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# Large Eddy Simulation (LES) Applied to Advanced Engine Combustion Research


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**Support Provided by the DOE**
**Office of Energy Efficiency and Renewable Energy**
**Vehicle Technologies Program**
**is Gratefully Acknowledged**

# Overview

## Timeline

- Project provides fundamental research that supports advanced engine development
- Focused on next generation simulations, models, flow-solvers, and workflow for model validation using Large Eddy Simulation
- Project scope, direction, and continuation evaluated annually

## Barriers

- Two sets of barriers addressed
  1 – Lack of fundamental knowledge of both Diesel and GDI combustion regimes
  – Understanding coupled effects of fuel-injection, turbulent-mixing, heat-transfer, chemical-kinetics, and geometry on combustion and emissions over broad operating ranges

  2 – Lack of predictive models for engine combustion design and control
  – Efficient and routine use of advanced High-Performance-Computing (HPC) codes and computer architectures

## Budget

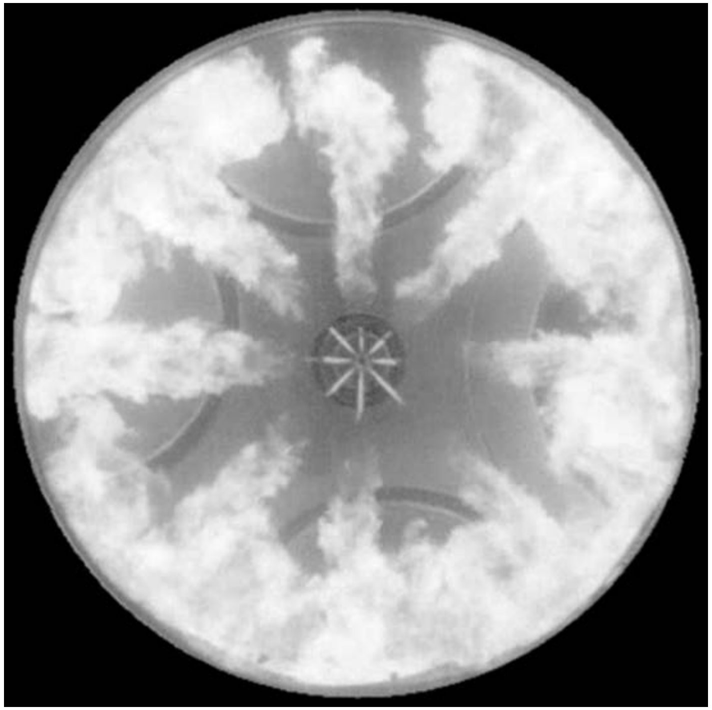
- Total Project Funding
  - FY15 – \$390K
  - FY16 – \$390K

## Partners

- CRF Engine and UQ Groups
- Penn State, Stanford, Michigan CERFACS (e.g., DOE/NSF/FOA)
- DOE Office of Science
- Project Lead: Joe Oefelein

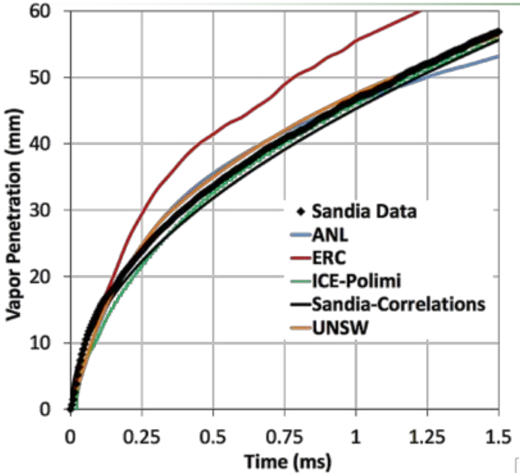
# Relevance … need for advanced model development is well recognized

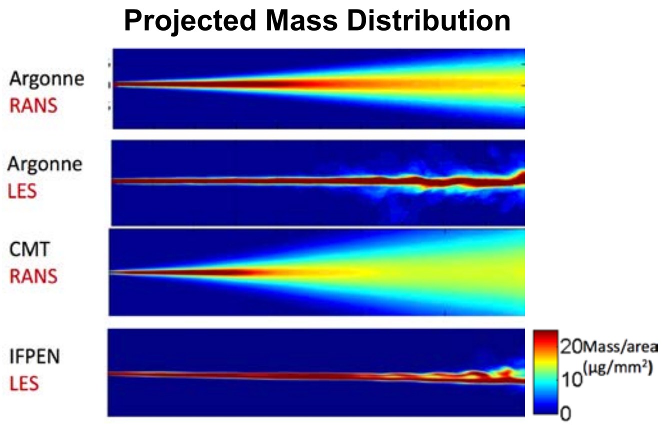
- Challenges … treatment of nonlinear, strongly coupled, multiphysics/multiscale phenomena
  - High-Reynolds-number turbulence and scalar-mixing processes (Re > 100,000)
  - High-pressure mixed-mode combustion
  - Compressible, acoustically active flow
  - Complex geometries, heat transfer
  - Complex fuels, multiphase flow
- Current models not predictive, current solvers do not scale on advanced HPC architectures
  - Coupled system of sub-models must be treated simultaneously since accuracy of simulations is limited by least accurate sub-model
  - Cost of simulations must be reduced and fidelity (resolution, models) increased through improved use of the full hierarchy of HPC resources
- A new generation of models and flow solvers combined with additional data and improved workflow aimed at model validation is required
  - Experimental data alone insufficient for validation
  - High-resolution LES combined with first principles models and UQ can provide next level of precision

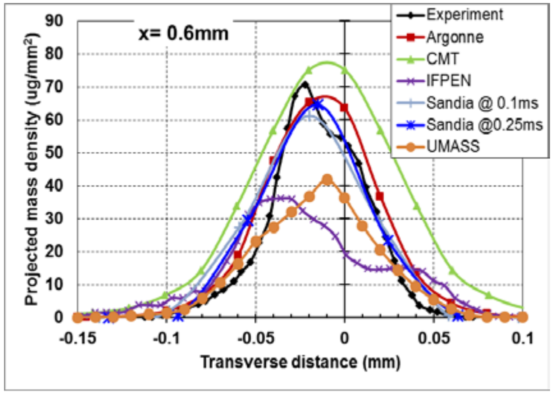


Diesel spray combustion imaging through transparent piston (Mark Musculus, Sandia)

# Deficiencies in model development have been demonstrated for years

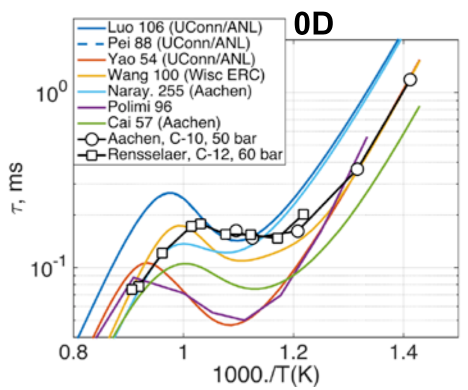


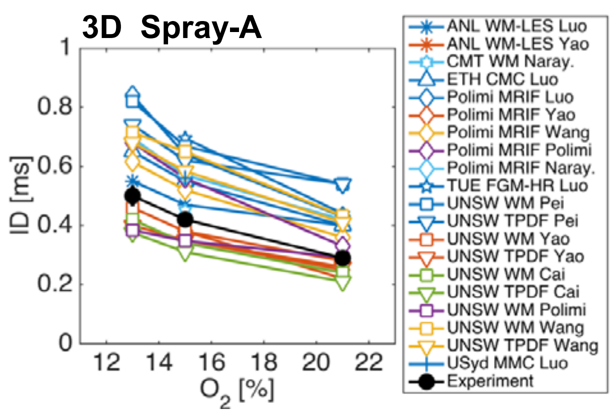



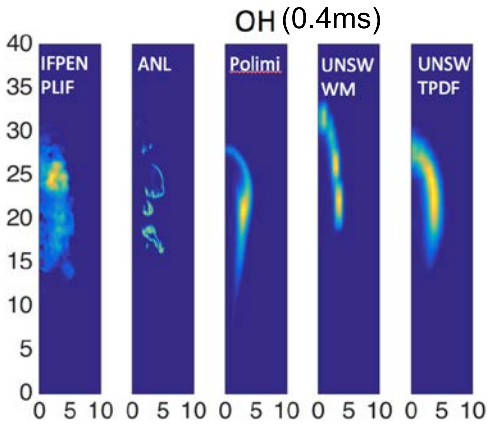




**Inconsistencies in non-reacting calculations observed in all ECN workshops (here ECN4)**

- Correct vapor penetration but large scatter in other quantities




**Similarly, large scatter is observed in reacting calculations**

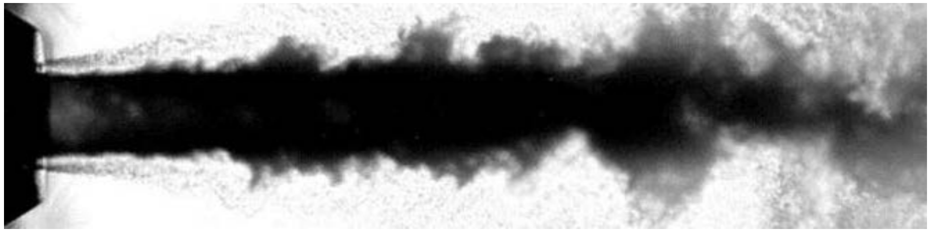
- Large variability between chemical mechanisms and shock tube data, and scatter in ignition delay (ID) in Spray-A simulations



**There is a distinct lack of discriminating data due to many competing effects in both models and numerical methods ...**

# Milestones

- Subtask 6.1 (FY2016-17) LES of transient Diesel fuel injection, ignition, combustion, and emissions
- Subtask 6.2 (FY2016-18) LES of transient Gasoline Direct Injection spray dynamics, combustion, and emissions
- Subtask 6.3 (FY2017-18) LES of the LTGC engine with emphasis on temperature stratification
- Subtask 6.4 (FY2018) LES of the LTGC engine including direct injection and combustion

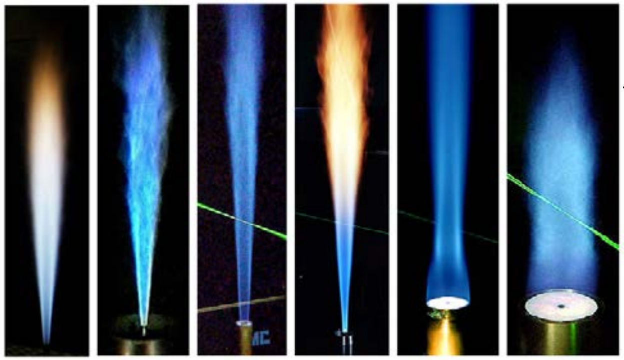


**Milestones aimed toward detailed calculations in (optical) engine geometries with advanced treatment of detailed physics and turbulence phenomena not account for in current codes; e.g., "low"-pressure versus "high"-pressure fuel injection processes**

# Approach/Strategy

**Basic** ← **Next Generation Code Framework (RAPTOR)** → **Applied**

**DOE Basic Energy Sciences Program**



**TNF Workshop**
www.ca.sandia.gov/TNF

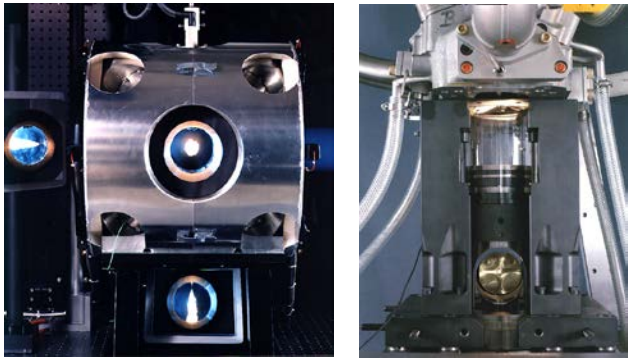
**Detailed jet flame data for model development but low Reynolds number and simple fuels**

