



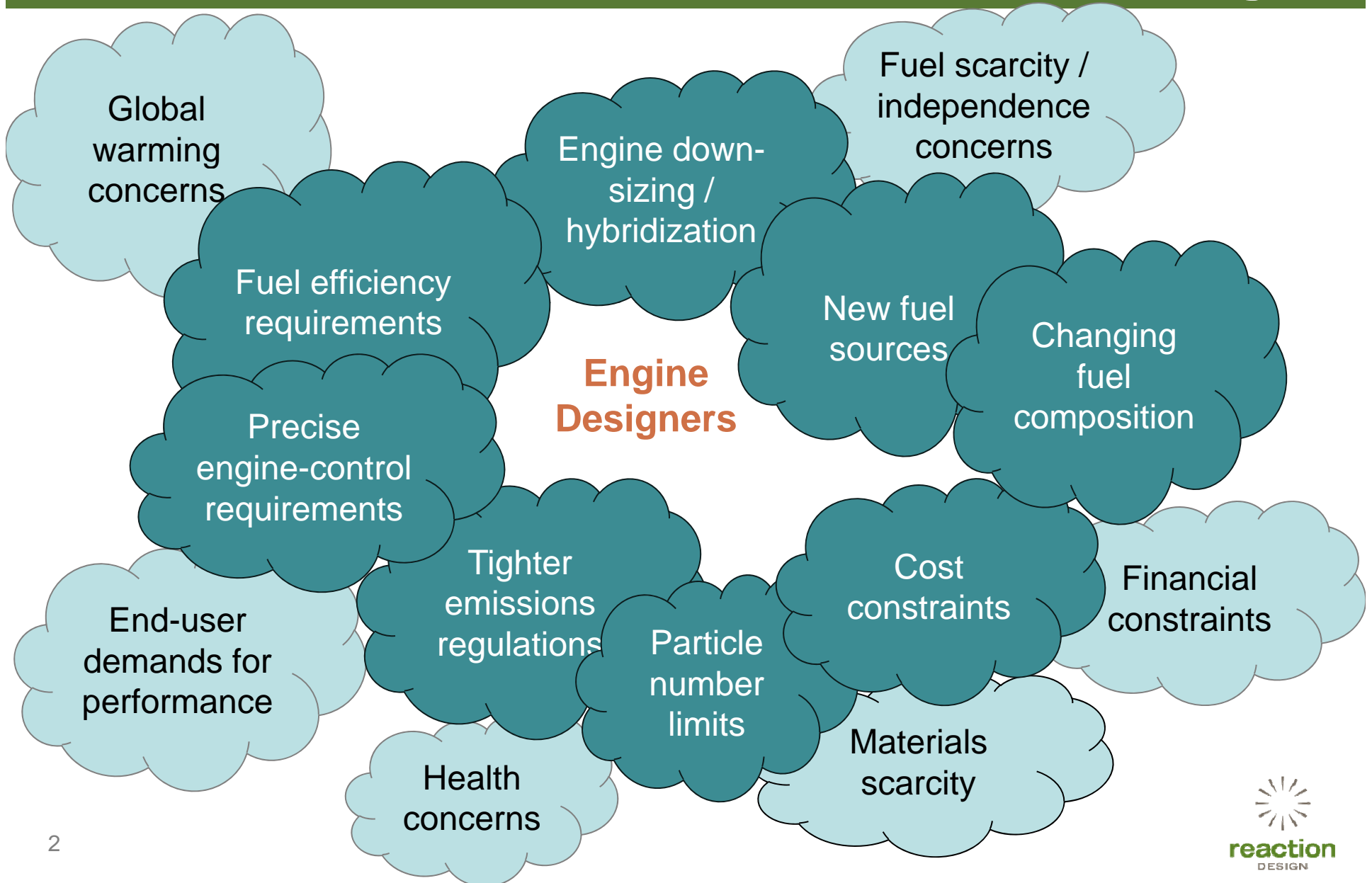
# Efficient-clean-combustion design demands new approaches to combustion simulation

Ellen Meeks

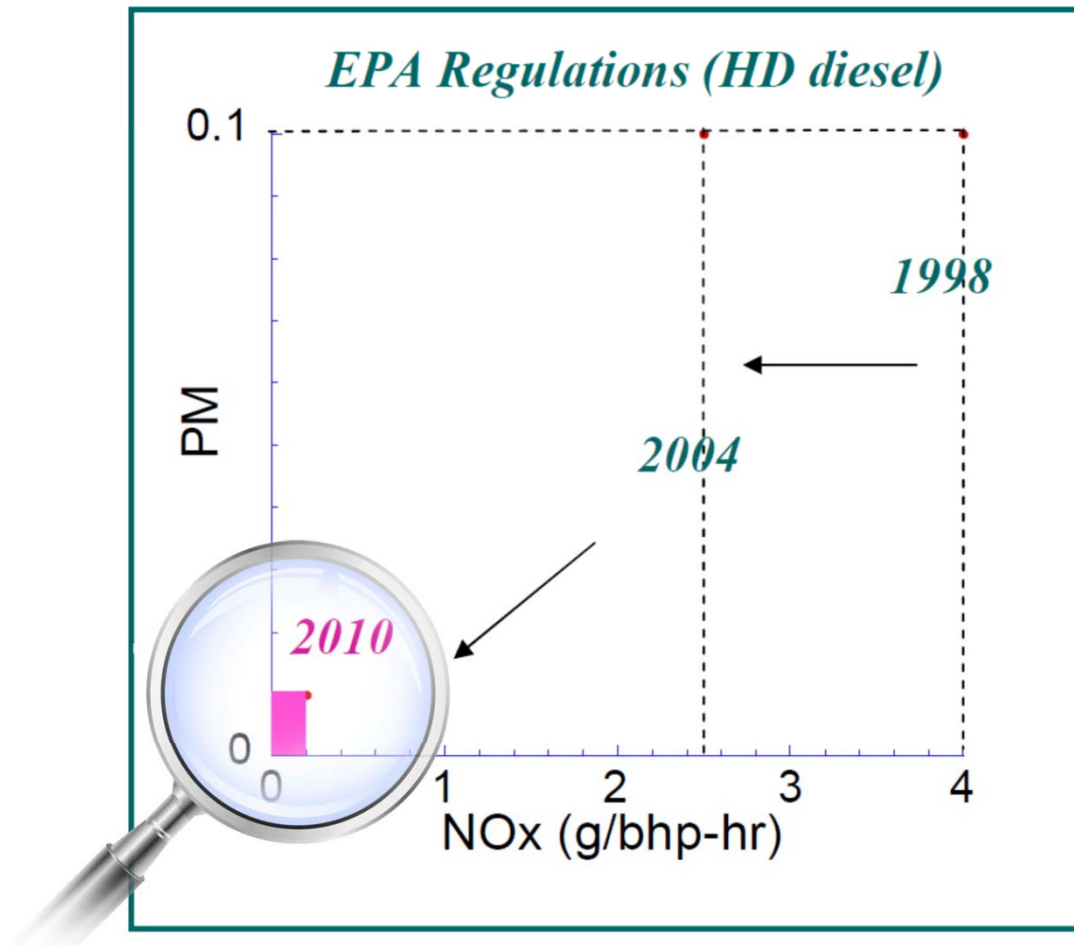


LEADING THE WAY TO CLEAN COMBUSTION DESIGN

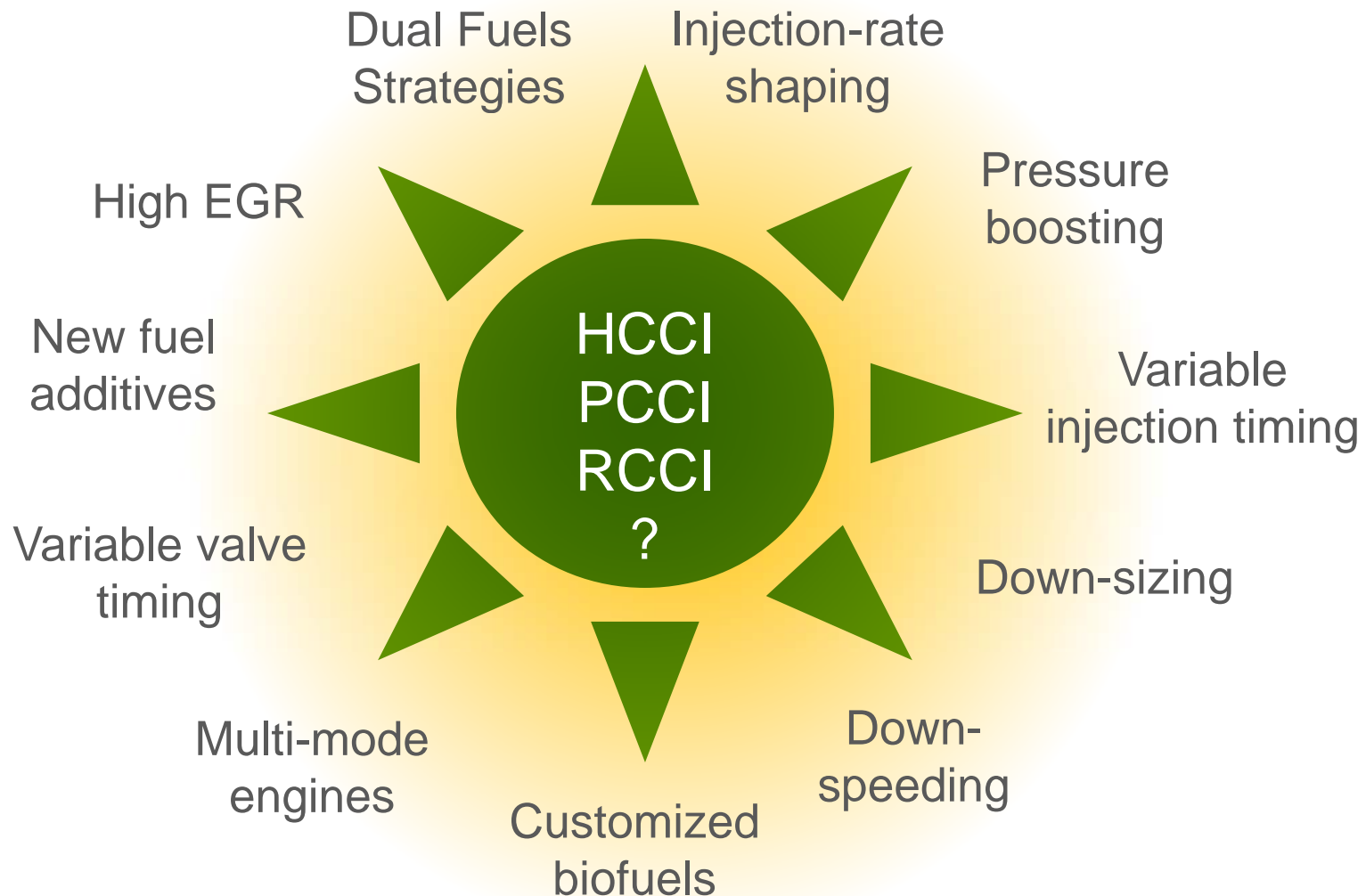
# For the engine designer, A requirements “storm” has been brewing



