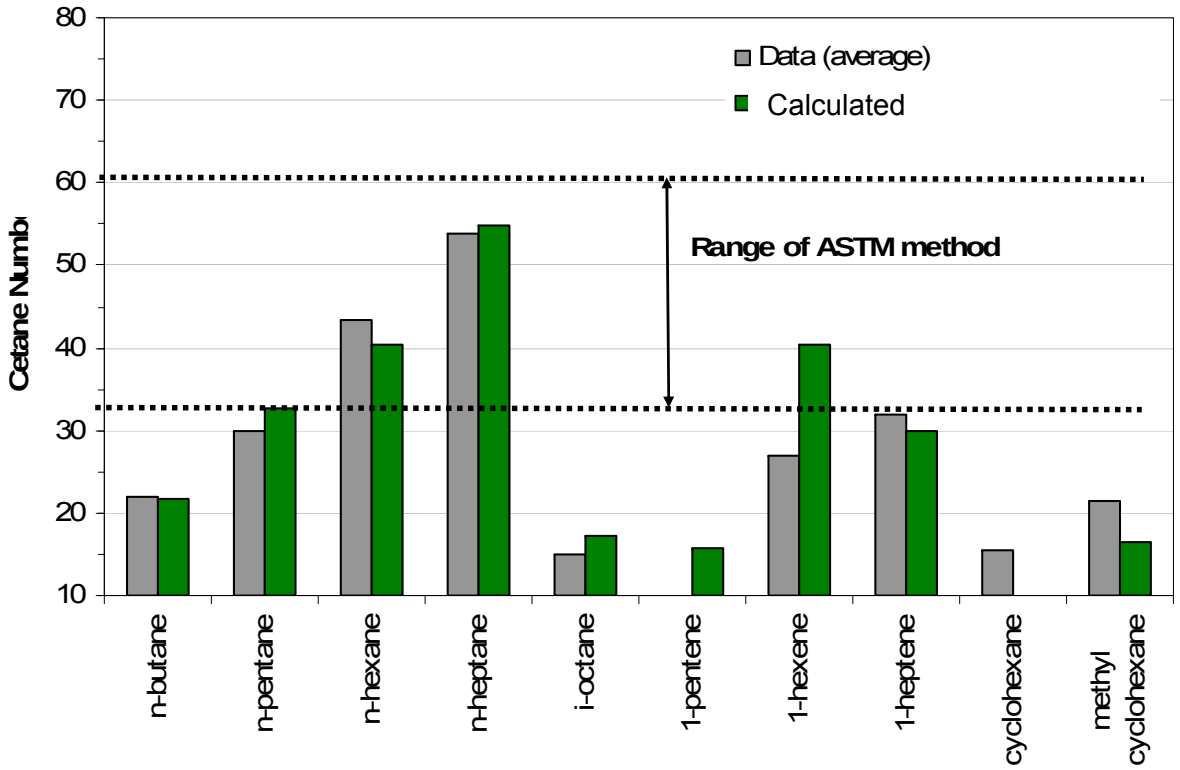
# Preliminary results show good predictive capability for a range of fuels

- **Comparison to experiment**
  - Same multi-component mechanism used for all cases
  - Data averaged from Murphy et al. (2004), NREL Compendium of Experimental Cetane Number Data



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# ON and CN Calculators will provide means of testing surrogate blend properties

- Use to match real-fuel properties
- Based on simulation, can be used for arbitrary fuel mixture
- Additional test for detailed mechanisms of surrogate-fuel mixtures and components

# Several new capabilities are in progress, particularly for automotive applications

- **Fuel analysis tools**
  - Octane Number Calculator
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- **Mechanism Reduction facility**
  - Skeletal vs. severe-reduction methods
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- **More performance improvements**
  - Sparse-matrix solver for large mechanisms

# Mechanism reduction is very important for practical simulation of realistic fuels

- **Skeletal mechanism**
  - Subset of species and elementary reactions from the original master mechanism
- **Severely reduced mechanism**
  - Lumped species and/or reactions
  - Assumptions:
    - Partial equilibrium
    - Quasi-steady-state
    - etc.