**Re ≈ *O(10,000)***

**Device relevant measurements but limited due to complex geometry, flow, and fuels**

**Re > *O(100,000)***

**DOE Vehicle Technologies Program**

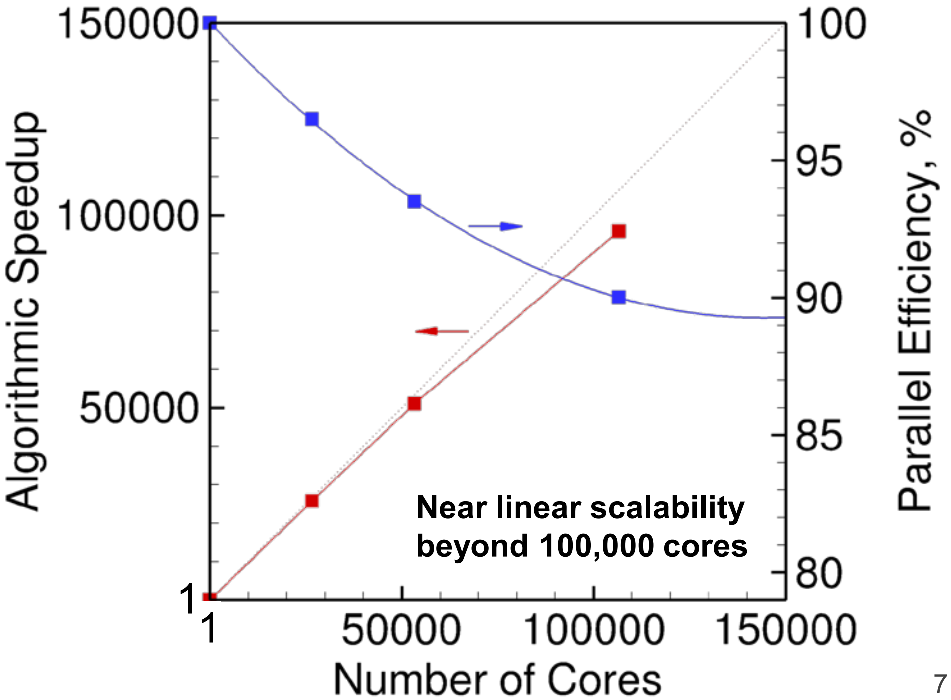


**Engine Combustion Network**
www.ca.sandia.gov/ECN

- **Complement advanced experiments with unique simulation capabilities using high-fidelity LES and first-principles models**
  - **Match detailed geometric and operating conditions, retain full governing physics**
  - **Establish one-to-one correspondence between measured and modeled results**
  - **Validate using available experimental data, then extract**
    - **Data and insights not available from experiments alone**
    - **Data required to develop affordable models for engineering**
- **Use full hierarchy of high-performance computing resources (both local and DOE platforms) with next generation massively-parallel code framework**

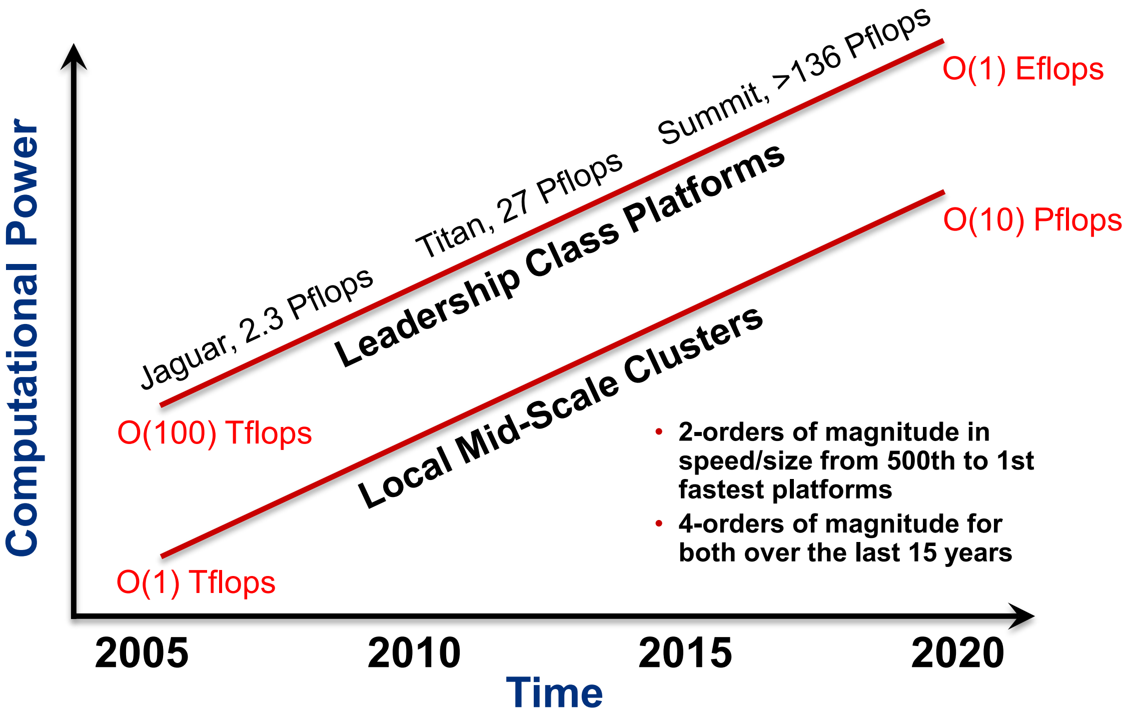
# Theoretical-Numerical Framework
## (RAPTOR: A first-principles DNS solver optimized for LES)

- **Theoretical framework … (Comprehensive physics)**
  - Fully-coupled, compressible conservation equations
  - Real-fluid equation of state (high-pressure phenomena)
  - Detailed thermodynamics, transport and chemistry
  - Multiphase flow, spray (Lagrangian-Eulerian)
  - Dynamic SGS modeling (No Tuned Constants)
- **Numerical framework … (High-quality numerics)**
  - Staggered finite-volume differencing (non-dissipative, discretely conservative)
  - Dual-time stepping with generalized preconditioning (all-Mach-number formulation)
  - Detailed treatment of geometry, wall phenomena, transient BC's
- **Hybrid-parallel programming model … (Highly-scalable)**
  - Demonstrated performance on hierarchy of HPC platforms (e.g., scaling on ORNL TITAN)
  - MPI at block/node level, OpenMP/OpenACC at flux/operator level, GPU acceleration of sub-model kernels (properties, chemistry, turbulence, etc.)



# RAPTOR selected for ORNL Center for Accelerated Application Readiness

- Oak Ridge Leadership Computing Facility "CAAR" Program, 2015 – 2018
  - Objective is to port RAPTOR to next generation multicore/GPU SUMMIT architecture
    - OLCF provides staff and postdoc (Sankaran et al.)
    - Matching effort at Sandia (Oefelein et al., BES)
    - Three-year Application Readiness Phase (2015-17)
    - Early Science "Grand-Challenge" Phase (2018)
- Milestones proposed for this project in FY16 – FY18 are the major focal point




**Titan**
- 18,688 Nodes
- 1.4 TF/Node
- AMD Opteron™ NVIDIA Kepler™
- 9 MW Power

**Summit**
- >3,400 Nodes
- 40 TF/Node
- IBM POWER9™ NVIDIA Volta™
- 10 MW Power

# Technical Accomplishments and Progress

# Technical path … systematic treatment of coupled system(s) of sub-models

**First Principles LES (RAPTOR)**
- Comprehensive physics (accuracy)
- Non-dissipative numerics (optimal for LES)
- Complex geometry (high-quality)
- Massively-parallel (highly-scalable)

Grid Interface (Complex Geometry)

Unstructured Multiblock Connectivity

SPMD Distributed Communication Shell (MPI)

SMP Shared Memory Shell (OpenMP/OpenACC)

Input

Multistage Integrator

Preconditioned Dual-Time-Stepping (All-Mach-Number Formulation)

Spatial Differencing Operators

Staggered Finite-Volume Scheme (Body-Fitted Coordinates)

Lagrangian Particle Integrator

Output

System Library

Math Library (Portable)

Model Library (Portable)

Data Processing Interface

**Detailed results and physical insights**

**Advanced grid generation**
- Complex geometry and topologies
- Dynamic mesh movement, AMR

**Liquid atomization, spray formation**
- Level-set/volume-of-fluid development
- Lagrangian treatment of dense sprays

**Lagrangian particle dynamics**
- Secondary breakup, two-way coupling
- Multicomponent drop vaporization

**Multicomponent mixture properties**
- Real-fluid gas/liquid equations of state
- Detailed thermodynamics and transport

**Turbulence and scalar mixing**
- Dynamic modeling, inverse methods
- Implicit, explicit filtering

**Turbulent combustion**
- Turbulence-chemistry interactions
- Complex fuels, mixed mode combustion

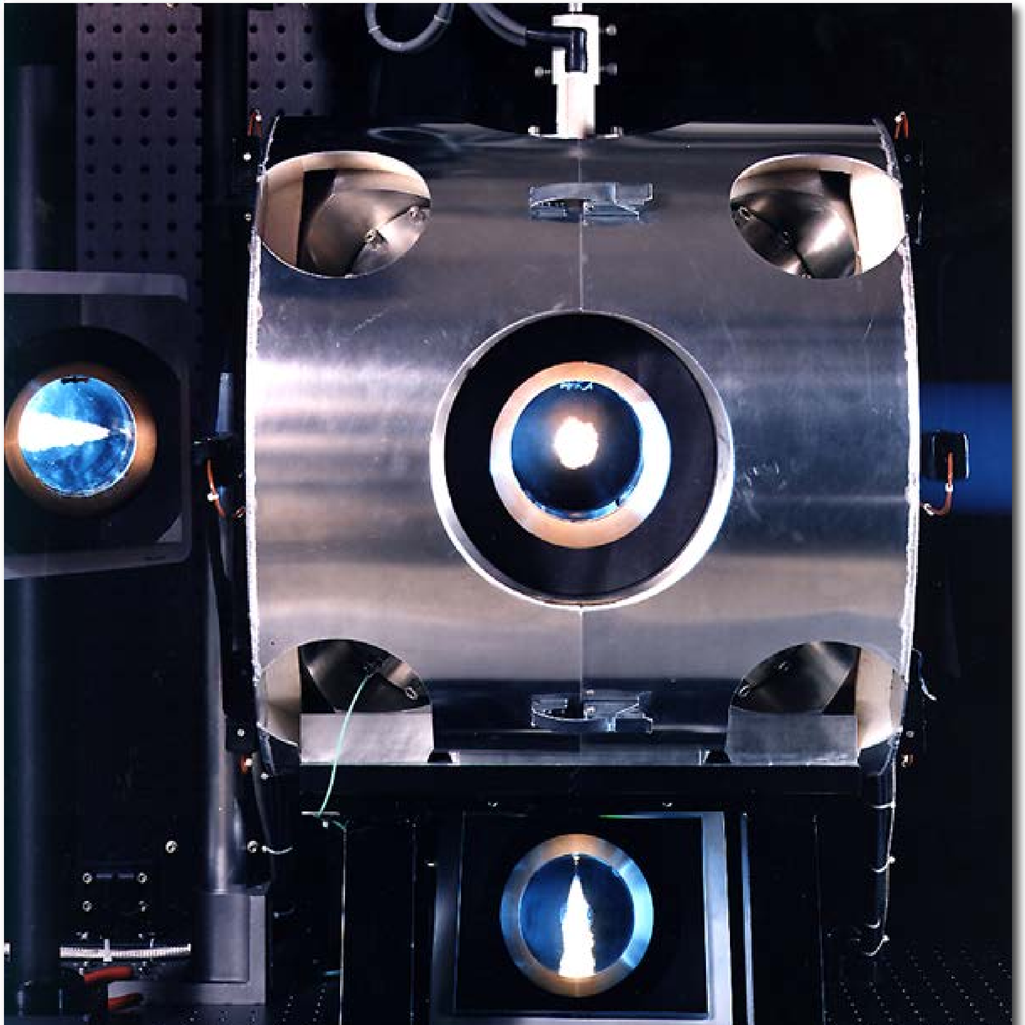
**Heat transfer and wall turbulence**
- Thermal radiation-turbulence interactions
- Transient wall-flow interactions

**Chemical kinetics and emissions**
- Detailed, skeletal mechanisms
- Optimized model mechanisms

**In-situ visualization and analysis**
- Massively-parallel data management
- Advanced mathematical data reduction

## Technology Transfer Mechanisms
- Development of advanced sub-model framework combined with UQ
- Near DNS benchmark data that provides insights not available from experiments
- Next generation multiphysics/ multiscale simulation code

# First principles LES of Diesel ignition and combustion … Spray-A ($C_{12}H_{26}$-Air)



Sandia high-pressure combustion vessel (Pickett et al.)