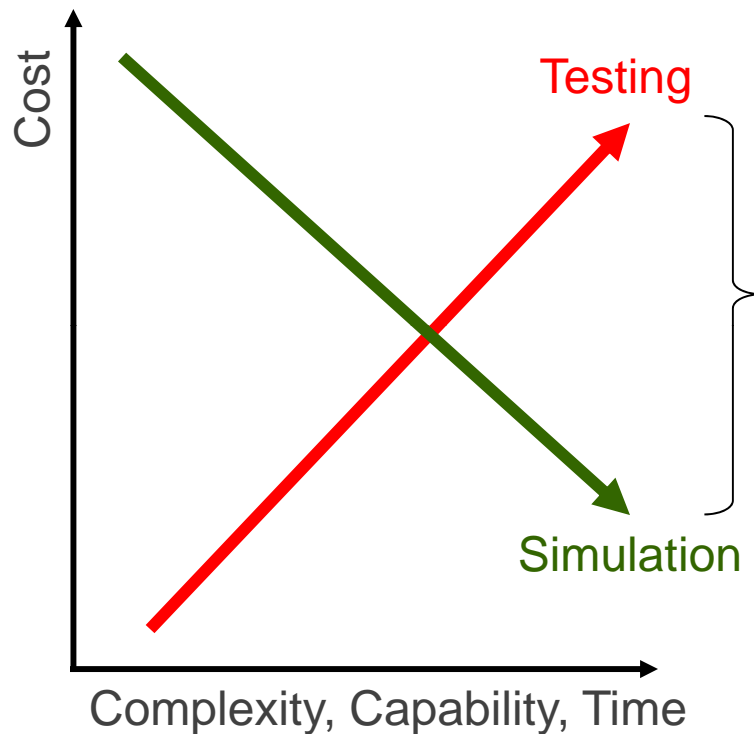
# Any new goals must be achieved without straying out of the NO<sub>x</sub>-Soot “box”



# Innovation is increasing design complexity

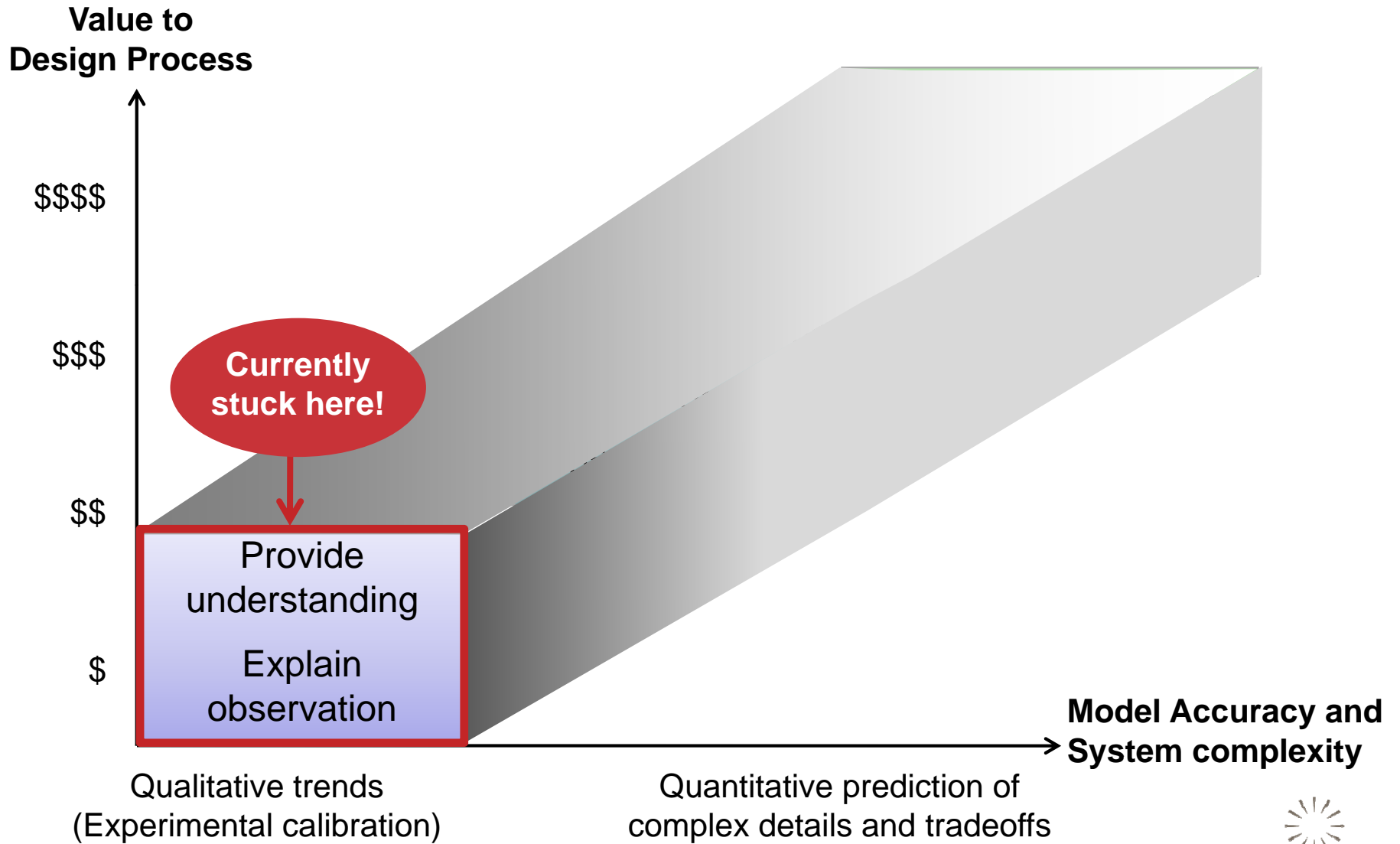


# With more complexity, there's more opportunity for simulation to reduce cost

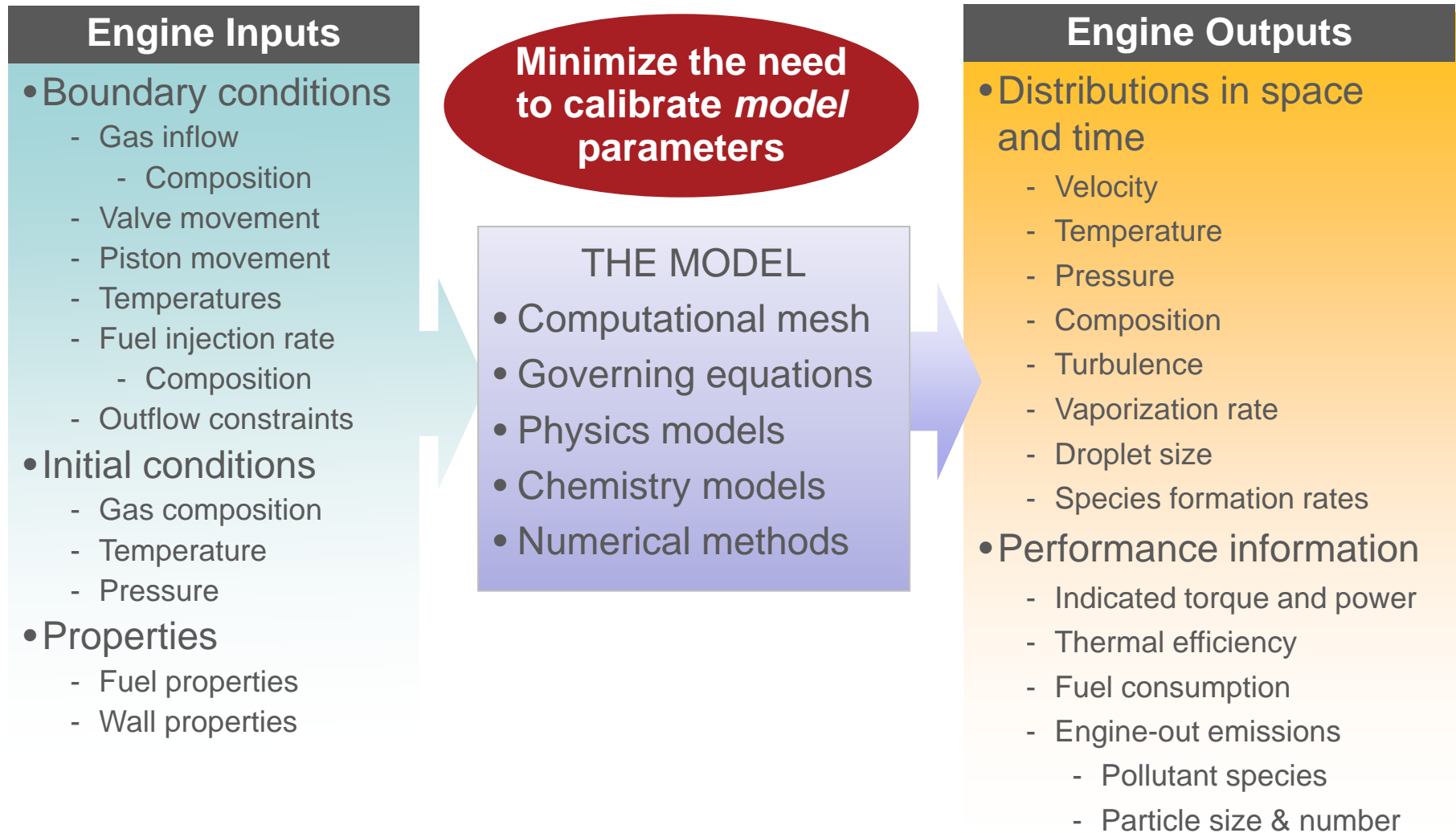


- **Opportunity to:**
  - Reduce risk
  - Improve use of testing
  - Speed development
  - Facilitate innovation