# We have tested several methods for automated reduction

- **Two skeletal methods have been implemented**
  - Directed Relation Graph (DRG) *
    - Based on species rates of production
  - Principal Component Analysis (PCA) **
    - Based on reaction-rate sensitivity analysis

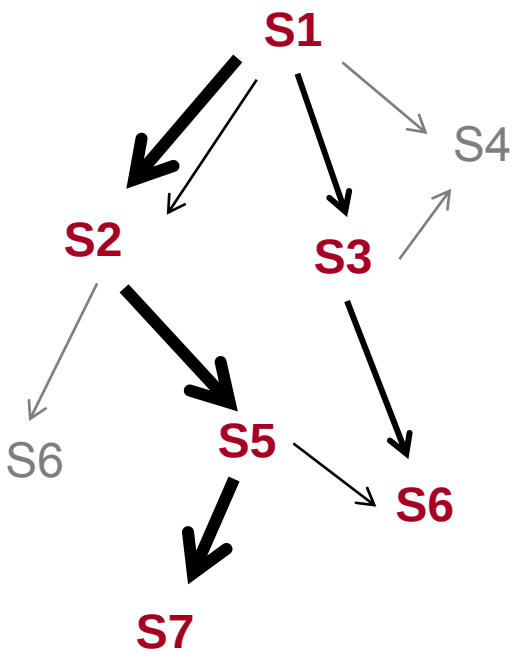
** Lu and Law, 2005; 2006*
*** Vajda, Valko,Turanyi; 1985*

# Mechanisms can be reduced to skeletal form for a particular range of conditions

- **Automation of reduction process**
  - Iterate method's error controls to determine smallest possible mechanism to achieve desired targets
    - Allow "derived" targets
  - Example targets:
    - Crank angle for 10% heat release, within 1 degree
    - Emissions of $NO_x$ within 50 ppm
  - Ranges of conditions set in CHEMKIN parameter study
    - Choice of reactor model
    - Parameter study varying equivalence ratio, pressure, temperature
    - Run first with full "master" mechanism

# The DRG method reduces paths based on species production and destruction rates

- **Analyze a "baseline" solution that uses the fully detailed mechanism**
  - Start with the Fuel & Oxidizer species
  - Determine which production path is above tolerance setting for each species
  - Repeat as "tree" of species is descended
  - Remove reactions that are below tolerance
  - Remove species that no longer contribute
- **Our implementation considers all points in the solution(s)**
  - Allows coverage of full transient analysis, as well as range of operating conditions



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# Test case for 5-component gasoline surrogate mechanism

- **Wide range of operating conditions**
  - Equivalence ratio 0.1 to 2.0
  - Temperature 600K to 1800K
  - Pressure 0.5atm to 60atm
- **384 cases used in reduction**
  - For each case, 100 time points considered
    - Total of 38,400 sampling points operated on during reduction
- **"Master" mechanism is gasoline surrogate blend**

| Fuel Component | (mole%) |
|---|---|
| n-heptane | 8 |
| iso-octane | 60 |
| Toluene | 20 |
| Methyl cyclohexane | 8 |
| 1-pentene | 4 |

RON=93.7
MON=90.6

# Gasoline Surrogate Base Kinetic Mechanism

- **1380 species, 6138 reactions**
  - Based on LLNL mechanism*
  - Updated mechanism and added missing reaction pathways
  - Includes low- and high-temperature pathways
  - Includes NOx pathways from GRI mechanism**
  - Includes PAH pathways from Appel et al.***