**Injection and Initial Conditions**

| | |
|---|---|
| Fuel Temperature: | 363 *K* |
| Chamber Temperature: | 900 *K* |
| Chamber Pressure: | 60 *bar* |
| Peak Velocity: | 600 *m/s* |
| Peak $Re_d$: | O(100,000) |
| Nozzle Diameter: | 0.09 *mm* |
| Chamber Volume: | $(1000d)^3$ |

**Available Data**

- Rate of injection
- Rayleigh scattering images
- Schlieren movies
- Liquid length versus time
- Vapor length versus time

# Filtered conservation equations

- Mass:

$$\frac{\partial}{\partial t}(\theta\overline{\rho}) + \nabla\cdot(\theta\overline{\rho}\tilde{\mathbf{u}}) = \overline{\dot{\rho}_s}$$

- Momentum:

$$\frac{\partial}{\partial t}(\theta\overline{\rho}\tilde{\mathbf{u}}) + \nabla\cdot\left[\theta\left(\overline{\rho}\tilde{\mathbf{u}}\otimes\tilde{\mathbf{u}} + \frac{\mathcal{P}}{M^2}\mathbf{I}\right)\right] = \nabla\cdot(\theta\vec{\vec{\mathcal{T}}}) + \overline{\dot{\mathbf{F}}}_s$$

- Total Energy:

$$\frac{\partial}{\partial t}(\theta\overline{\rho}\tilde{e}_t) + \nabla\cdot[\theta(\overline{\rho}\tilde{e}_t + \mathcal{P})\tilde{\mathbf{u}}] = \nabla\cdot\left[\theta\left(\vec{\mathcal{Q}}_e + M^2(\vec{\vec{\mathcal{T}}}\cdot\tilde{\mathbf{u}})\right)\right] + \theta\overline{\dot{Q}}_e + \overline{\dot{Q}}_s$$

- Species:

$$\frac{\partial}{\partial t}(\theta\overline{\rho}\tilde{Y}_i) + \nabla\cdot(\theta\overline{\rho}\tilde{Y}_i\tilde{\mathbf{u}}) = \nabla\cdot(\theta\vec{\mathcal{S}}_i) + \theta\overline{\dot{\omega}}_i + \overline{\dot{\omega}}_{s_i}$$

- Spray Source Terms
- Composite Stresses/Fluxes
- Chemical Source Terms

# Mixed dynamic Smagorinsky model for turbulence and scalar mixing

- Eddy Viscosity:

$$\mu_t = \overline{\rho} C_R \Delta^2 \Pi_{\tilde{\mathbf{S}}}^{\frac{1}{2}} \qquad \Pi_{\tilde{\mathbf{S}}} = \tilde{\mathbf{S}} : \tilde{\mathbf{S}} \qquad \tilde{\mathbf{S}} = \frac{1}{2}\left(\nabla \tilde{\mathbf{u}} + \nabla \tilde{\mathbf{u}}^T\right)$$

- Stress Tensor:

$$\vec{\vec{\mathcal{T}}} = (\overline{\tau} - \mathbf{T}) = (\mu_t + \mu)\frac{1}{Re}\left[-\frac{2}{3}(\nabla \cdot \tilde{\mathbf{u}})\mathbf{I} + \left(\nabla \tilde{\mathbf{u}} + \nabla \tilde{\mathbf{u}}^T\right)\right] - \overline{\rho}\left(\widetilde{\tilde{\mathbf{u}} \otimes \tilde{\mathbf{u}}} - \tilde{\tilde{\mathbf{u}}} \otimes \tilde{\tilde{\mathbf{u}}}\right) - \frac{1}{3}\overline{\rho} q_{\mathrm{sfs}}^2 \, \mathbf{I}$$

- Energy Flux:

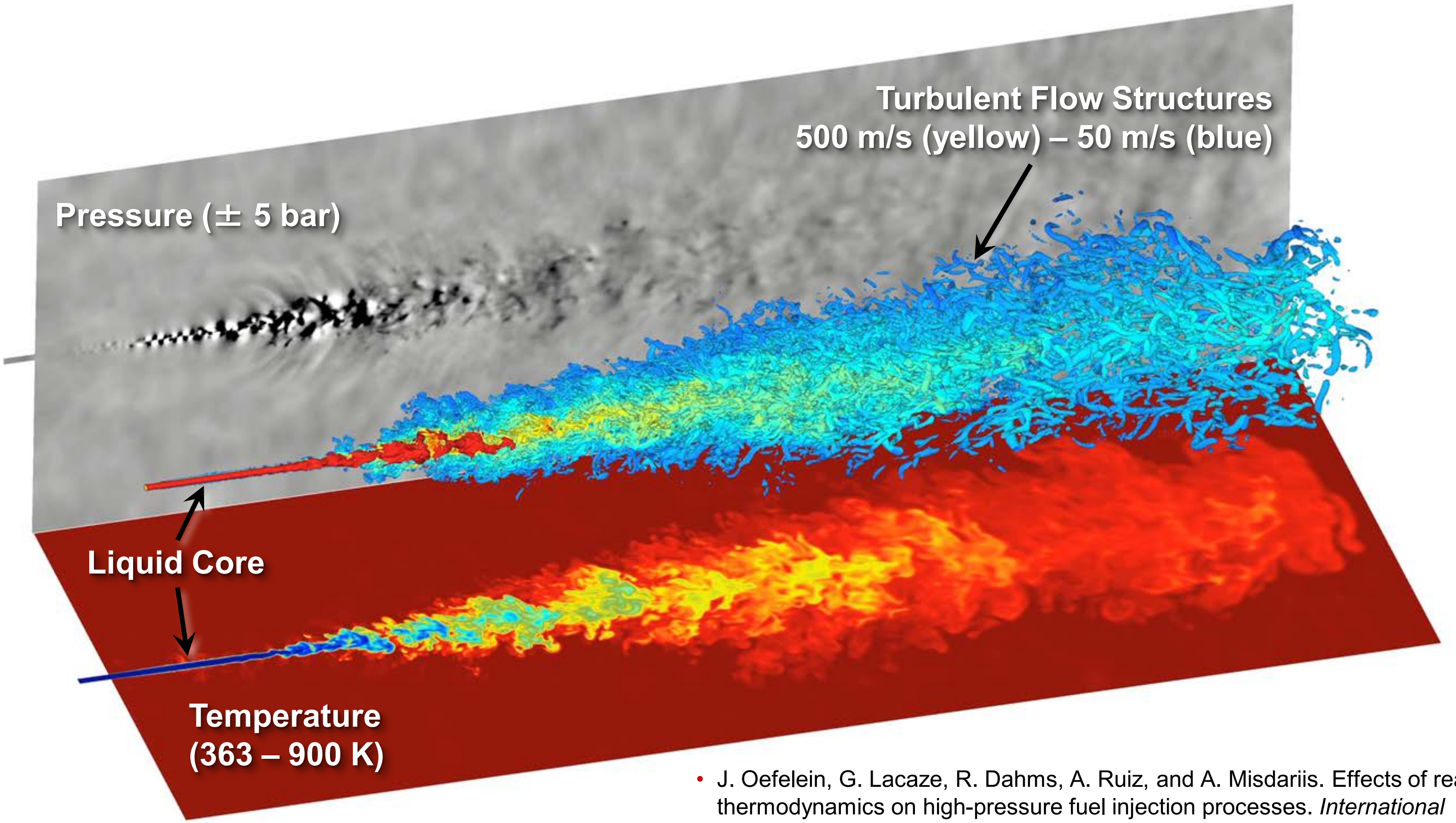
$$\vec{\mathcal{Q}}_e = (\overline{\mathbf{q}}_e - \mathbf{Q}) = \left(\frac{\mu_t}{Pr_t} + \frac{\mu}{Pr}\right)\frac{1}{Re}\nabla \tilde{h} + \sum_{i=1}^{N} \tilde{h}_i \vec{\mathcal{S}}_i - \overline{\rho}\left(\widetilde{\tilde{h}\tilde{\mathbf{u}}} - \tilde{\tilde{h}}\tilde{\tilde{\mathbf{u}}}\right)$$

- Mass Flux:

$$\vec{\mathcal{S}}_i = (\overline{\mathbf{q}}_i - \mathbf{S}_i) = \left(\frac{\mu_t}{Sc_{t_i}} + \frac{\mu}{Sc_i}\right)\frac{1}{Re}\nabla \tilde{Y}_i - \overline{\rho}\left(\widetilde{\tilde{Y}_i\tilde{\mathbf{u}}} - \tilde{\tilde{Y}}_i\tilde{\tilde{\mathbf{u}}}\right)$$

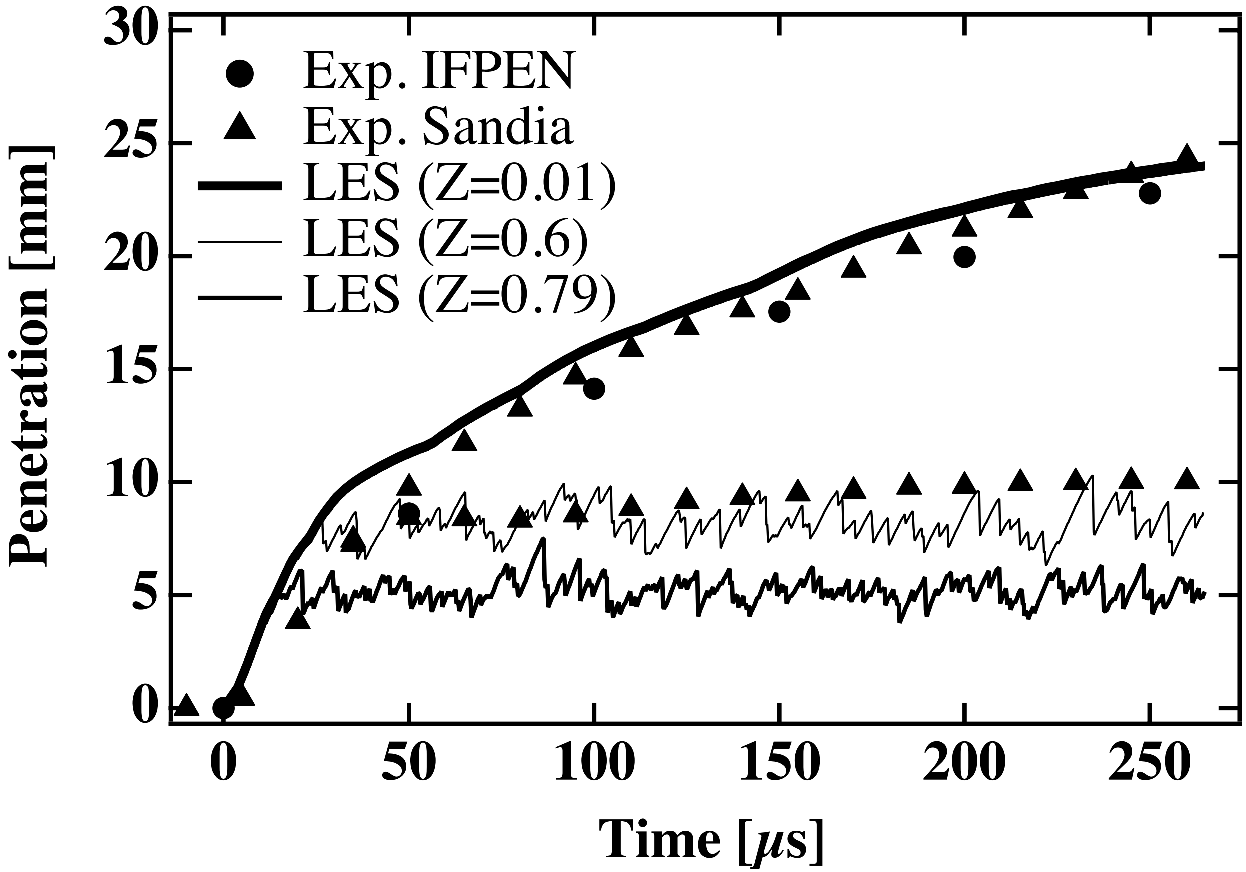
Coefficients $C_R$, $Pr_t$, and $Sc_{t_i}$ evaluated dynamically as functions of space and time

# Transient evolution of jet reveals details of turbulence and scalar-mixing

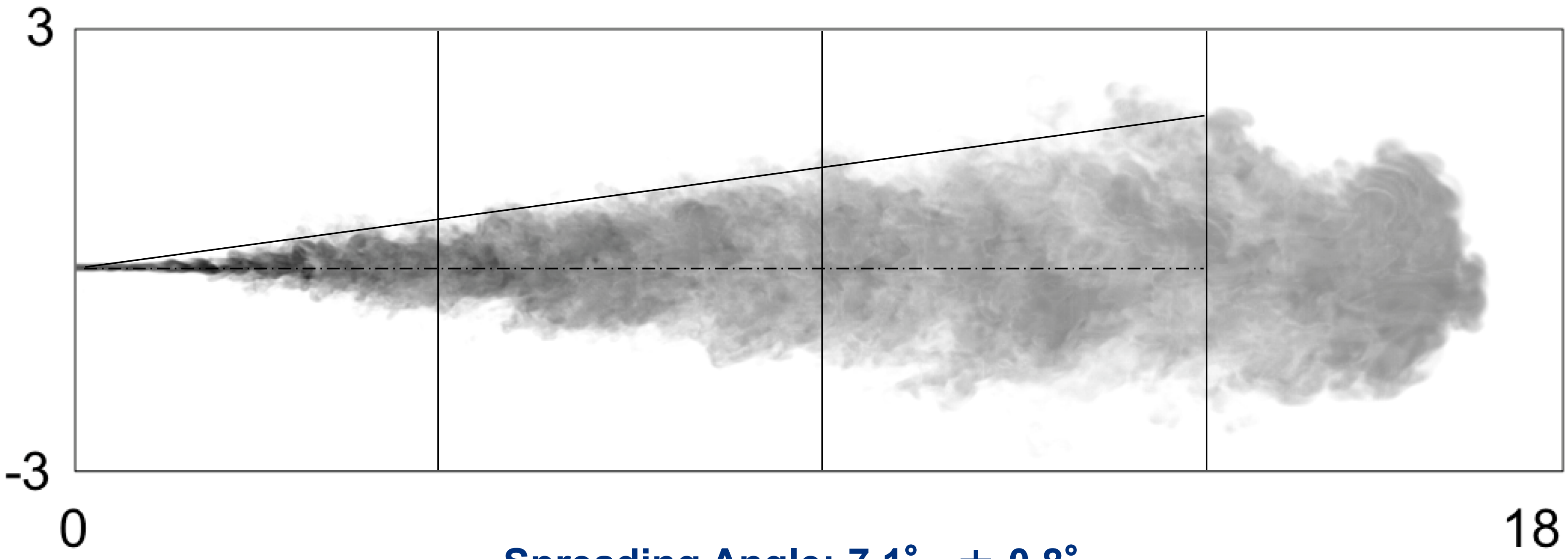



- J. Oefelein, G. Lacaze, R. Dahms, A. Ruiz, and A. Misdariis. Effects of real-fluid thermodynamics on high-pressure fuel injection processes. *International Journal of Engines*, **7**(3):1–12, 2014.
- G. Lacaze, A. Misdariis, A. Ruiz, and J. C. Oefelein. Analysis of high-pressure diesel fuel injection processes using LES with real-fluid thermodynamics and transport. *Proceedings of the Combustion Institute*, **35**:1603–1611, 2015.