# Value of simulation depends on accuracy



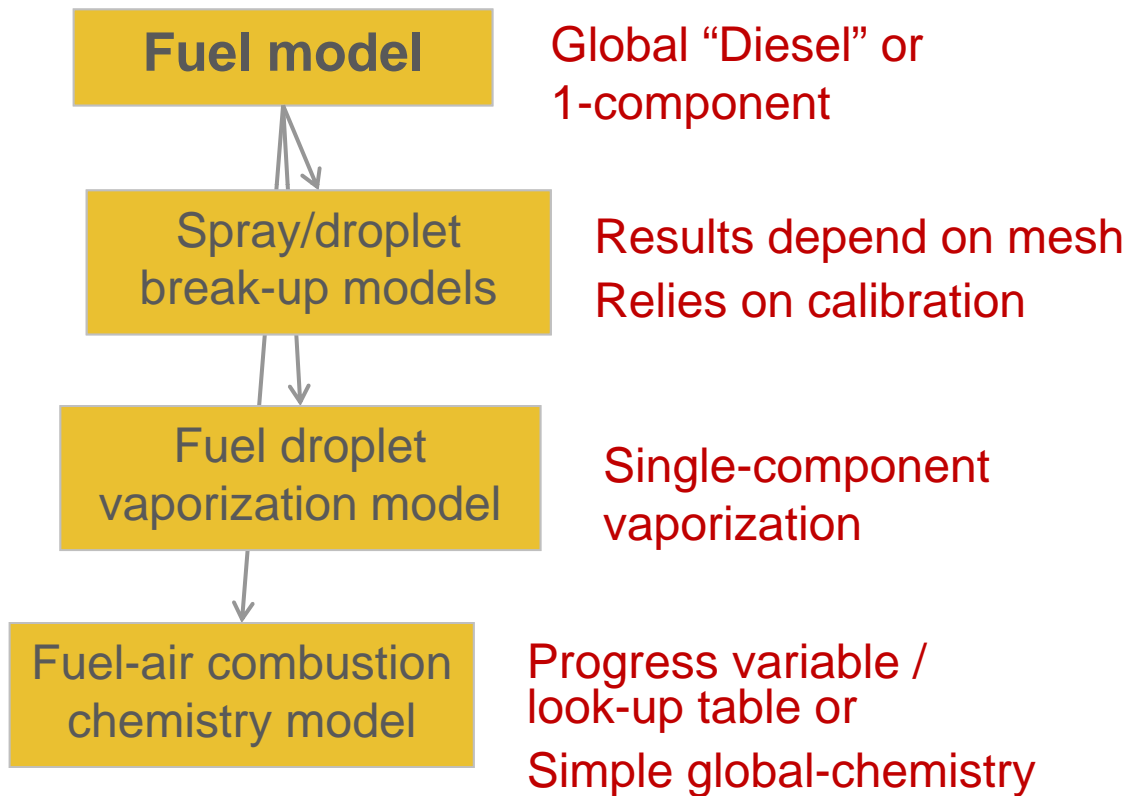
# An accurate model predicts engine outputs based on *engine* inputs





# Current practice cannot predict design needs

## Existing Model Approaches



## Unable to even approximate:

- Effects of fuel variability on:
  - Ignition
  - Efficiency
- Behavior of a new fuel
- Effects of multiple injections
- Emissions details (at 2010 levels)
  - CO, UHC, NO<sub>x</sub>
  - Soot precursors
  - Aldehydes, phenols, ...

# Traditional barriers to using better fuel-chemistry and fuel-spray models in CFD

- **Real fuels are too complex**
  - Don't know how to represent fuel differences
  - Don't have reliable models of the fuel chemistry
  - Don't have reliable models of the fuel spray / vaporization
  
- **Simulations are too time-consuming**
  - Detailed mechanisms are too large to be practical
  - Chemistry takes up >80% of calculation
  - Can't afford more chemistry detail
  - Must have very refined mesh to get good spray

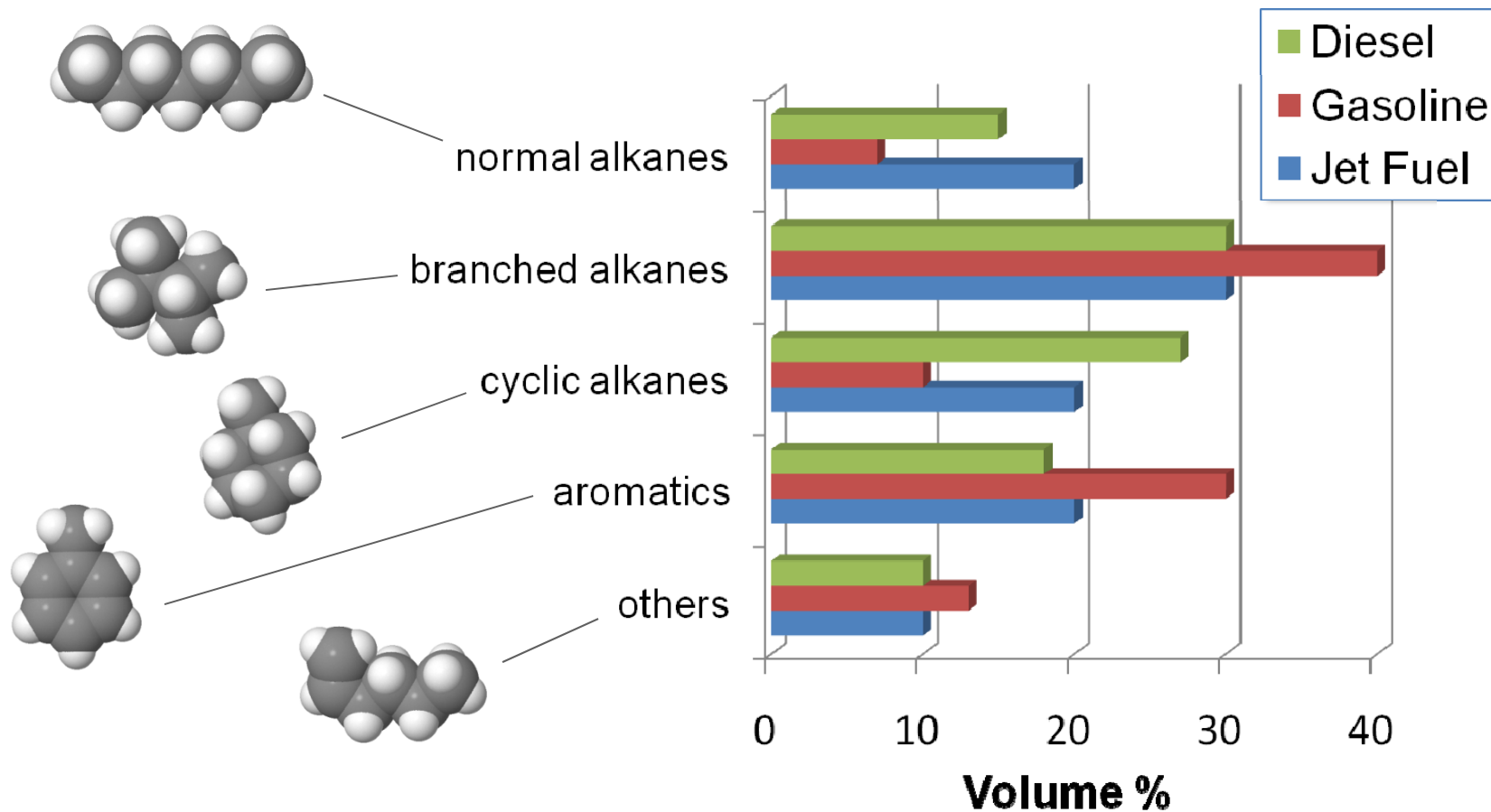
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  - Can't afford more chemistry detail
  - Spend too much time calibrating spray models

# Recent developments address these issues

- **There is a wealth of knowledge about fuels**
  - Surrogate (model) fuels represent fuel differences
  - There are many validated models now available
  - Good spray models are available that have been validated against detailed experimental data

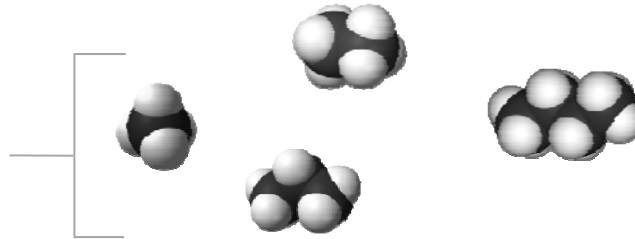
# The concept of “Surrogate Fuel” is now widely accepted in combustion science