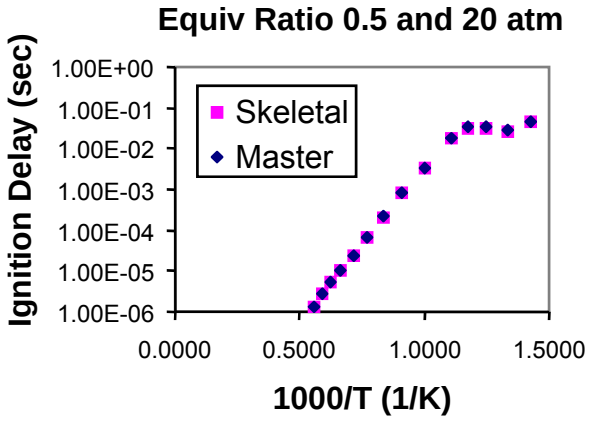
*C. V. Naik, W. J. Pitz, M. Sjoberg, J. E. Dec, J. Orme, H. J. Curran, J. M. Simmie, and C. K. Westbrook, SAE Fall Powertrain and Fluid Systems Conference & Exhibition, SAE2005-01-3742, 2005.

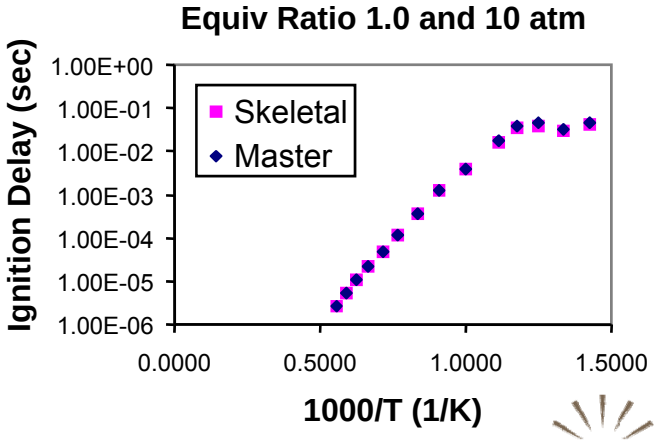
**G. P. Smith, D. M. Golden, M. Frenklach, N. W. Moriarty, B. Eiteneer, M. Goldenberg, C. T. Bowman, R. K. Hanson, S. Song, W. C. Gandiner, Jr., V. V. Lissianski, and Z. Qin, http://www.me.berkeley.edu/gri_mech/

***J. Appel, H. Bockhorn, and M. Frenklach, Combustion and Flame, vol. 121, pp. 122-136, 2000

# Application of DRG to ignition-delay simulations shows good accuracy

- **384 Cases used in reduction**
  - Equivalence ratio 0.1 to 2.0
  - Temperature 600K to 1800K
  - Pressure 0.5atm to 60atm
- **Results show good results for ~60% reduction**
  - Start: 1328 species, 5835 reactions
  - Finish: 560 species, 2818 reactions
- **Relative mean-square-root error is 3.9%**
  - Largest error is 24%
  - 19 cases above 10% error