# Good agreement with vapor and "liquid" penetration data

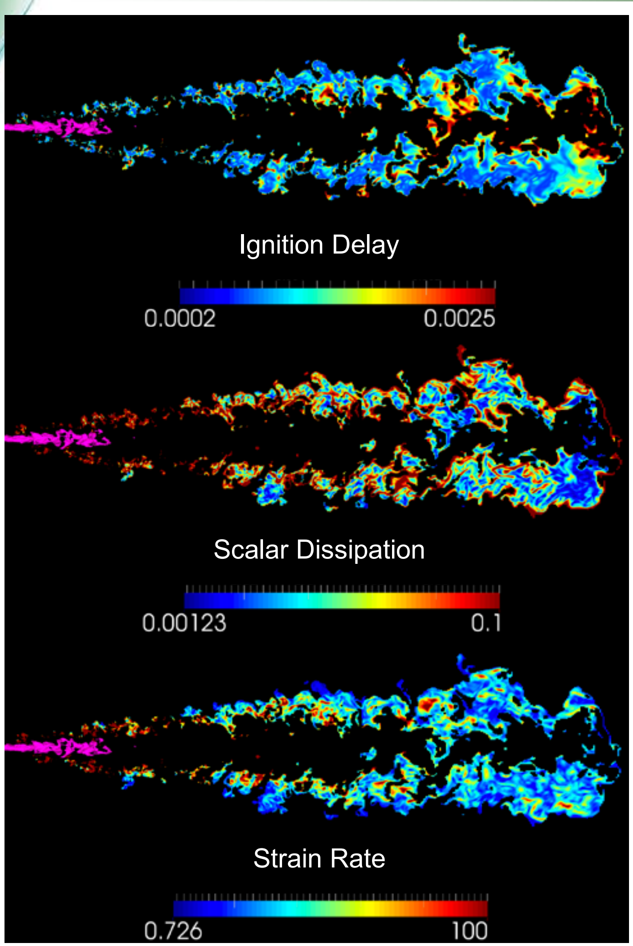


# Also good agreement with jet spreading angle

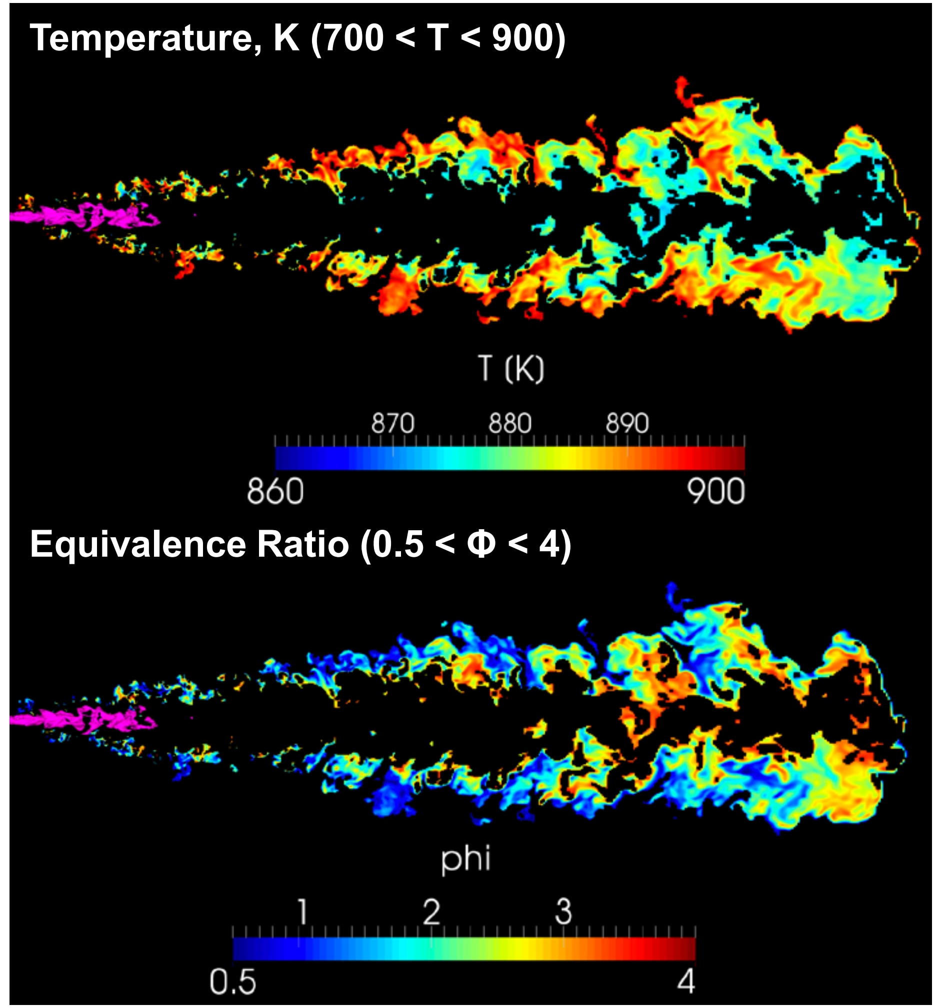



**Spreading Angle: 7.1° ± 0.8°**

# Results reveal transient mixture state just prior to autoignition (≈ 260 μs)




**Identification of flammable regions used to identify conditions where the chemical model must perform accurately**



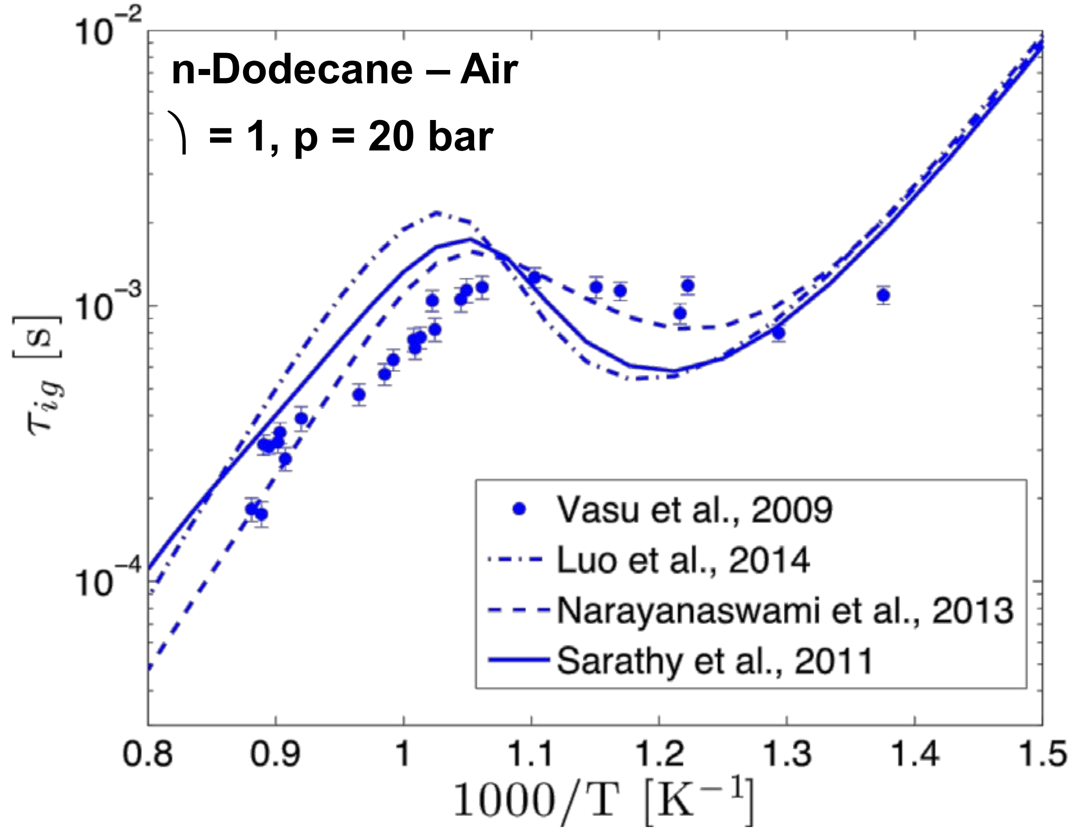

**Autoignition most likely to occur where ignition delay time, scalar dissipation rate, and strain rate are simultaneously minimized**

**Pressure: 60±5 bar**

# Selection of candidate mechanisms presents interesting questions

- Sarathy et al., 2011
  - 2-methyl-alkanes and n-alkanes up to C12 (2755 species and 11173 reactions)
  - Validated for n-dodecane – air auto-ignition delay times …
    - Against experimental data
    - Up to 20 bar from low to high temperatures (600 – 1500 K)
- Narayanaswami et al., 2013
  - Skeletal mechanism (255 species and 2289 reactions)
  - Reduced from Sarathy et al., 2011
    - Directed relation graph with error propagation (DRGEP) and isomer lumping
    - Modification of some reaction rates based on recent theoretical and experimental analysis
  - Validated for n-dodecane – air auto-ignition delay times
    - Against experimental data and detailed mechanism
    - Up to 20 bar from low to high temperatures (600 – 1500 K)
- Luo et al., 2014
  - Skeletal mechanism (105 species and 420 reactions)
  - Reduced from Sarathy et al., 2011
    - DRG with expert knowledge (DRGX) and DRG-aided sensitivity analysis (DRGASA)
  - Validated for n-dodecane – air auto-ignition delay times
    - Against experimental data and detailed mechanism
    - Up to 20 bar and from low to high temperatures (600 – 1500 K)

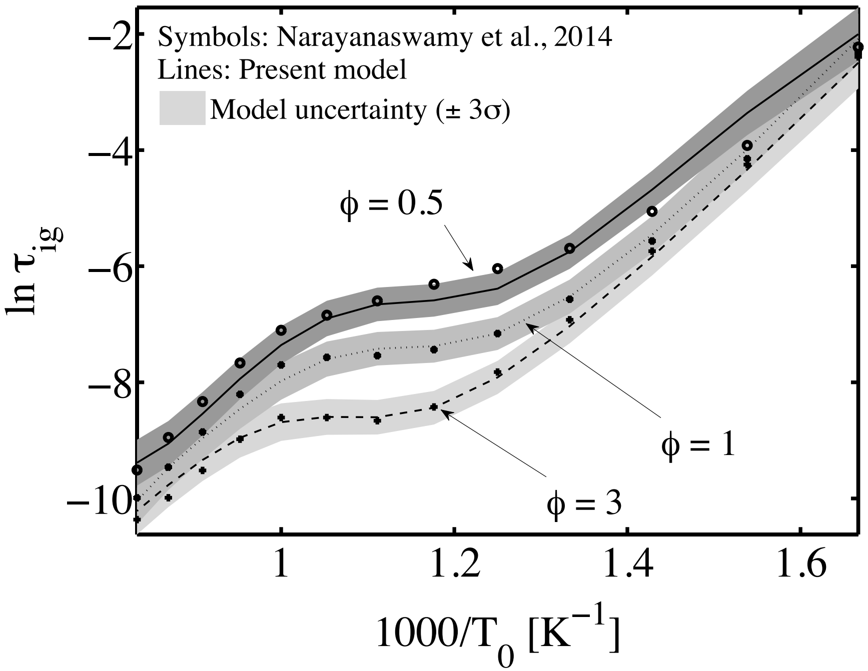
# There is a wide range of variability between mechanisms




e.g., Predicted ignition delay time (even within designed ranges) exhibit notable differences, particularly in NTC region and at high temperatures

# Given variability, UQ used to optimize chemical models for simulations

- **Objective**
  - Design model around specified range of operating conditions (p, T, phi) using detailed reference mechanism
  - Optimize model to capture specific chemical characteristics (e.g., ignition delay, flame propagation, selected emissions)
  - Minimize implementation cost for CFD
- **Approach**
  - Start with simplest model form such as models that follow Arrhenius laws for reaction rates (Westbrook et al. 1981, Misdariis et al. 2014)
  - Functionalize pre-exponential factors and activation energies w.r.t. operating conditions
  - Use Bayesian inference to fit the most probable surfaces over specified range of conditions
  - Calculate uncertainties relative to reference and add model complexity as needed




**Approach provides "simplest" least expensive model optimized to provide selected characteristics with error bars on predictions**

**Here 12 species, 5 step model optimized for ignition delay using Narayanaswamy et al. as reference**

L. Hakim, G. Lacaze, M. Khalil, H. N. Najm, and J. C. Oefelein. Modeling auto-ignition transients in reacting Diesel jets. *ASME 2015 Internal Combustion Engine Division Fall Technical Conference*, Paper 2015-1120, November 8-11 2015. Accepted for publication in the *Journal of Engineering for Gas Turbines and Power*.