# Alternative fuels can also be well represented by a handful of molecules

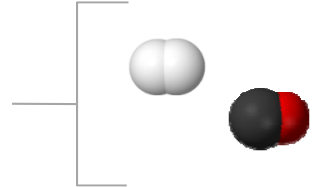
- **Natural gas / LNG**

- Small alkanes,  $C_1$ - $C_4$



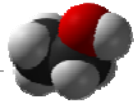
- **Syngas**

- H<sub>2</sub> / CO



- **Bio-fuels**

- Alcohols

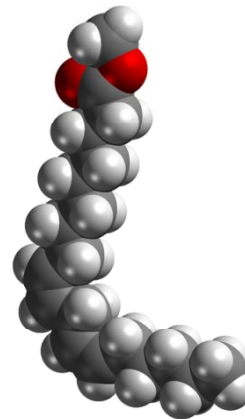


- Methyl esters

- Furans

- Algae

- Similar to crude oil-derived fuels



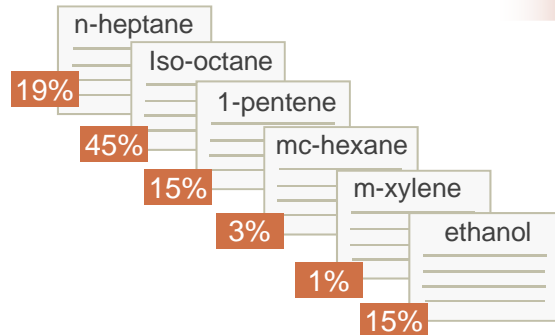
# A surrogate blend can match any combination of fuel properties

**Desired Fuel Properties**

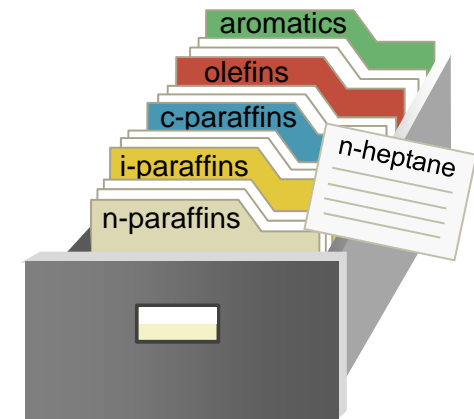
Set target characteristics  
Class composition  
Heating value  
Octane / Cetane #  
H/C ratio, O content  
Boiling points  
Sooting threshold index

Match with fuel palette  
Select surrogate components  
optimize blend

**Surrogate fuel composition**



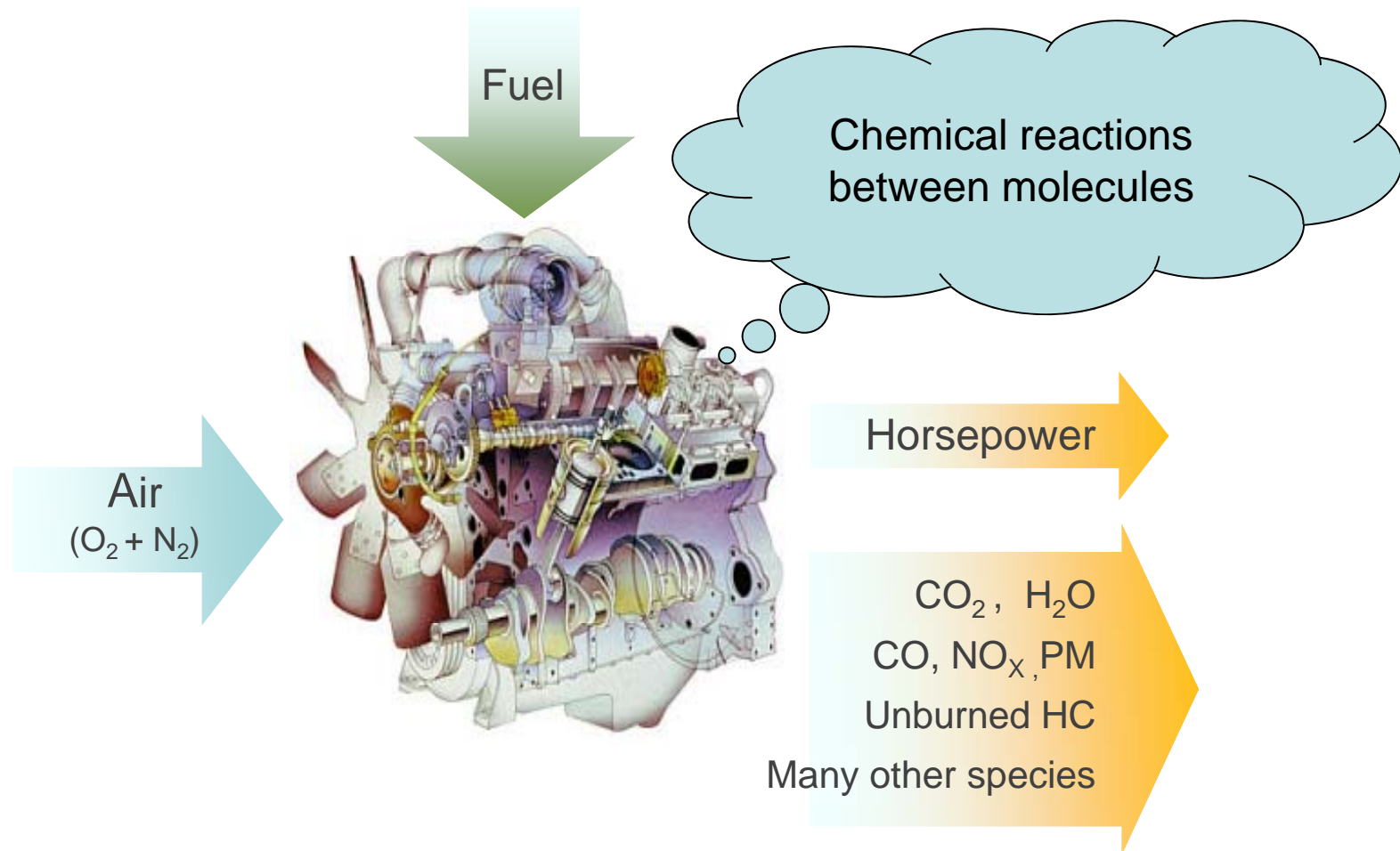
Database of Model Fuel Properties



**Fuel Model for Simulation**

# A chemistry “mechanism” is key to describing the surrogate-fuel behavior

- The engine as a chemical plant:



# There is a recent upsurge in availability of reaction mechanisms for liquid fuels

- **Examples of sources:**

- LLNL Combustion Chemistry group, funded by DOE
  - Pioneering work on automotive fuels mechanisms
- Model Fuels Consortium (MFC), funded by industry
  - Unified mechanism / database including > 30 fuel components & emissions-formation mechanisms
  - Focused on automotive fuels
- MURI Project on Surrogate Fuels, funded by U.S. AFOSR
  - Focused on Conventional and F-T jet fuels
- CEFRC, funded by DOE
  - Focused on fundamental kinetics for non-petroleum fuels
- Other academic and research institutions

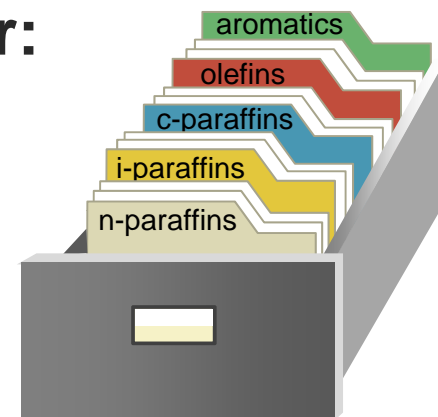
# Example: MFC Mechanism Database

## Validated Liquid-fuel Components

Fuel component	Relevant to modeling:		
	Gasoline	Diesel	Jet Fuel
n-heptane	✓	✓	
n-decane	✓	✓	✓
n-dodecane		✓	✓
n-hexadecane		✓	
i-octane	✓	✓	✓
heptamethylnonane		✓	✓
Toluene	✓	✓	✓
n-propylbenzene	✓	✓	✓
o-xylene	✓	✓	✓
m-xylene	✓	✓	✓
p-xylene	✓	✓	✓
naphthalene		✓	
1-methylnaphthalene	✓	✓	✓
Cyclohexane	✓	✓	✓
Methylcyclohexane	✓	✓	✓
Decalin	✓	✓	✓
1-pentene	✓	✓	
2-pentene	✓	✓	
1-hexene	✓	✓	✓
2-hexene	✓	✓	✓
3-hexene	✓	✓	✓
2-methyl-2-butene	✓	✓	✓
Ethanol			
Butanol			
DME			
Methylbutanoate			
Methylstearate			
ETBE			
NOx	✓	✓	✓
PAH pathways	✓	✓	✓
Soot	✓	✓	✓