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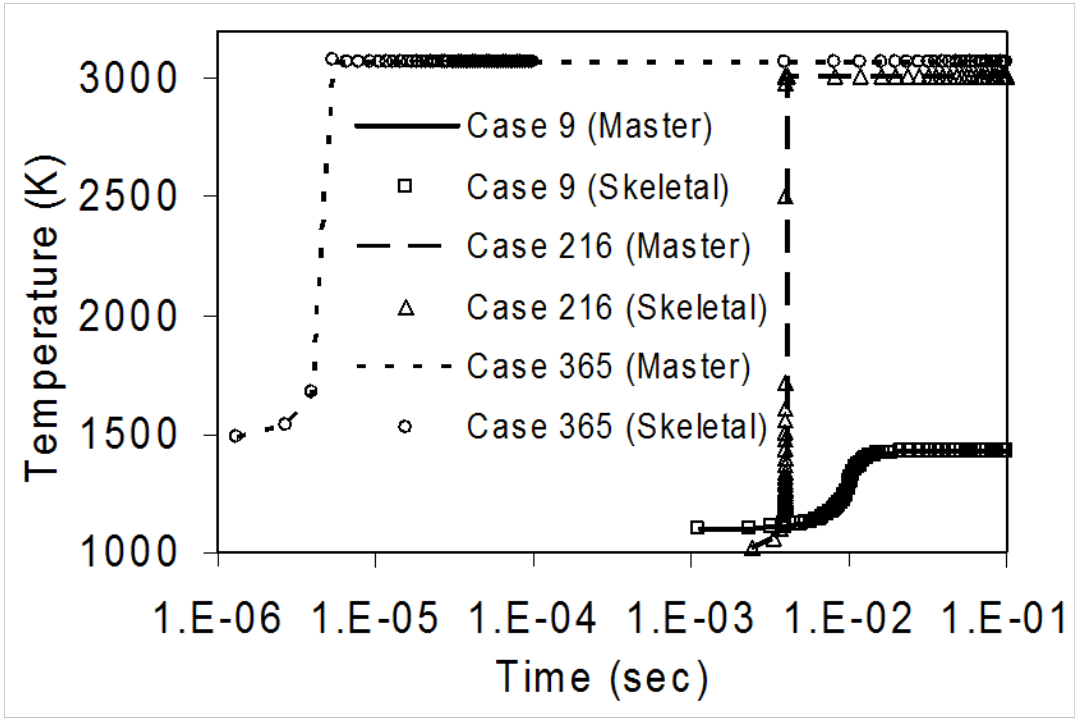
# Detailed temperature profiles agree well for single-zone engine model

- **Skeletal mechanism predicts same temperature profile as master mechanism**
- **Wide range of conditions**
  - P=0.5-60 atm, phi=0.1-2, T=1000-1500 K



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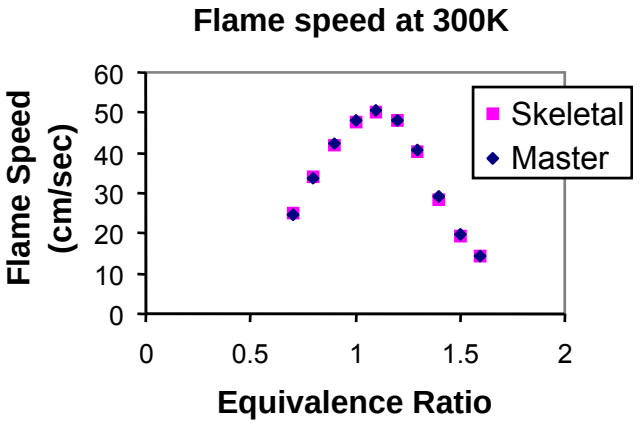
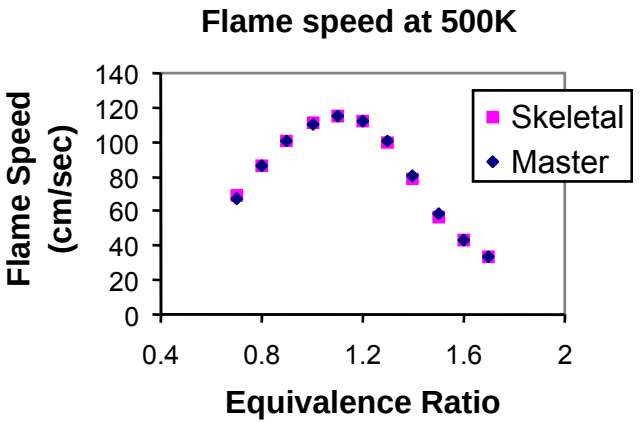
# More reduction can be achieved for high-temperature conditions (flames)

- **55 Cases used in n-heptane mechanism reduction**
  - Equivalence ratio 0.7 to 1.7
  - Temperature 300K to 700K
  - Pressure 1atm
- **Good results for ~80% reduction**
  - Start: 561 species, 2539 reactions
  - Finish: 121 species, 538 reactions
- **Relative mean-square-root error is 2.2%**
  - Largest error is 9.6%
  - 3 cases over 5% error