# Chemical model is combined with new combustion closure for LES

Stochastic Reconstruction Model:

- Filtered chemical source terms evaluated using modeled instantaneous scalar field, $\phi_i(\mathbf{x}, t)$, and time-dependent filter kernel

$$\bar{\dot{\omega}}_i(\mathbf{x}, t) = \int_t^{t+\Delta t} \left\{ \iiint_{V(\tau)} \mathcal{G}(\mathbf{y}-\mathbf{x}, \tau-t; \delta\mathbf{y}, \delta\tau)\, \dot{\omega}_i(\phi_1, \phi_2, \ldots; \mathbf{y}, \tau)\ dV \right\} d\tau$$

where

$$\phi_i(\mathbf{x}, t) = \tilde{\phi}_i(\mathbf{x}, t) + \phi_i''(\mathbf{x}, t)$$

- Correlated velocity and scalar fluctuations generated stochastically using Cholesky decomposition on subfilter time scales as function of subfilter variances and covariances

$$\begin{aligned} \phi_1 &= \tilde{\phi}_1 + a_{11} r_1 \\ \phi_2 &= \tilde{\phi}_2 + a_{21} r_1 + a_{22} r_2 \\ \phi_3 &= \tilde{\phi}_3 + a_{31} r_1 + a_{32} r_2 + a_{33} r_3 \\ &\vdots \end{aligned}$$

where $r_i$'s are normal deviates with zero mean and unit variance ( $\overline{r_i} = 0$ , $\overline{r_i r_j} = \delta_{ij}$ )

# Modeled instantaneous fluctuations facilitate formation of ignition kernels

- Normal deviates are functions of subfilter variances and covariances

$$a_{ii} = \left( R_{ii} - \sum_{j=1}^{i-1} a_{ij}^2 \right)^{1/2} \qquad a_{ij} = \left( R_{ij} - \sum_{k=1}^{j-1} a_{ik} a_{jk} \right) / a_{jj}$$

where

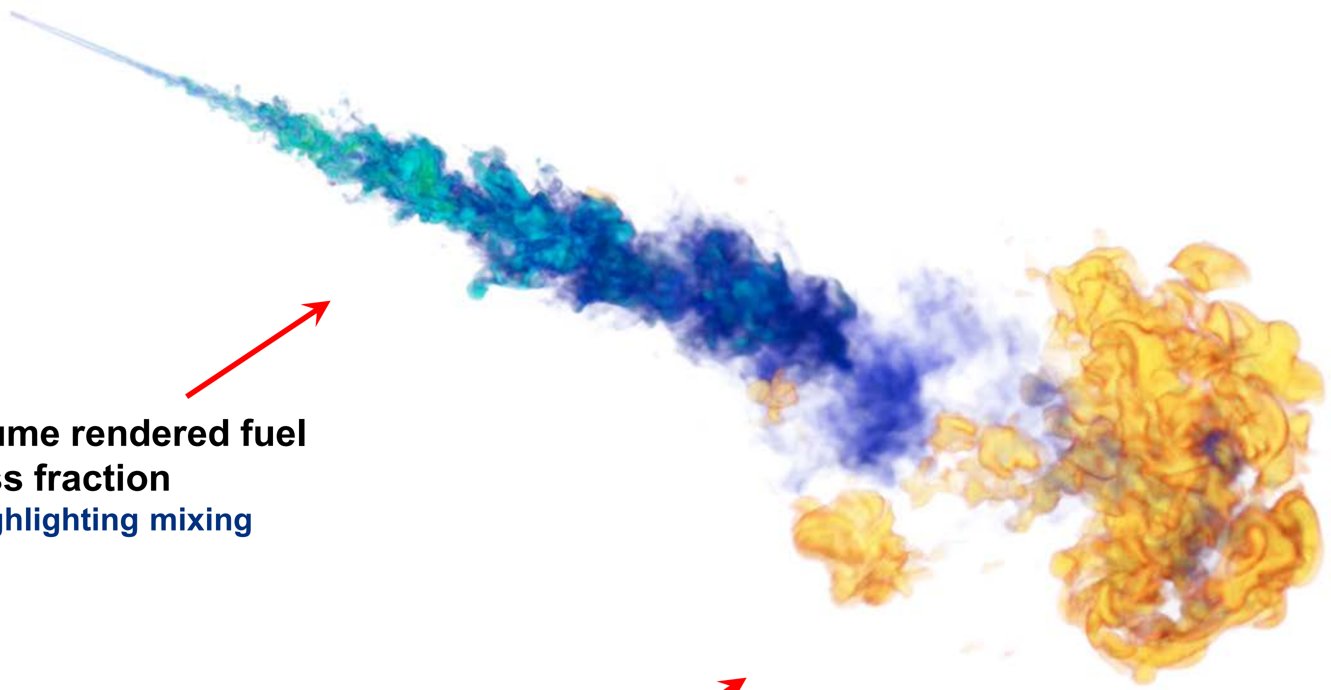
$$R_{ij} = (\widetilde{\phi_i \phi_j})_{\rm sfs} = \overline{\rho \phi_i \phi_j} - \bar{\rho} \tilde{\phi}_i \tilde{\phi}_j$$

$$R_{ij} = \left( \begin{array}{c|cccc|c|ccc}
0 & & & & & & & \cdots & \\
\hline
0 & (\widetilde{u^2})_{\rm sfs} & & & & & & \cdots & \\
0 & (\widetilde{vu})_{\rm sfs} & (\widetilde{v^2})_{\rm sfs} & & & & & \cdots & \\
0 & (\widetilde{wu})_{\rm sfs} & (\widetilde{wv})_{\rm sfs} & (\widetilde{w^2})_{\rm sfs} & & & & \cdots & \\
\hline
0 & (\widetilde{hu})_{\rm sfs} & (\widetilde{hv})_{\rm sfs} & (\widetilde{hw})_{\rm sfs} & & (\widetilde{T^2})_{\rm sfs} & & \cdots & \\
\hline
0 & (\widetilde{Y_1 u})_{\rm sfs} & (\widetilde{Y_1 v})_{\rm sfs} & (\widetilde{Y_1 w})_{\rm sfs} & & (\widetilde{Y_1 T})_{\rm sfs} & (\widetilde{Y_1^2})_{\rm sfs} & \cdots & \\
\vdots & \vdots & \vdots & \vdots & & \vdots & \vdots & \ddots & \vdots \\
0 & (\widetilde{Y_{N-1} u})_{\rm sfs} & (\widetilde{Y_{N-1} v})_{\rm sfs} & (\widetilde{Y_{N-1} w})_{\rm sfs} & & (\widetilde{Y_{N-1} T})_{\rm sfs} & (\widetilde{Y_{N-1} Y_1})_{\rm sfs} & \cdots & (\widetilde{Y_{N-1}^2})_{\rm sfs}
\end{array} \right)$$

- Terms $R_{ij}$ obtained using approximate deconvolution with assumed scalar spectrum
- Fluctuations generated asynchronously on subfilter-scale in time at frequencies consistent with local eddy lifetimes and transit times

# Modeled instantaneous fluctuations facilitate formation of ignition kernels

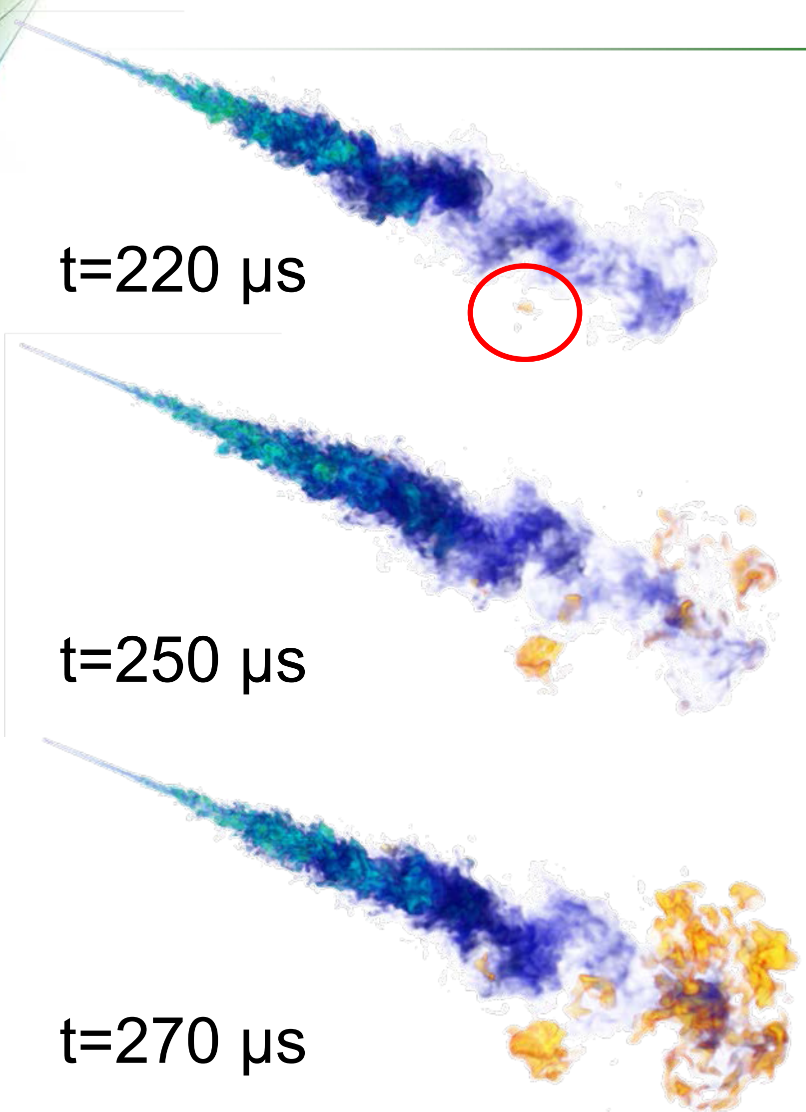
L. Hakim, G. Lacaze, and J. C. Oefelein. Large eddy simulation of autoignition transients in a model Diesel injector configuration. *SAE World Congress*, Paper 2016-01-0872, April 12-14, 2016.



**Volume rendered fuel mass fraction**
- **Highlighting mixing**

**Volume rendered temperature**
- **Highlighting ignition kernel development**

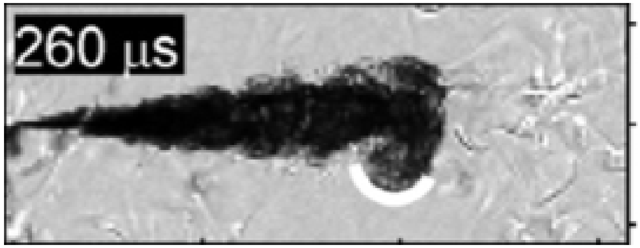
# Ignition sequence




**First kernel**, diameter ≈ 500 μm (too small to be optically detected in experiment)
Location: tip of the jet, off-axis

**Independent kernels appear**, diameter ≈ 500μm to 2mm (still very small for optical detection)
Location: tip of the jet, off-axis