- **Self-consistent set of chemistry models for:**

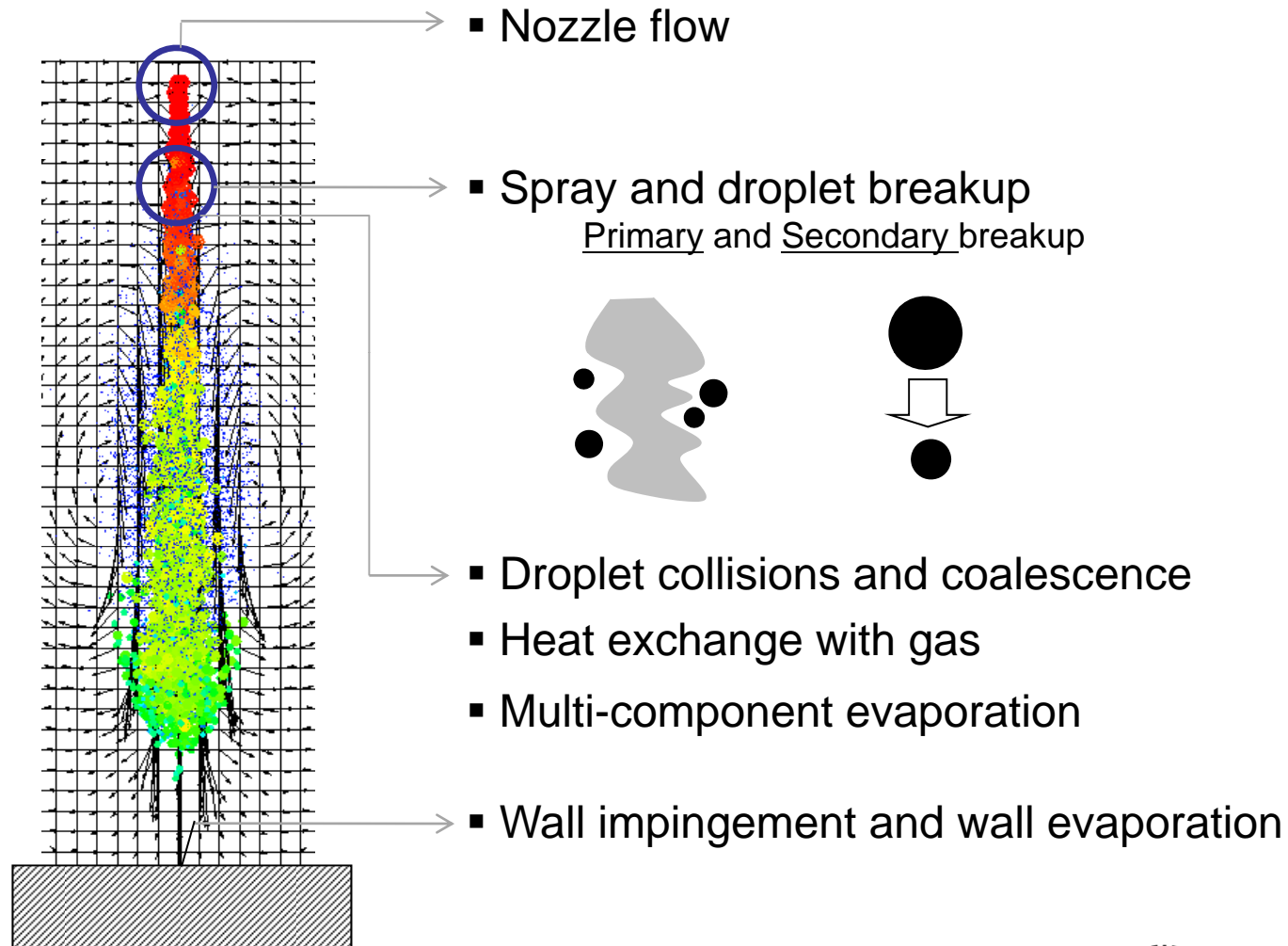
- Liquid fuels
- Gaseous fuels
- Emissions formation



- **Validated against data from over 400 fundamental experiments**

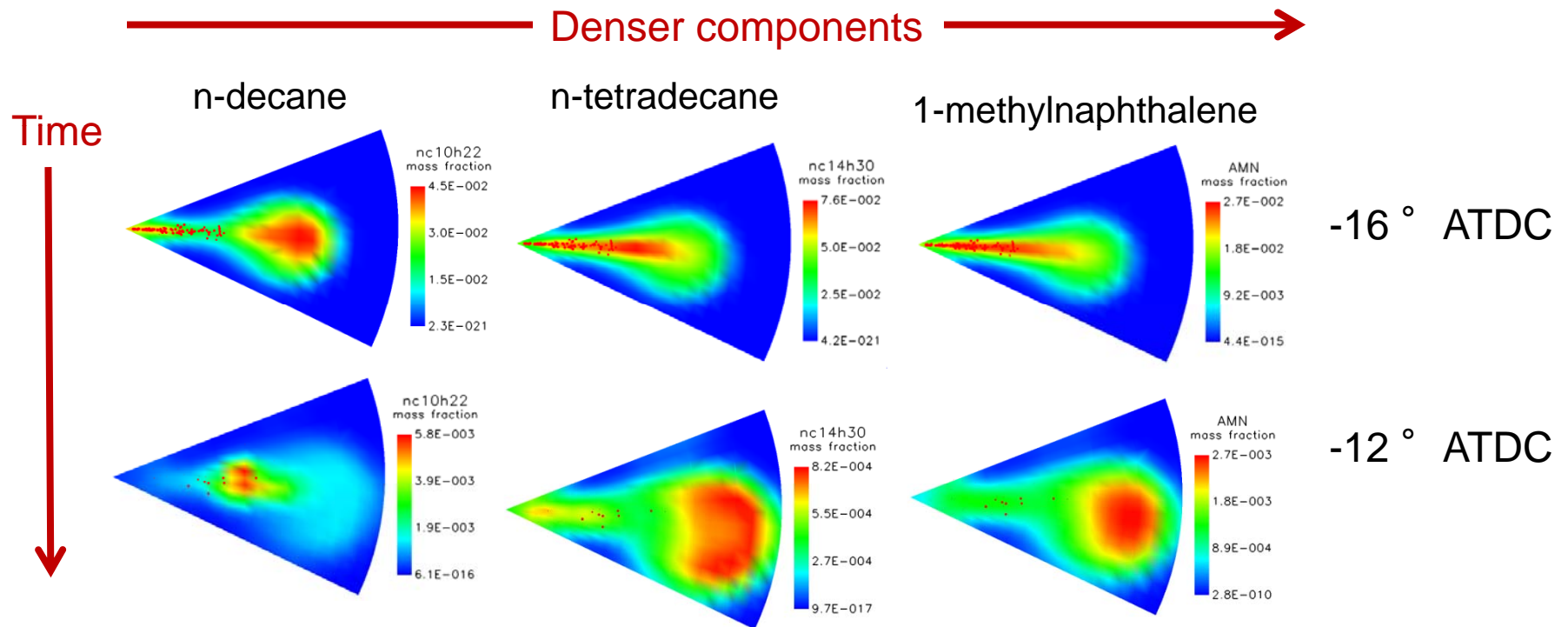
Ref: SAE2010-01-0545, SAE2010-01-0541

# Physical models have also advanced to capture details of fuel-injection phenomena



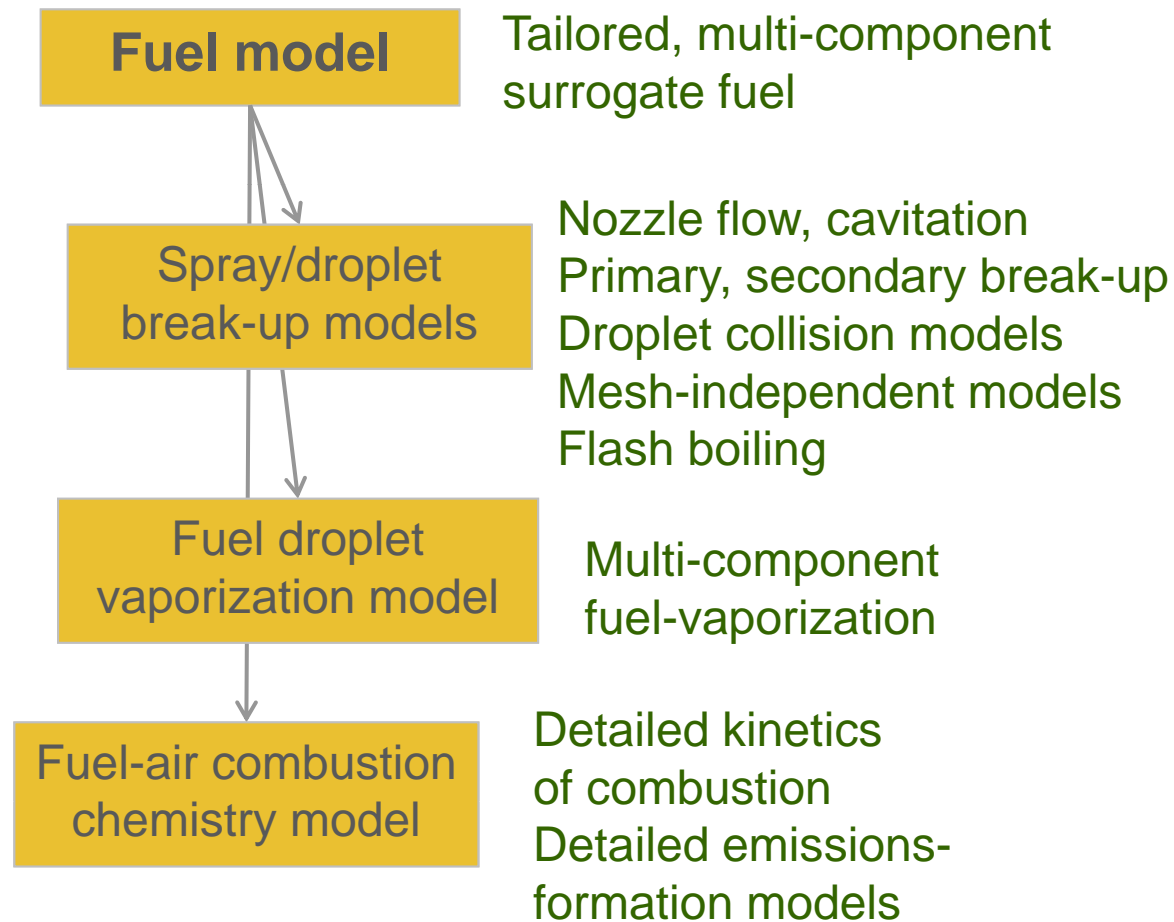
# Multi-component surrogate fuels can capture vaporization stratification

## Vapor Fractions of Multi-component Fuel for LTC Diesel Engine



# Detailed fuel models provide predictions that are otherwise unattainable

## Accurate Model Components



## Can Predict:

- Effects of fuel variability
  - Ignition timing
  - Combustion phasing
  - Efficiency
- Behavior of a new fuel
- Effects of multiple injections
- Emissions details (at 2010 levels)
  - CO, UHC, NO<sub>x</sub>
  - Soot precursors
  - Aldehydes, phenols