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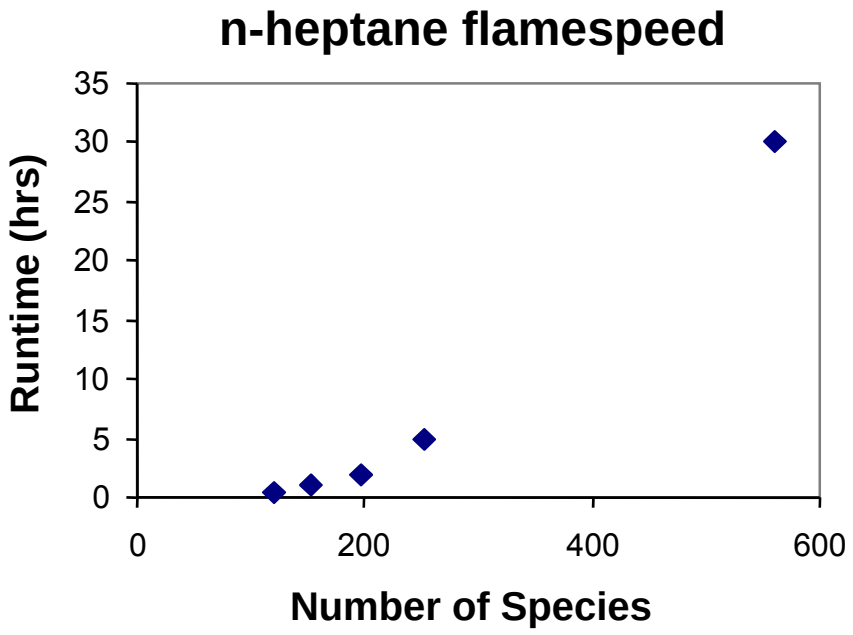
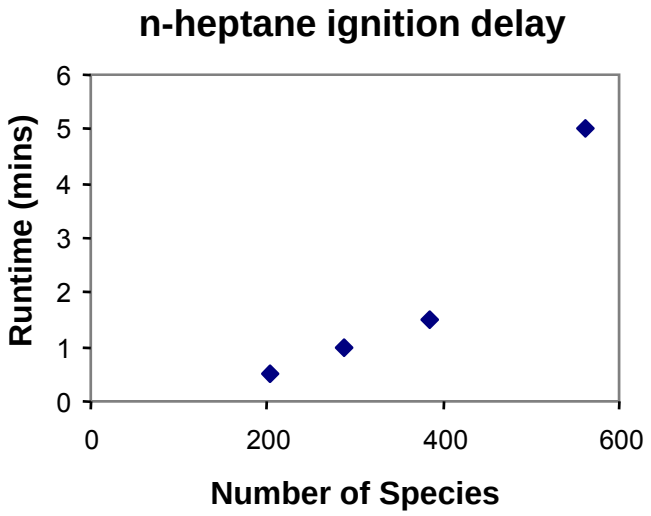
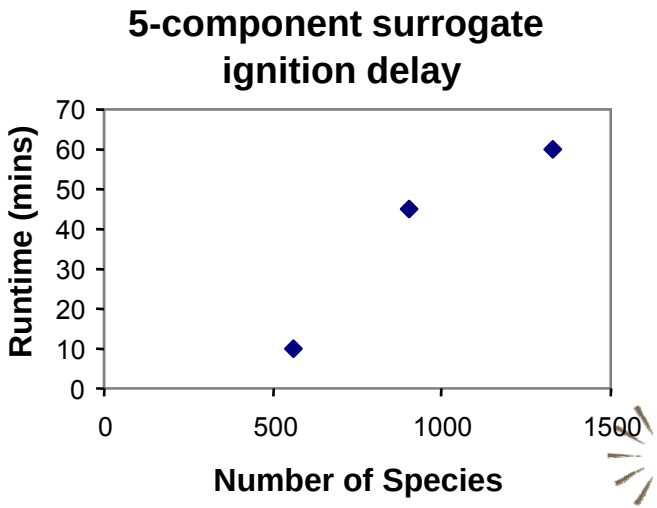
# Timing comparisons show how mechanism size relates to CPU time