**Many small kernels present in the "jet tip" region … impact on schlieren?**

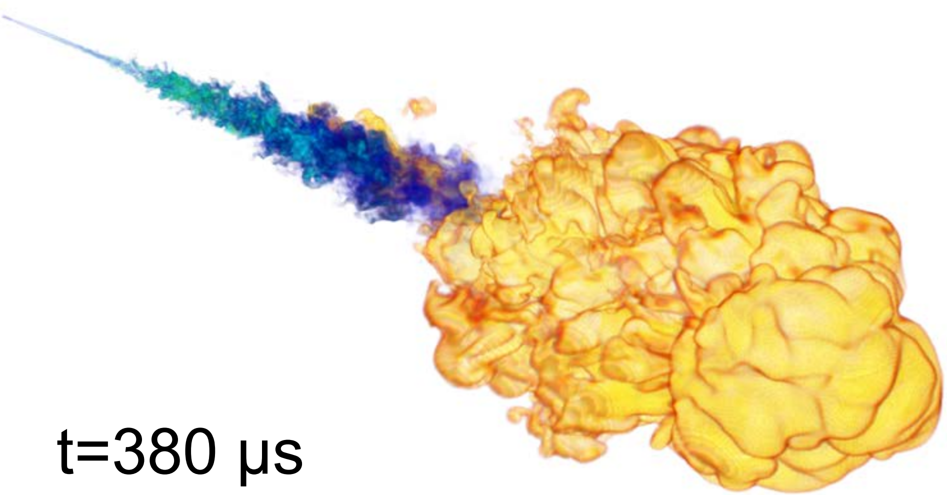



**Schlieren images by Skeen *et al.*, PCI, 2015**

# Ignition sequence

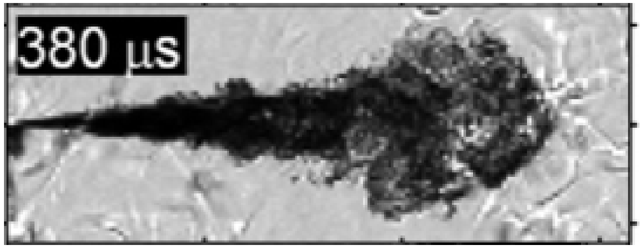
t=300 μs

**Single flame structure with upstream independent kernels,** flame expends through dilatation and autoignition



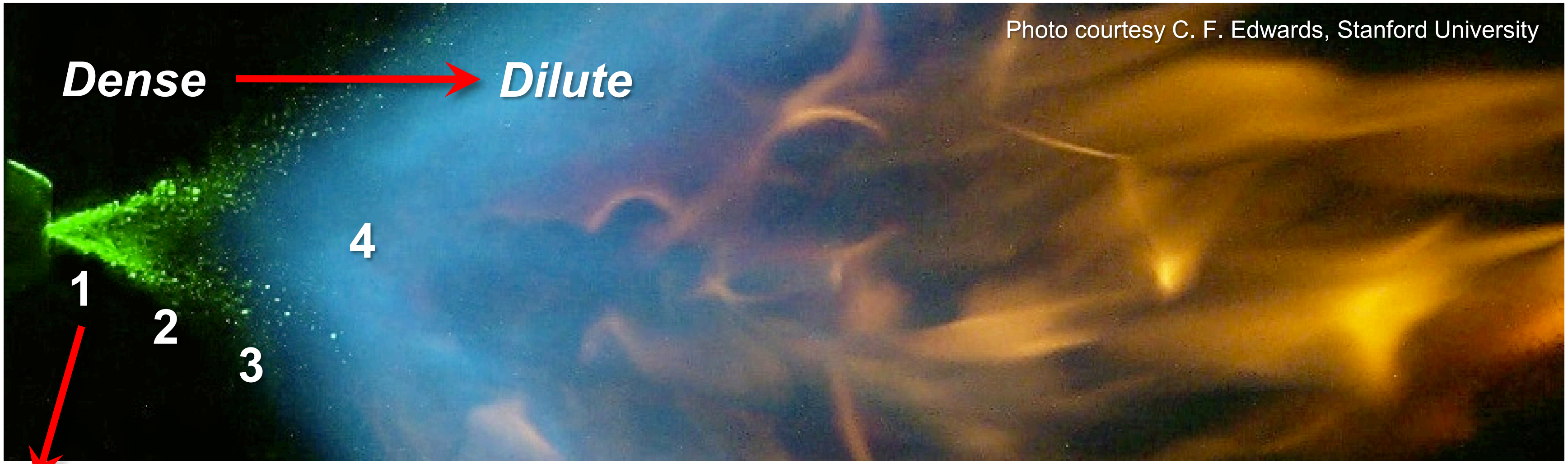
t=380 μs

**Main flame region at the jet extremity,** autoignition locations observed ahead of main front




**Schlieren images by Skeen *et al.*, PCI, 2015**

# Systematic treatment of GDI sprays in progress (Lagrangian-Eulerian method)




**1. Primary atomization (sheet, filament and lattice formation)**

**2. Secondary breakup (including particle deformation, coalescence)**

**3. Dilute spray dynamics**
   a. Drop dispersion
   b. Multicomponent drop vaporization
   c. Two-way coupling between gas and dispersed liquid phase
      − Turbulence modulation (damping of turbulence due to particle drag effects)
      − Turbulence generation (production of turbulence due to particle wakes)

A new dense spray formulation based on space-time filtering has been implemented

Current focus is on advanced treatment of secondary breakup and dilute spray dynamics

**4. Turbulent mixed-mode combustion**
   a. Complex high-pressure hydrocarbon chemistry
   b. Emissions and soot

# Detailed modeling of filtered void fraction and interphase source terms

- Mass:

$$\frac{\partial}{\partial t}(\theta\overline{\rho}) + \nabla\cdot(\theta\overline{\rho}\tilde{\mathbf{u}}) = \overline{\dot{\rho}}_s$$

- Momentum:

$$\frac{\partial}{\partial t}(\theta\overline{\rho}\tilde{\mathbf{u}}) + \nabla\cdot\left[\theta\left(\overline{\rho}\tilde{\mathbf{u}}\otimes\tilde{\mathbf{u}} + \frac{\mathcal{P}}{M^2}\mathbf{I}\right)\right] = \nabla\cdot(\theta\vec{\vec{\mathcal{T}}}) + \overline{\dot{\mathbf{F}}}_s$$

- Total Energy:

$$\frac{\partial}{\partial t}(\theta\overline{\rho}\tilde{e}_t) + \nabla\cdot[\theta(\overline{\rho}\tilde{e}_t + \mathcal{P})\tilde{\mathbf{u}}] = \nabla\cdot\left[\theta\left(\vec{\mathcal{Q}}_e + M^2(\vec{\vec{\mathcal{T}}}\cdot\tilde{\mathbf{u}})\right)\right] + \theta\overline{\dot{Q}}_e + \overline{\dot{Q}}_s$$

- Species:

$$\frac{\partial}{\partial t}(\theta\overline{\rho}\tilde{Y}_i) + \nabla\cdot(\theta\overline{\rho}\tilde{Y}_i\tilde{\mathbf{u}}) = \nabla\cdot(\theta\vec{\mathcal{S}}_i) + \theta\overline{\dot{\omega}}_i + \overline{\dot{\omega}}_{s_i}$$

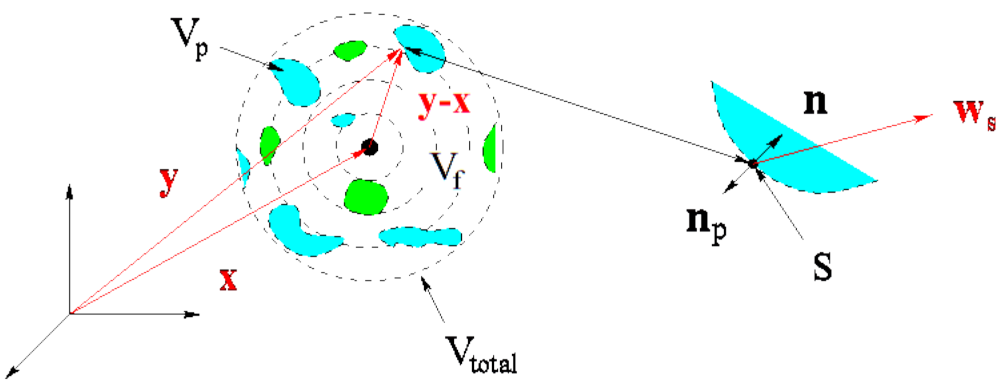
- Spray Source Terms
- Composite Stresses/Fluxes
- Chemical Source Terms

# Detailed modeling of filtered void fraction and interphase source terms

$$\overline{\dot{\mathcal{H}}}_s(\mathbf{x},t) = \underbrace{\int_t^{t+\Delta t} \underbrace{\sum_p \mathcal{G}(\mathbf{y}_p-\mathbf{x},\tau-t) \underbrace{\left\{ \oiint_{S(\mathbf{y}_p,\tau)} \vec{\psi}(\mathbf{y}_p,\tau)\cdot\mathbf{n}_p\, dS \right\}}_{(i)}}_{(ii)} d\tau}_{(iii)}$$

| $\overline{\dot{\mathcal{H}}}_s(\mathbf{x},t)$ | $\oiint_{S(\mathbf{y}_p,\tau)} \vec{\psi}(\mathbf{y}_p,\tau)\cdot\mathbf{n}_p\, dS$ |
|---|---|
| $\bar{\dot{\rho}}_s(\mathbf{x},t)$ | $-\left\{\dfrac{dm_p}{d\tau}\right\}$ |
| $\overline{\dot{\mathbf{F}}}_s(\mathbf{x},t)$ | $-\left\{\dfrac{dm_p}{d\tau}\mathbf{u}_p + m_p\dfrac{d\mathbf{u}_p}{d\tau}\right\}$ |
| $\bar{\dot{Q}}_s(\mathbf{x},t)$ | $-\left\{\dfrac{dm_p}{d\tau}e_{t_p} + m_p\dfrac{de_{t_p}}{d\tau}\right\}$ |
| $\bar{\dot{\omega}}_{s_i}(\mathbf{x},t)$ | $-\left\{\dfrac{dm_p}{d\tau}Y_{i_p} + m_p\dfrac{dY_{i_p}}{d\tau}\right\}$ |

$(i)$ Instantaneous rate of exchange across drop interfaces at remote points $\mathbf{y}_p$ and times $\tau$
$(ii)$ Spatially filtered effect of remote exchange processes on discrete points $\mathbf{x}$ at times $\tau$
$(iii)$ Filtered effect of temporal disturbances that occur over the interval $t \le \tau \le t+\Delta t$

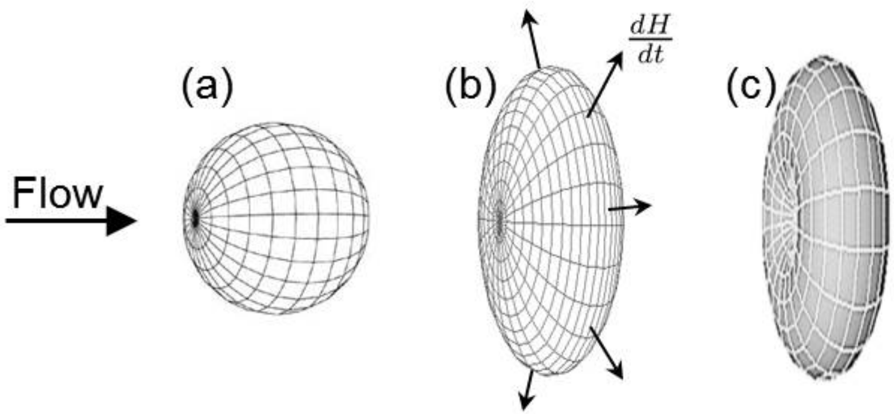



- **Form of source terms derived through mathematical formalism of LES using time-dependent filter kernel**
- **Filtering performed within a given fluid phase but not across phase boundaries**
- **Drop mass, volume, and (assumed) topology are fully accounted for (e.g., no need to assume "point particle limit")**
- **Lagrangian ODE's (drop dynamics) integrated on subfilter time scales using modeled instantaneous scalar field (consistent with stochastic reconstruction model used in combustion closure) … no adjustable constants**

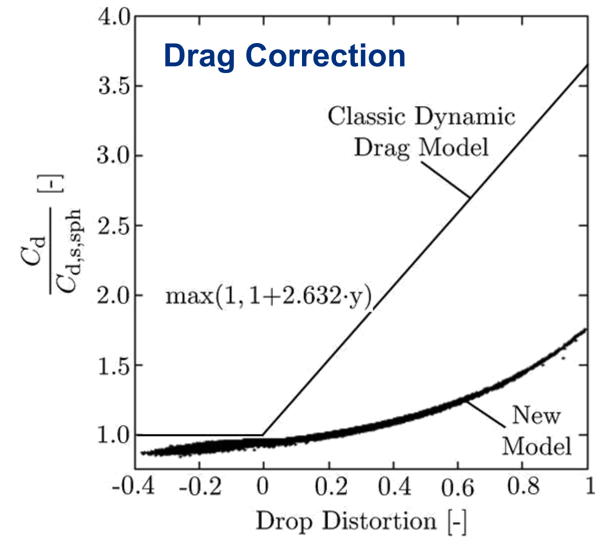
# Sensitizing drops to subfilter time scales facilitates model improvements

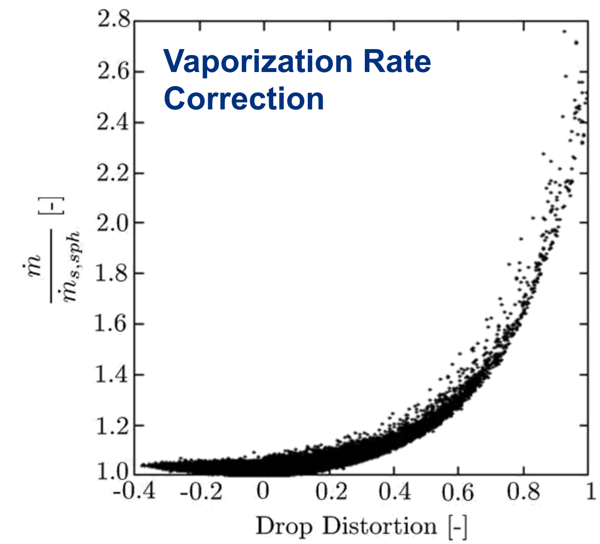
**Physical drops (not parcels) are tracked**