# But what about simulation time?

- **Real fuels are too complex**
  - Don't know how to represent fuel differences
  - Don't have good models of the chemistry
  - Don't know if we can believe the detailed models
- **Simulations are too time-consuming**
  - Detailed mechanisms are too large to be practical
  - Can't afford more chemistry detail
  - Spend too much time calibrating spray models

# Effective simulation must be efficient

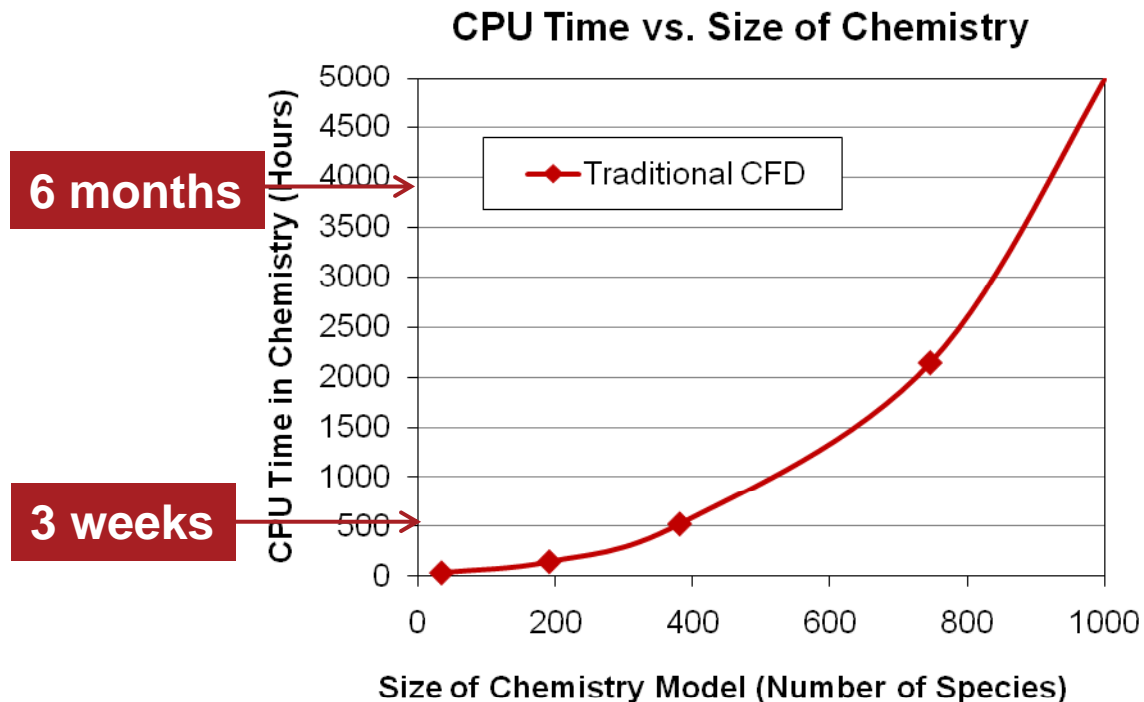
- **Engineering timescale**
  - Turn-around time < ~15 hours
    - “I go home at night and the next morning I have a solution”
- **Reasonable (available) compute resources**
  - ~8 to 32 CPUs per run
- **Reliable convergence**
  - Allow jobs to run unattended
  - Enables parameter studies
  - Enables optimization
  - Enables use in controller design

# Progress on many fronts help eliminate the tradeoff between speed and accuracy

- **More accurate solution of flow**
  - Better mesh quality, automated mesh generation
- **Multi-core and multi-CPU computers**
  - Parallel-processing without access to super computers
- **Advanced chemistry-solution techniques**
  - Dramatically reduce chemistry-solution time
- **Better spray representation**
  - More accuracy without refinement of grid around spray

# Attempts to directly couple chemistry to flow are typically very inefficient

- Solvers are not tailored to chemistry



## Nature of Chemistry

- Disparate timescales
- Minor species have large impact on major species
- Each species interacts with only a fraction of others

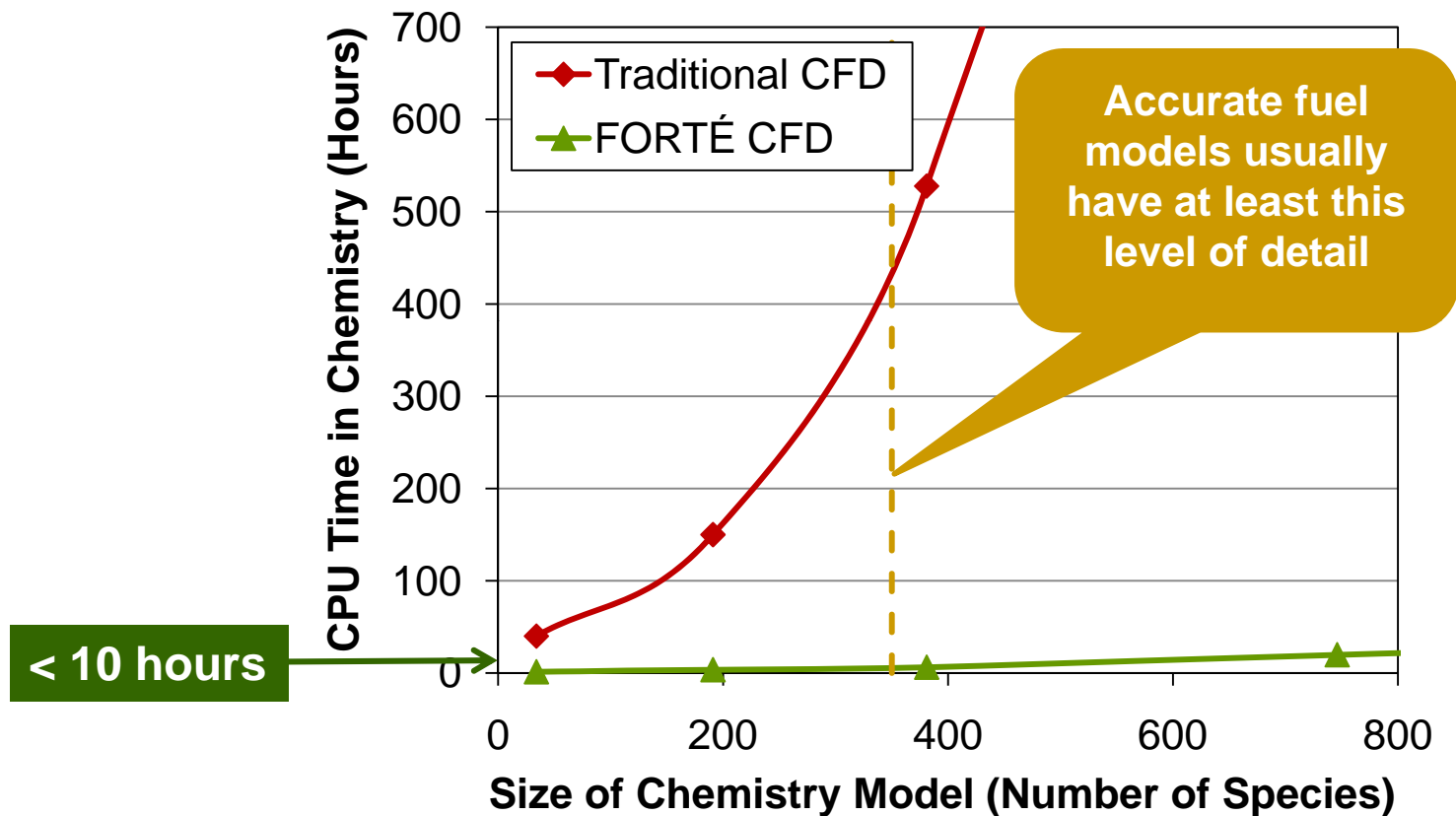
- Solution time  $\sim (\text{Number of Molecules})^3$
- Convergence can be very unstable

# Advanced solution techniques completely change the chemistry scaling

- **Use of sparse matrix solver\***
  - **Changes Scaling from  $N^3$  →  $N$**
- **On-the-fly mechanism reduction\***
  - **Reduces chemistry time by ~10 – 100X**
- **On-the-fly data clustering\* calculations**
  - **Reduces chemistry time by ~10 – 100 X**

\*From: L. Liang et al. IMEM 2009

# Advanced solution techniques completely change the chemistry scaling

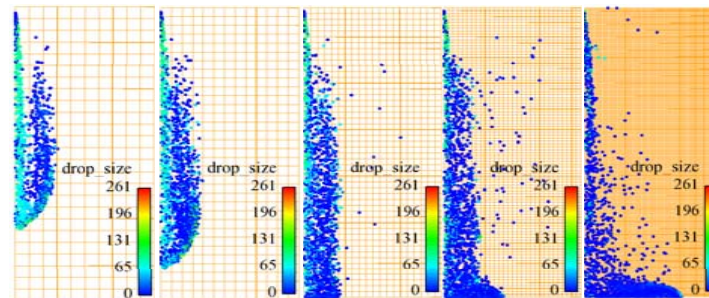
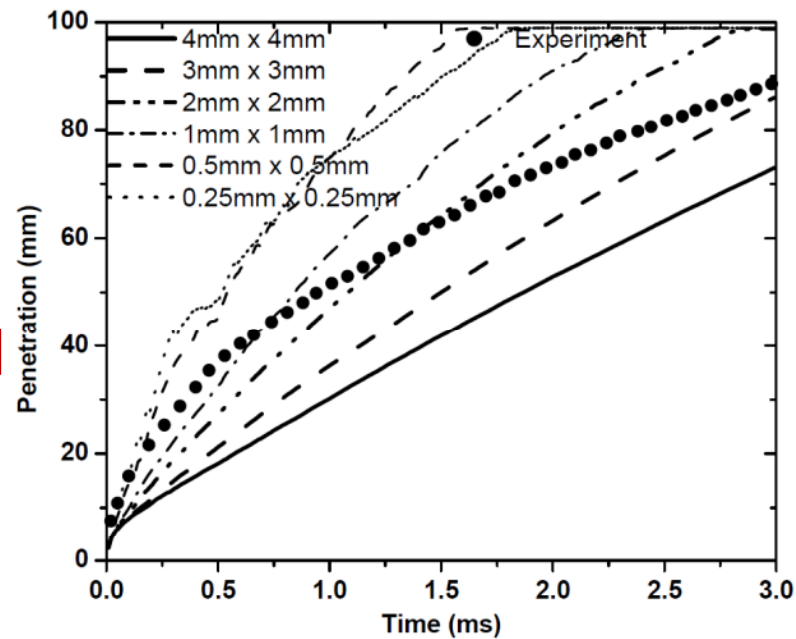