- **Reduction of species results in significant reduction of CPU time**



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# Operating conditions considered

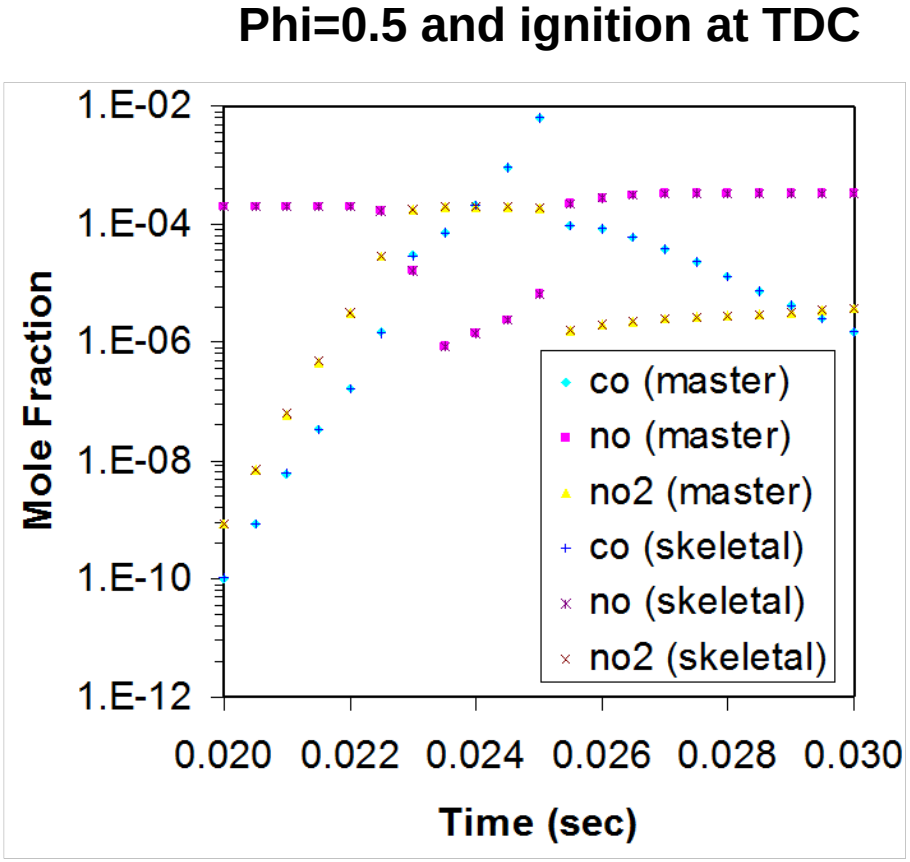
- **Gasoline HCCI Target conditions (8 multi-zone runs):**
  - Equivalence ratio=0.1, 0.2, 0.5, 1
  - Initial temperature adjusted so that ignition occurs at TDC and at TDC-10CAD
  - Mass distribution of 10 zones sames as that of Aceves et al., (SAE 2000-01-0327)

| Zone # | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| Region | Crevice | | | | | Boundary Layer | | Core | | |
| Mass % | 2 | 1 | 1 | 1 | 2 | 5 | 10 | 18 | 25 | 35 |

- **Engine characteristics:**
  - Starting pressure = 1 bar
  - Engine speed = 1200 rpm
  - Displacement volume = 1600 $cm^3$
  - Engine compression ratio = 15.0
  - Starting crank angle = 180
  - EGR = 20%
  - Engine connecting rod to crank radius ratio = 3.7

# Results show that, for emissions, DRG works well only up to ~44% reduction

- **Results are good for 44% skeletal reduction with DRG**
  - 1380 species → 774
  - 6138 reactions → 3572
  - 170 hours run-time → 52
  - All results within 10% relative tolerance and 0.01 ppm absolute tolerance
    - 658 species and 3182 reactions with 20% relative tolerance and 1 ppm absolute tolerance
- **Reduction size limited due to need for keeping more pathways to get $NO_x$ and CO right**