**System of drop models (e.g., drag, vaporization) now modified to include drop non-sphericity**

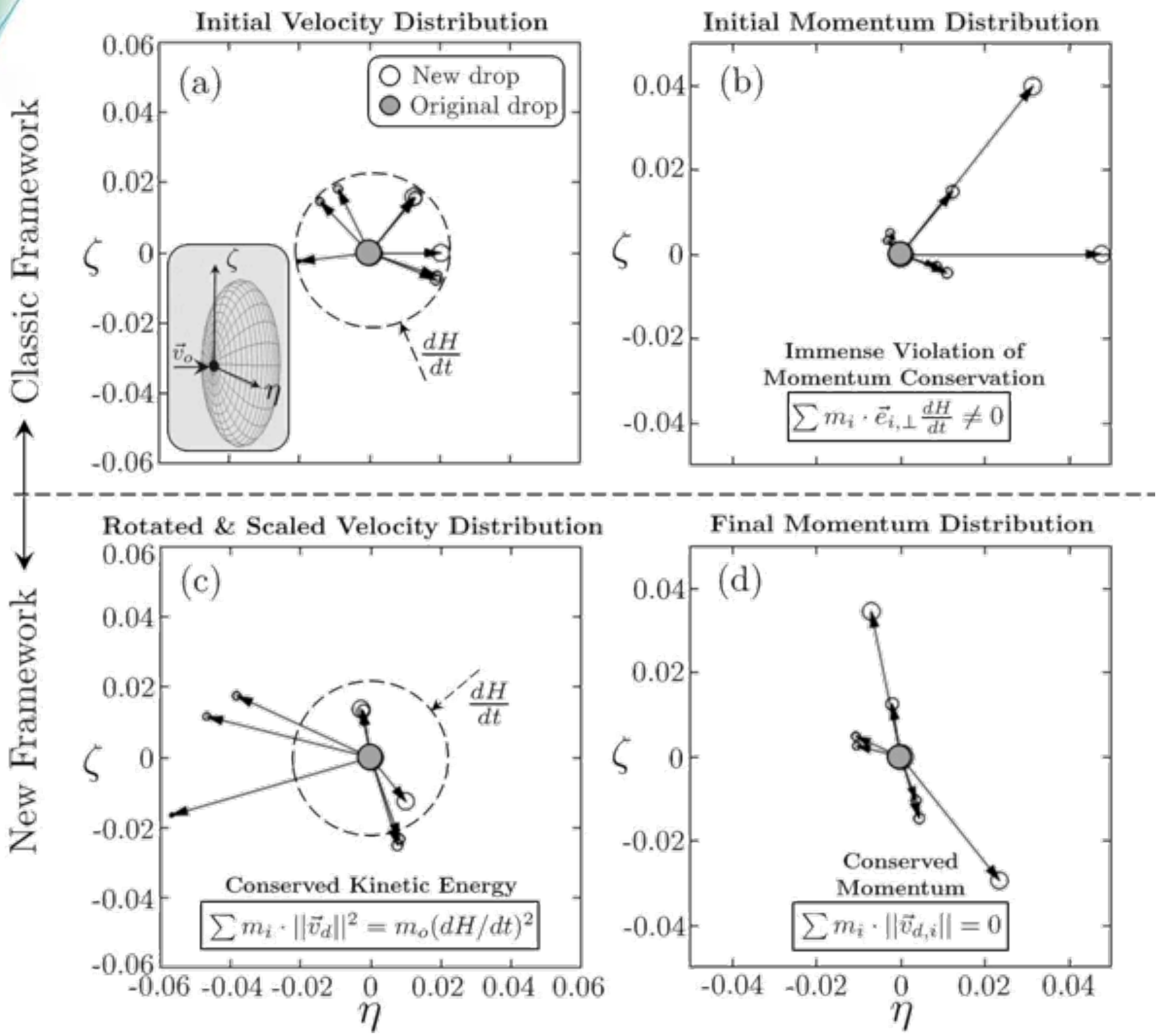



- R. N. Dahms and J. C. Oefelein. The significance of drop non-sphericity in sprays. *International Journal of Multiphase Flow*, 2016. Submitted.
- R. N. Dahms and J. C. Oefelein. Development of high-fidelity models for liquid fuel spray atomization and mixing processes in transportation and energy systems. *Sandia National Laboratories Technical Report SAND2015-3314*, 2015.



# Improved breakup model also derived that conserves momentum




**Normalized drop velocity and momentum distributions**

a) Initial drop velocity distribution

b) Corresponding momentum distribution after multiplication of the velocities in (a) with the respective drop masses (Momentum contributions do not cancel, thus momentum conservation is significantly violated)

c) Drop velocity distribution after rotation of the initial solution in (a) to enforce momentum conservation and scaling to maintain energy conservation

d) Conserved momentum distribution after the rotation and scaling operation

**Fully-coupled LES of ECN Spray G in progress using new model framework.**

# Response to previous year reviewer comments

- **Comment**: The project and approach are very important since current CFD codes still have significant limitations. Project should move as quickly as possible toward in-cylinder calculations and include heat transfer and wall effects (and eventually coupling with material stresses).
- **Response**: We are working toward full engine geometries (see milestones on slide 5). Concurrently, we are developing first principles models for heat transfer and wall effects (see slides 10 and 32). Code has the capability, the current rate limiting factor is funding level and related staffing.
- **Comment**: There is good coordination with government laboratories and academia. Would like to see more interaction with industry and CFD code vendors.
- **Response**: We are attempting to establish closer interactions. Our goal is to complement what current commercial/industry design codes already provide, not reproduce more of the same. This involves providing data and insights not available from experiments and developing the workflow required to overcome the major obstacles for development of predictive models listed in slide 33.
- **Comment**: This project would benefit from placing the capabilities of RAPTOR in the context of other widely used codes which ostensibly make the same claims regarding high-fidelity predictions.
- **Response**: "High-fidelity" and "high performance computing" have become ambiguous terms. For example, RAPTOR is proven to perform with near linear scalability across platforms, including O(100,000) cores on leadership class architectures. This is compared to less than O(100) for other codes. RAPTOR is the only code designed using non-dissipative, fully-conservative numerics required for LES. Other codes are not, which significantly complicates the model validation process. Last, RAPTOR treats the fully-coupled compressible governing conservation equations over the widest range of conditions using first principles models with no tuned constants. The only adjustable parameters are spatial and temporal resolution and boundary conditions.
- **Comment**: All reviewers would like to see faster progress. One reviewer stated project appears to be limited in funding, another stated that the "budget of nearly $500K is probably adequate.
- **Response**: We have attempted to build the team up over time by hiring staff. However, this has been stalled over the past year since our funding level has dropped. Current spend plan is $390K.

# Collaboration and coordination with other institutions

- ORNL-OLCF, Center for Accelerated Application Readiness (CAAR)
  - CAAR Partnership in Turbulent Combustion using the RAPTOR Code Framework: Application Readiness and Early Science on next generation leadership class platform (called SUMMIT)
- Penn State (Haworth), U Michigan (Sick), ORNL (Szybist)
  - Development and Validation of Predictive Models for In-Cylinder Radiation and Wall Heat Transfer
- Penn State (Haworth), U Merced (Modest)
  - Turbulence-Radiation Interactions in Reacting Flows: Effects of Radiative Heat Transfer on Turbulence
- Stanford (Ihme), U Michigan (Sick)
  - Development of a Dynamic Wall Layer Model for LES of Internal Combustion Engines
- CERFACS (Poinsot et al.)
  - Numerical Benchmarks and comparisons of High-Pressure High-Reynolds-Number Turbulent Reacting Flows using the AVBP and RAPTOR Codes

# Remaining challenges and barriers

- **Accuracy of simulations is complicated by**
  - Interdependence between different models
  - Model variability and numerical implementation
  - Competition between model and numerical errors
- **Many uncertainties exist in addition to model accuracy**
  - Error-prone numerical methods (especially in context of LES)
  - Poor grid quality and/or lack of appropriate spatial or temporal resolution
  - Incorrect and/or ill-posed boundary conditions or solution initialization
- **Data available for validation does not provide fidelity required to draw distinguishing conclusions due to harsh environments**
  - Penetration, flame lift-off measurements necessary but not sufficient, instantaneous imaging is qualitative
  - Progressive levels of model accuracy difficult to check (e.g., injection ➔ mixing ➔ combustion ➔ emissions)
- **Combined uncertainties make it difficult to draw conclusions regarding both model performance and implementation requirements**
- **A major goal of this work is to provide the data and workflow necessary to overcome these obstacles through high-resolution benchmarks**

# Proposed future work … move toward detailed simulations of optical engines

- Subtask 6.1 (FY2016-17) LES of transient Diesel fuel injection, ignition, combustion, and emissions
- Subtask 6.2 (FY2016-18) LES of transient Gasoline Direct Injection spray dynamics, combustion, and emissions
- Subtask 6.3 (FY2017-18) LES of the LTGC engine with emphasis on temperature stratification
- Subtask 6.4 (FY2018) LES of the LTGC engine including direct injection and combustion

**Milestones aimed toward detailed calculations in (optical) engine geometries with advanced treatment of detailed physics and turbulence phenomena not account for in current codes**

# Summary

- Primary focus is to complement development of predictive engineering models for RANS and LES at engine relevant conditions
  - Direct coupling with key target experiments (anchor)
  - Application of first-principles models at identical conditions
  - Development of computational benchmarks to understand model accuracy
  - Use of a unique code and full hierarchy of high-performance computing resources
- Two sets of barriers addressed
  - Lack of fundamental knowledge of both Diesel and GDI combustion regimes and related lack of predictive models for engine combustion design
  - Efficient and routine use of advanced high-performance computing architectures
- A new generation of flow solvers and models combined with additional data and improved workflow aimed at model validation is required
  - Experimental data alone insufficient for validation
  - High-resolution LES combined with first principles models and UQ are being applied to provide an additional level of precision
- Technology transfer mechanisms include
  - Development of advanced sub-model framework combined with UQ
  - Near DNS benchmark data that provides insights not available from experiments
  - Eventually a next generation multiphysics/multiscale simulation code
  - Working closer with industry in the area of model/solver development and validation

# Technical Back-Up Slides

# Bayesian inference method

- **Bayesian inference** is a method of **statistical inference** in which **Bayes rule** is used to update the probability for a hypothesis as evidence is acquired
- **Statistical inference** is the process of deducing properties of an underlying distribution by analysis of data
- **Here it provides a means to systematically compare models with the goal of identifying an optimal model, i.e.,**

$$y = f(\lambda) + \varepsilon$$

Reference data, $y$, are equal to model prediction, $f(\lambda)$, with error, $\varepsilon$
$\lambda$ are the input parameters of the model

- **Bayes rule** relates the odds of event A1 to the odds of event A2 before (prior to) and after (posterior to) conditioning on another event B

$$\underbrace{p(\lambda|y)}_{\text{Posterior}} = \frac{\overbrace{p(y|\lambda)}^{\text{Likelihood}}\ \overbrace{p(\lambda)}^{\text{Prior}}}{\underbrace{p(y)}_{\text{Evidence}}}$$

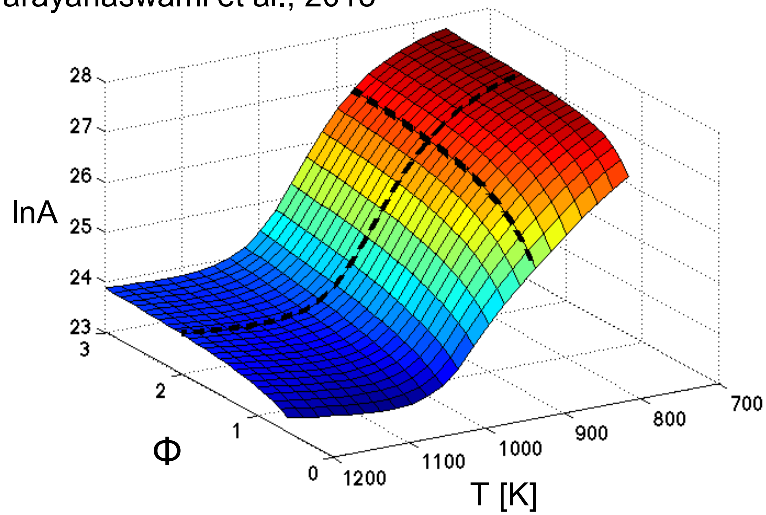
Gives joint PDF (**posterior**) on chosen parameters of interest (i.e., the probability of a hypothesis given the observed evidence)

- **Likelihood** obtained by running ensemble of model calculations while varying parameters
- **Prior** indicates the previous estimate of probability that a hypothesis is true before gaining the current evidence
- **Evidence** is a normalizing constant in the present context