# There has also been great progress on efficiency of accurate fuel-spray models

Old model:

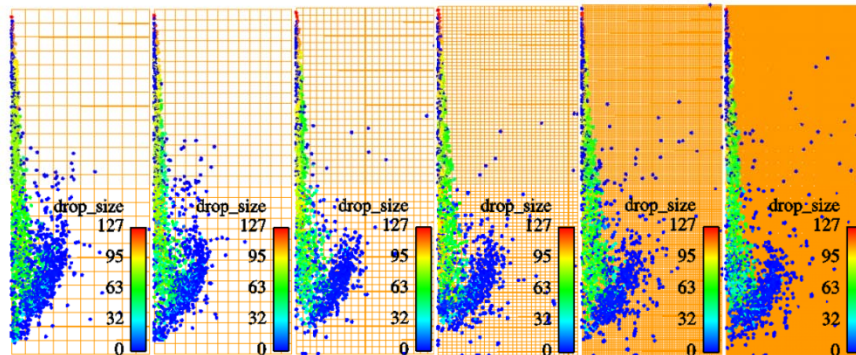
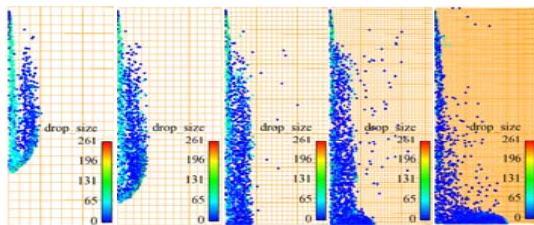
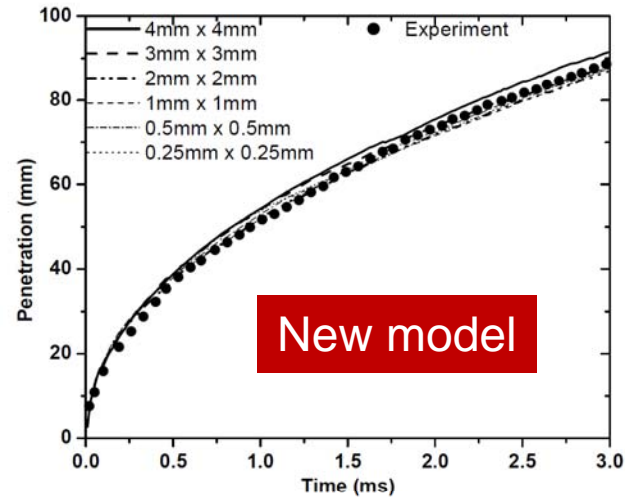
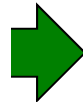
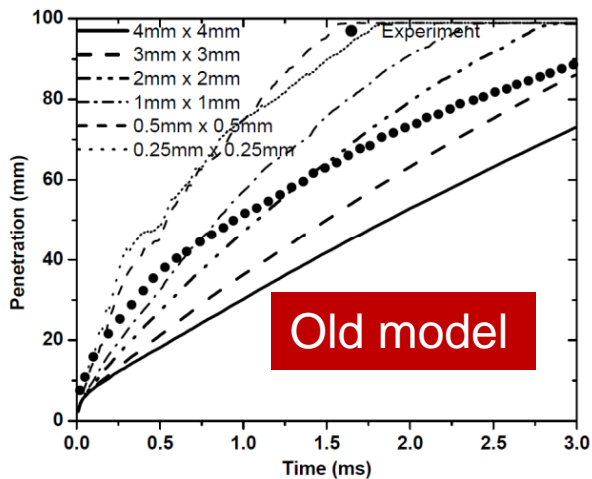
Results depend on grid size

Old model



# There has also been great progress on efficiency of accurate fuel-spray models

- Better physics for the droplet-vapor interaction



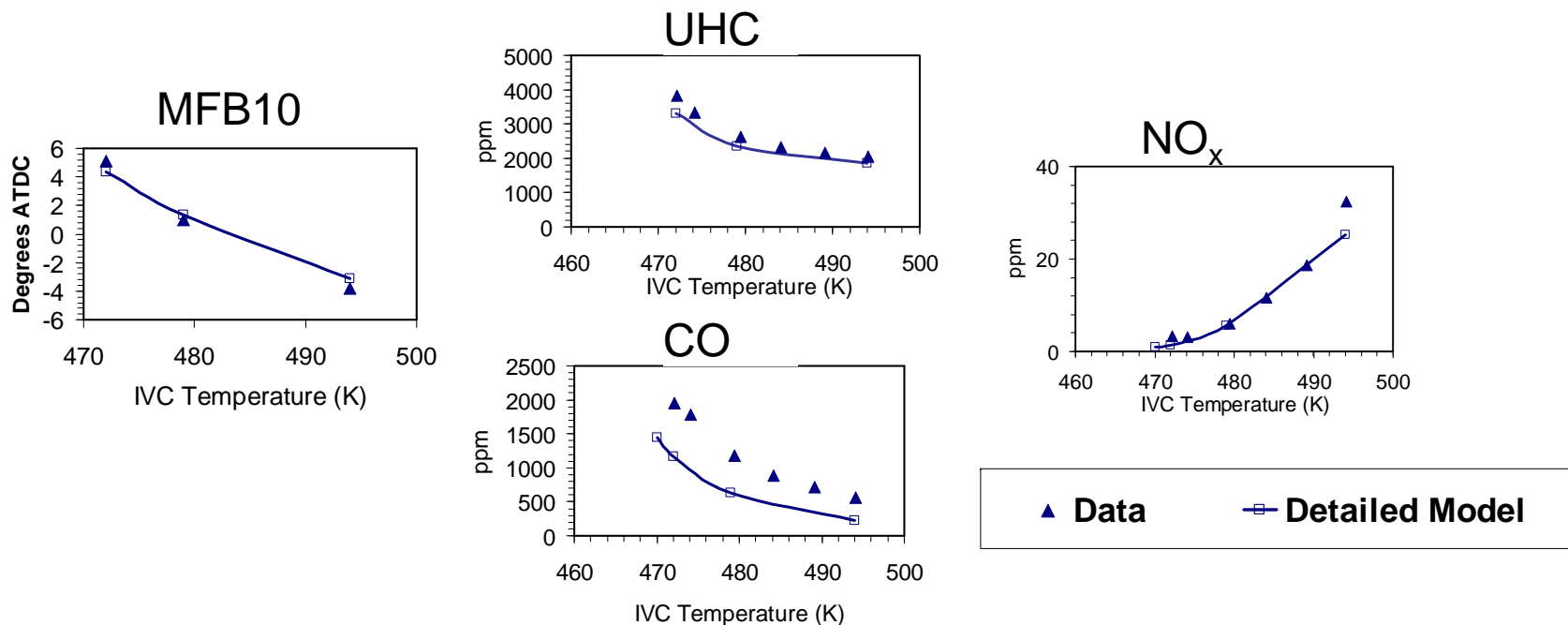
# Putting it all together:

- **Better physics & numerical methods enable  $\sim 10^3$  times faster solution**
  - With fuel-combustion detail intact
  - With advanced spray and vaporization
- **Accuracy at engineering timescales is possible**
  - Especially for kinetics-controlled engine modes
  - Provides insights not available through experiment alone
  - Enables focus of resources on other weak links
    - e.g., Turbulence models

# Example: Emissions predicted in HCCI

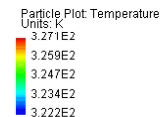
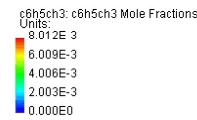
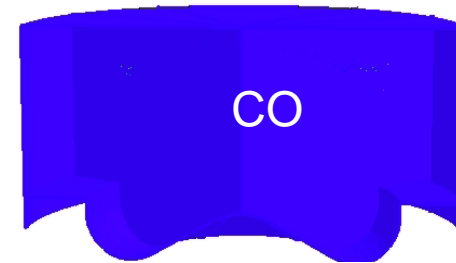
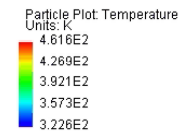
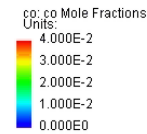
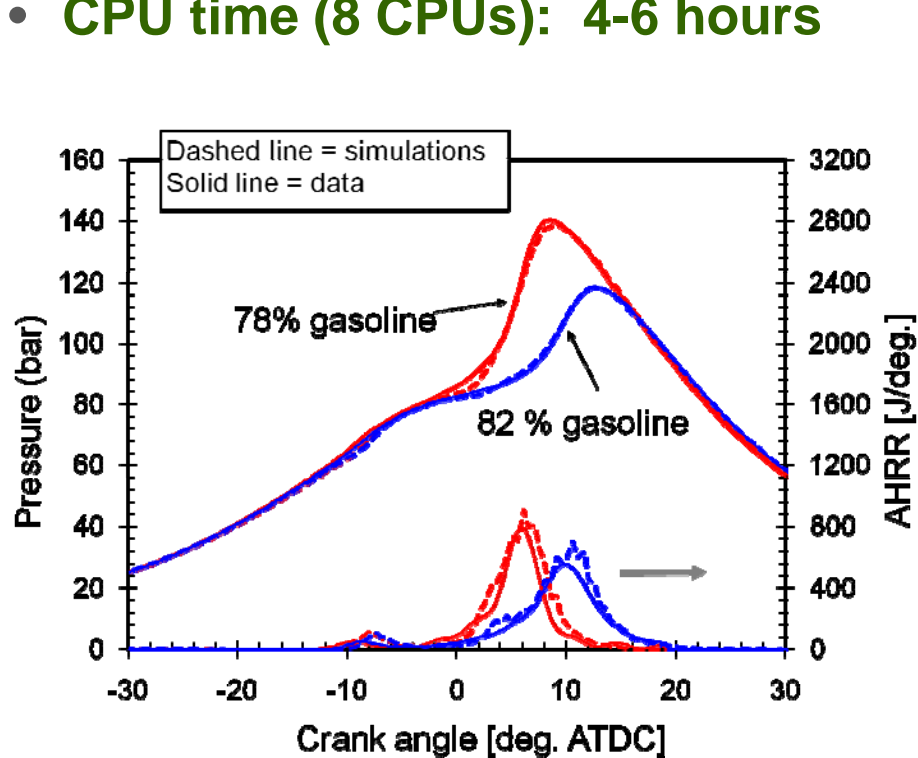
- Detailed PRF + ethanol mechanism (427 species)
- CPU Time (1 CPU): 13 hours [vs. Weeks with conventional CFD]