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# There are limits to how small you can get with a skeletal approach

- **Maximum reduction without compromising accuracy: 50-80%**
  - n-heptane ignition delay: 561 -> 256 species
  - n-heptane flamespeed: 561 -> 121 species
  - 5-component surrogate ignition delay: 1328 -> 560 species
  - 5-component surrogate emissions: 1380 -> 774
- **Further reduction results in significant error**
- **Skeletal methods are usually a “first step”**

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- **Fuel analysis tools**
  - Octane Number Calculator
  - Cetane Number Calculator
- **Mechanism Reduction facility**
  - Skeletal vs. severe-reduction methods
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- **More performance improvements**
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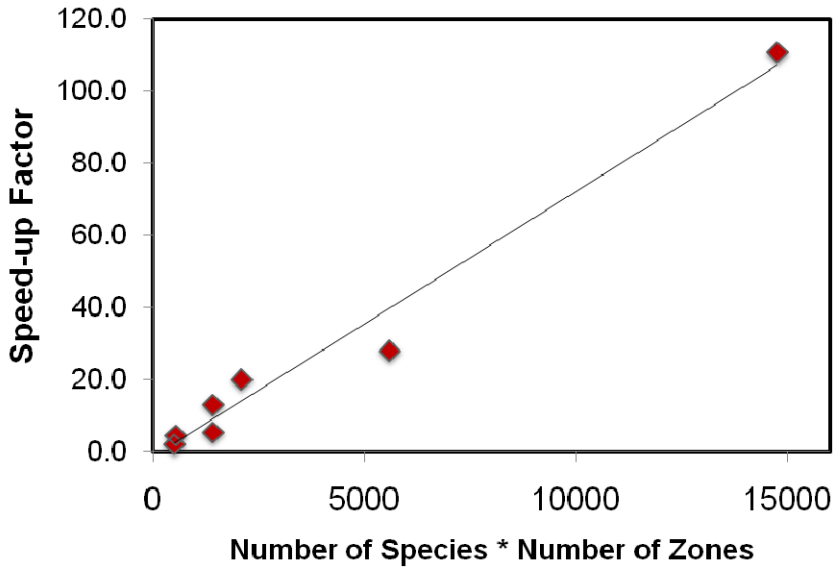
# Complementary efforts have been placed on further improvements to solver speed

- **Implementation of new sparse-matrix technology**
  - Important for large mechanisms
    - Species interaction matrix is sparse
  - Important for complex problems
    - Large reactor clusters in reactor networks
    - Multi-zone Engine simulations
- **Advanced methods of coupling kinetics to transport (CFD) simulations**

# Initial results for multi-zone engine simulations are very promising

- **Speed-up is relative to CHEMKIN-PRO**
- **Hours ⇨ a few minutes**
- **Days ⇨ ½ hour**

| Problem Description | # Species | # Zones | CPU time (h:m:s) | | Speed -up |
|---|---|---|---|---|---|
| | | | Before | After | |
| Closed system – MFC gasoline | 1440 | 1 | 0:11:36 | 0:02:03 | 5.7 |
| Closed system – n-hexadecane | 2116 | 1 | 0:20:15 | 0:01:00 | 20.3 |
| Multi-zone Engine – GRI-mech | 53 | 10 | 0:00:36 | 0:00:16 | 2.3 |
| Multi-zone Engine – n-heptane | 561 | 10 | 1:26:01 | 0:03:03 | 28.2 |
| Multi-zone Engine – 5-component | 1477 | 10 | 56:14:17 | 0:30:28 | 110.8 |




Benchmarks from a 64-bit Linux Blade server (Dual Core Xeon Processor, 4MB Cache, 2.0GHz, 1333MHZ FSB forPowerEdge 1955, 16GB RAM)



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# Summary:  Stay tuned – more on the way

- More speed
- Usability of larger mechanisms
- Automated mechanism reduction
- Practical tools for fuels analysis
- More advanced connectivity to multi-dimensional simulation