# Example … optimize 2-step mechanism making parameters (A, $E_a$) = f(T, Φ)

Narayanaswami et al., 2013

y = 




$$f(\lambda) = f(A, E_a, T, \phi) =$$

**$C_{12}H_{26} + 12.5O_2 \rightarrow 12CO + 13H_2O$ (1)**

**$CO + 0.5O_2 = CO_2$ (2)**

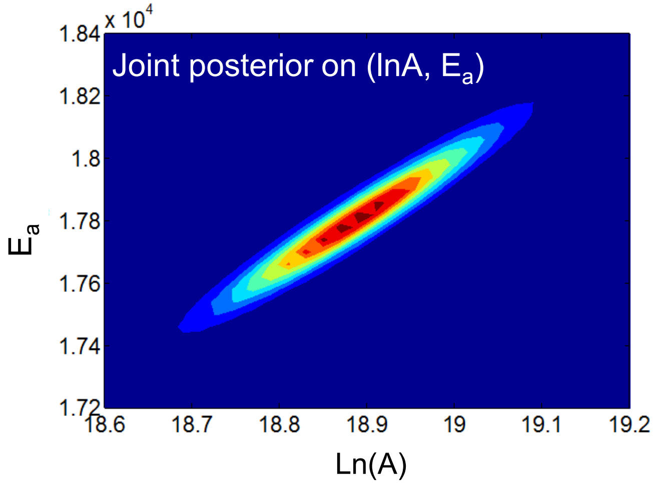
$$k_1 = AT^n \exp(-E_a/RT)[\mathrm{C_{12}H_{26}}]^{\mathrm{a}}[\mathrm{O_2}]^{\mathrm{b}}$$

$$k_2 = 3.98 \times 10^{14} \exp(-40/RT)[\mathrm{CO}]^1[\mathrm{H_2O}]^{0.5}[\mathrm{O_2}]^{0.25}$$

$$k_{-2} = 5.00 \times 10^8 \exp(-40/RT)[\mathrm{CO_2}]^1$$

Westbrook et al., CST, 1981
Dryer and Glassman, PCI, 1972

**Best A and $E_a$ parameters: p(A, $E_a$ | y) =**



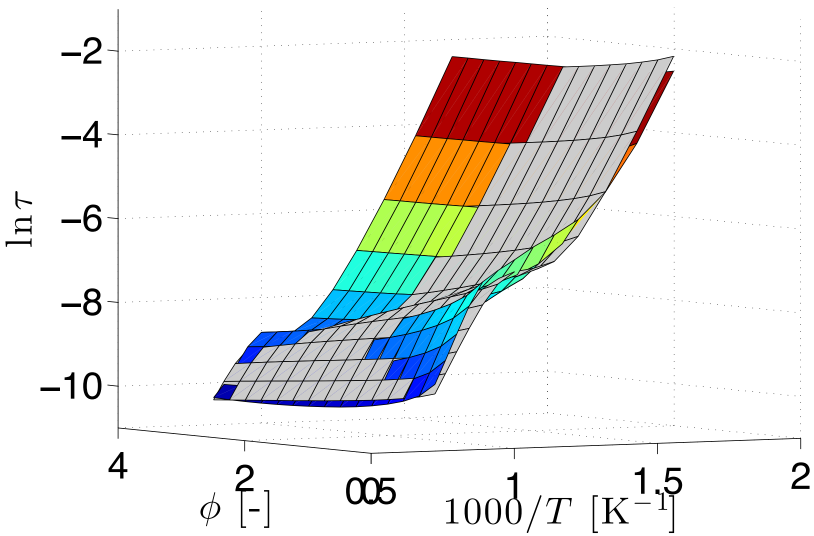
# Example … optimize 2-step mechanism making parameters (A, $E_a$) = f(T, Φ)

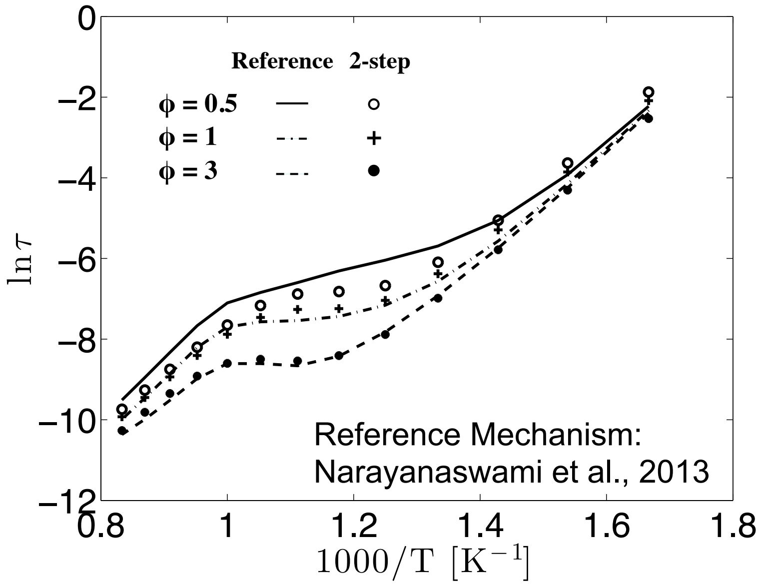
- **Using an 8-parameter expansion for $E_a$ and ln A:**

$$E_a = \eta_1$$

$$\ln A = \lambda_1 + \lambda_2 e^{\lambda_3 \phi} + \lambda_4 \tanh((\lambda_5 + \lambda_6 \phi) T_0 + \lambda_7)$$

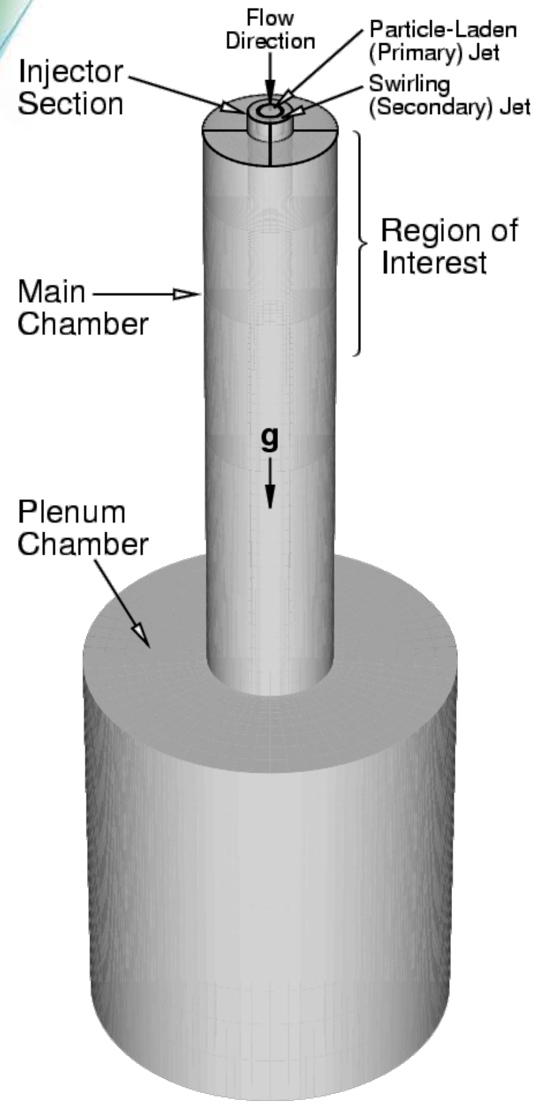
- **Bayesian inference is used to obtain best fit with quantified error**

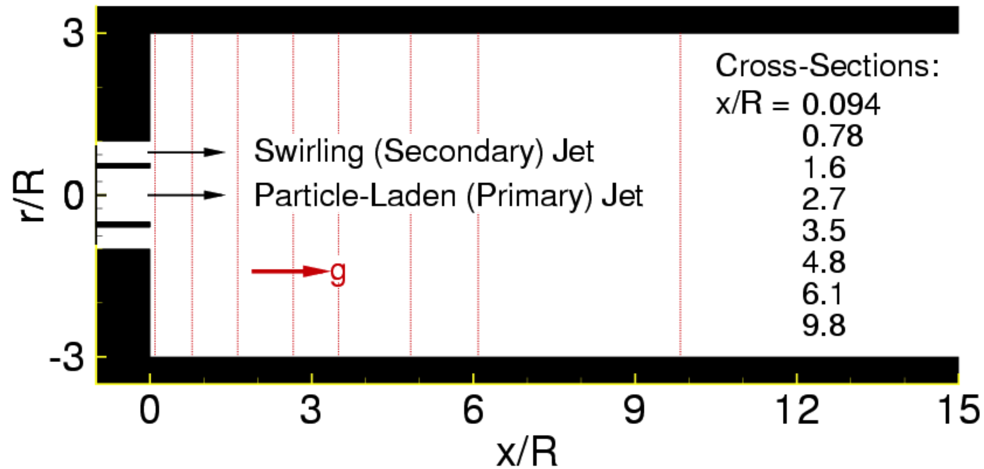


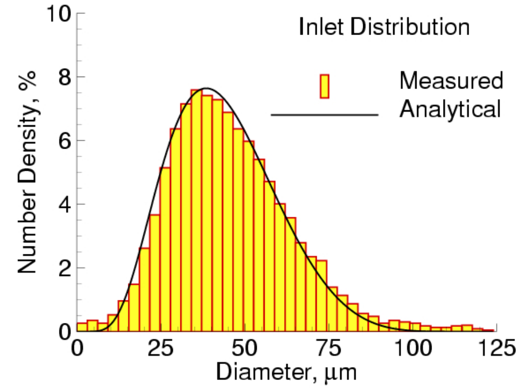




- **Challenge is to find best expansion possible with minimum parameters**

# Lagrangian spray modeling approach is being systematically validated



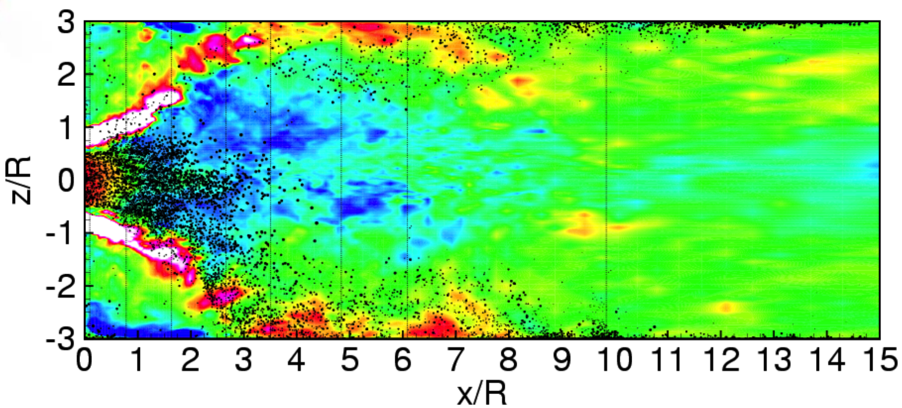



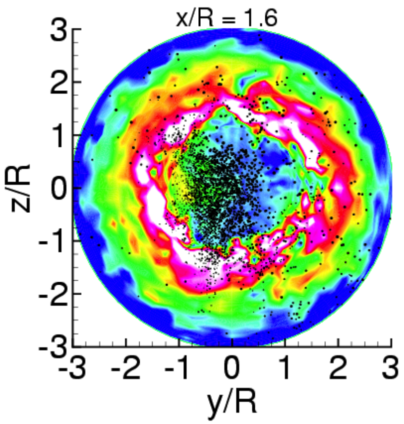



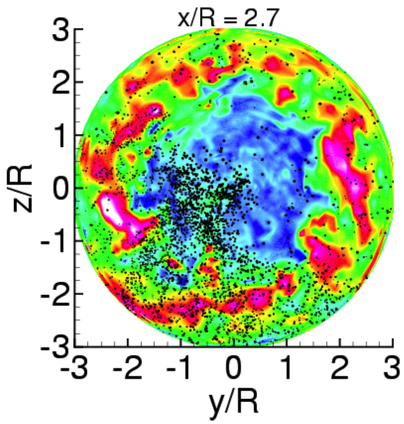

| | Case 1 | Case 2 |
|---|---|---|
| **Reynolds Number** | **26,200** | **27,250** |
| **Swirl Number** | **0.47** | **0.49** |
| **Loading Ratio** | **0.034** | **0.17 (5x)** |
| **Density Ratio** | **2152** | |

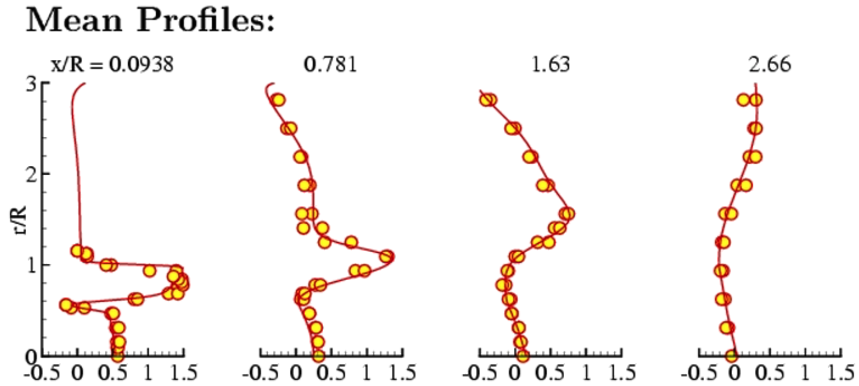
**$R_{ref}$ = 32 mm, $U_{ref}$ = 12.9 m/s**

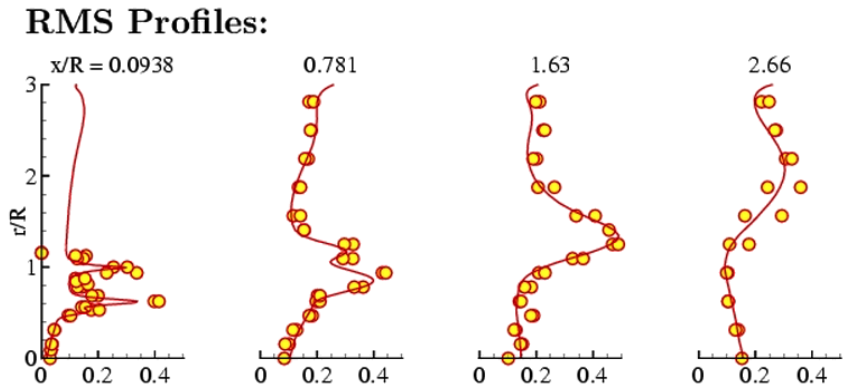
# Predictive accuracy demonstrated in complex flows with no model tuning




Time-averaged particle mean and RMS velocity profiles show good agreement with experimental measurements in a model axisymmetric combustor configuration

# End