Variation in IVC Temperature

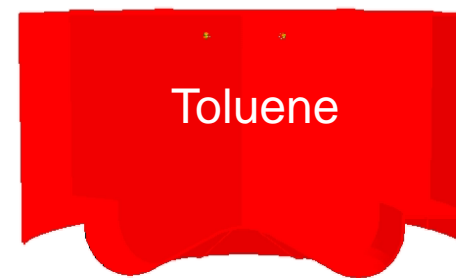


# Example: Dual fuel heavy-duty engine

- RCCI Simulation with 470-species for Diesel & Gasoline
- CPU time (8 CPUs): 4-6 hours



Time: 4.  
Reactio

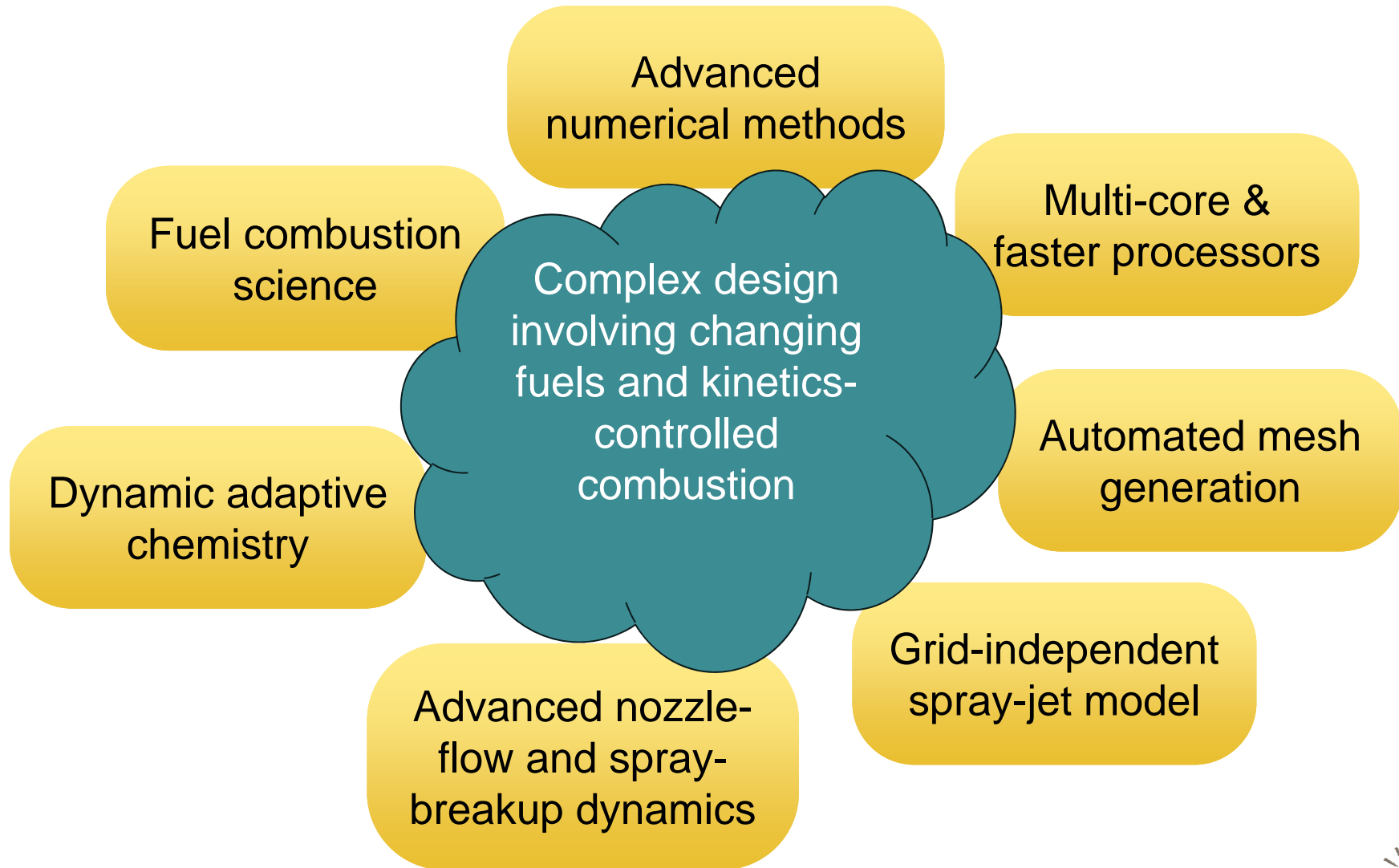


CO and UHC agree with experiment

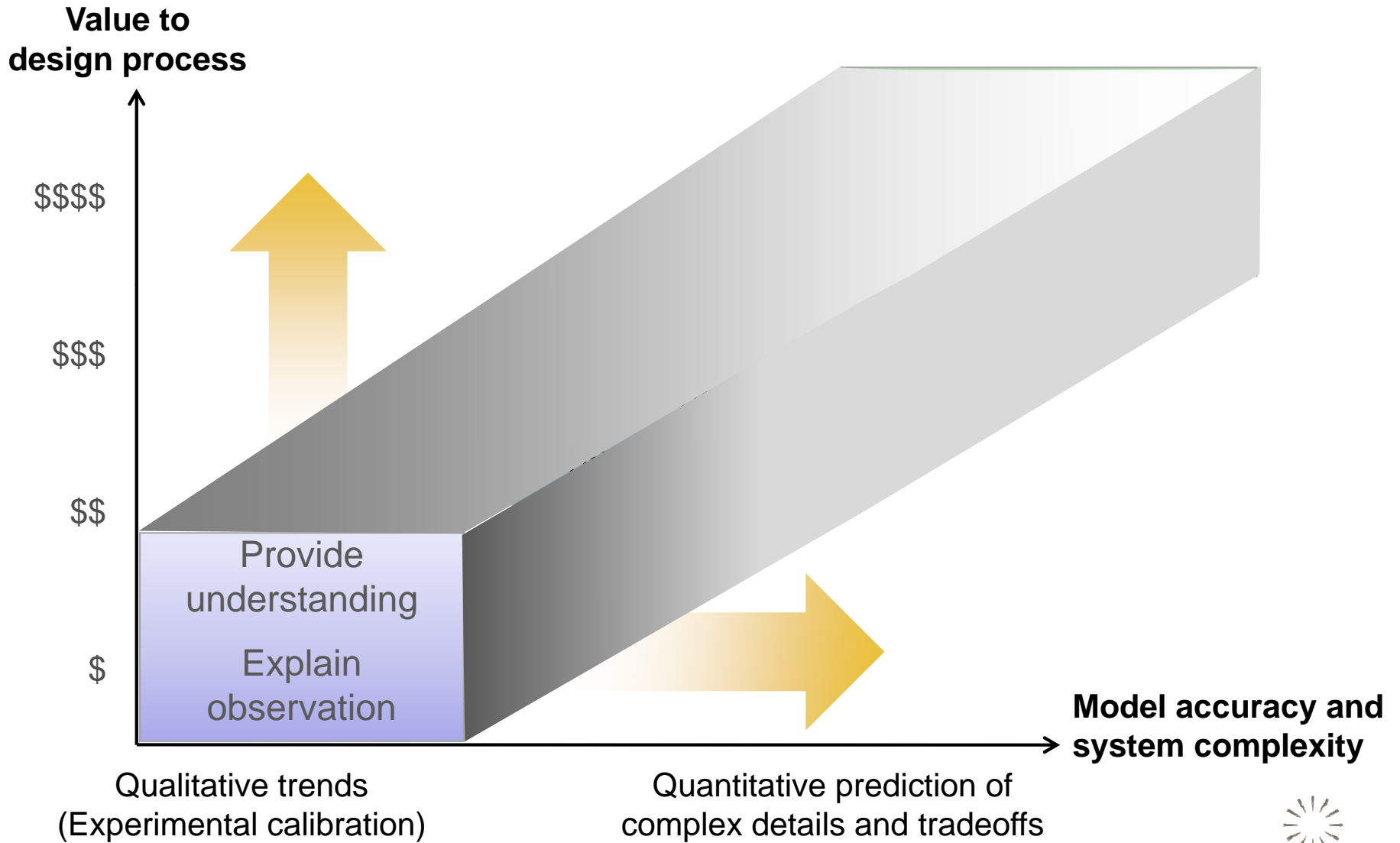
Time: 3.8497E-3, Crank Angle: -64.9724  
Reaction Design FORTÉ



# In summary: new methods enable study of advanced engine concepts



# Value of simulation depends on accuracy



# Acknowledgements

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**B. Bunting**



**Contributions from Reaction Design Team:**

**K. V. Puduppakkam, D. Hodgson, L. Liang, A. Modak,  
C. Naik, T. Garratt and V. Flores**