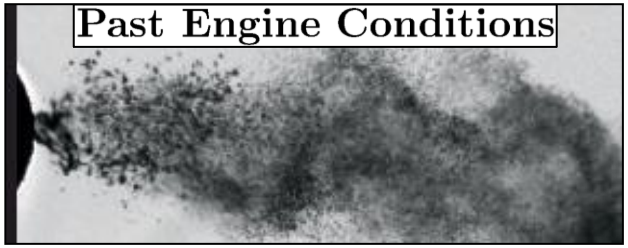
SAND2017-3224PE

Fuel injection under trans-critical conditions



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[1]*Combustion Research Facility*, **Sandia National Laboratories**, Livermore, CA

[2]**Argonne National Laboratory**, Lemont, IL

[3]**University of Brighton**, Brighton, UK

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Acknowledgement: Eric W. Lemmon, **NIST**, Boulder, CO
Mark Linne, **University of Edinburgh**, Edinburgh, UK
Andreas Dreizler, **TU Darmstadt**, Darmstadt, Germany

Outline

- **Introduction**
  Propulsion and power generation in the U.S.

- **Emerging “trans-critical” conditions in advanced devices**
  Requirement for a new capability for future engine design

- **Collaborative theoretical & experimental research**
  Theory: Mesoscale techniques in trans-critical injections

  Imaging: Developing microscopic high-speed imaging for validation

- **Results & outcome**
  (a) Predictive & affordable model for trans-critical conditions
  (b) Paradigm change in gas turbines, liquid rockets & diesel engines

- **Perspective & outlook**
  (a) Integration of advances into industry CFD
  (b) Control over injections independent of “trans-critical” conditions

Introduction

The role of combustion in modern society

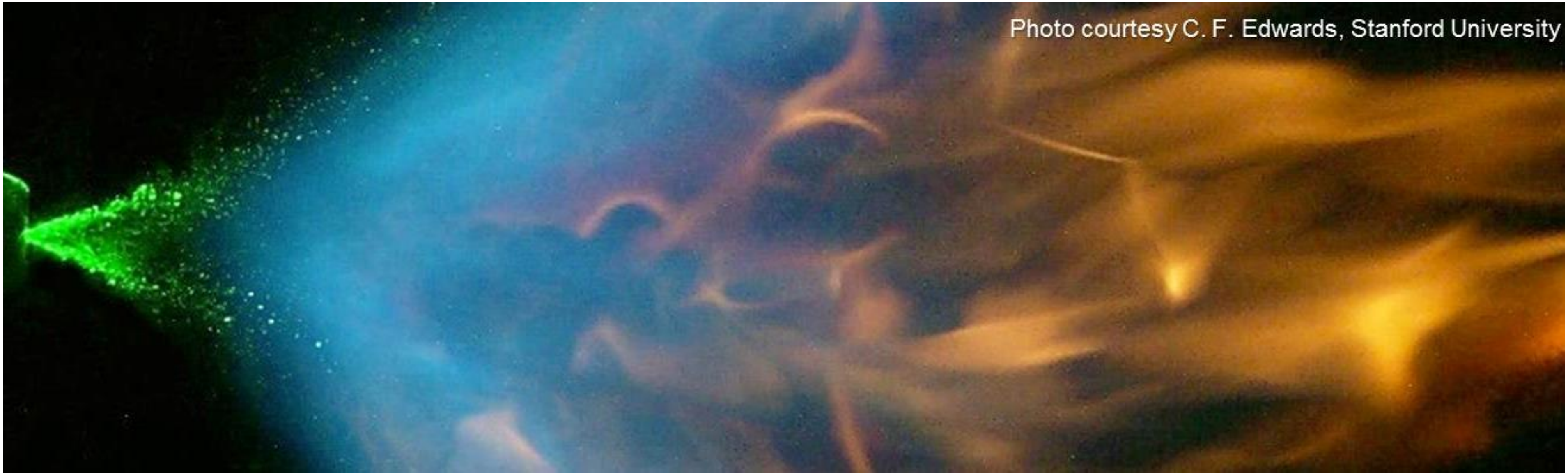
- **Combustion in the United States (propulsion & power generation)**
  - >90% reliance for all transportation
  - ~100% reliance for heavy duty trucks and airplanes
  - ~80% for primary energy generation
  - ~60% for electrical production

- **All-electric and plug-in hybrid transportation**
  - Less than 1% of current automotive sales despite promise in reducing vehicle emissions*
    (*Source: Argonne National Laboratory 2015)

- ***Further gains in clean & efficient combustion will have large economic and environmental impacts***

Introduction

Significance of mixture preparation to advanced combustion



- Close proximity between liquid injection & flame
  - ➢ **Fuel injection significantly determines combustion**

Introduction

Significance of mixture preparation to advanced combustion

- **Goals of advanced combustion strategies**
  - Reliable ignition & combustion
  - Optimal efficiency for minimal fuel consumption
  - Minimal harmful emissions (e.g., NOx, soot)

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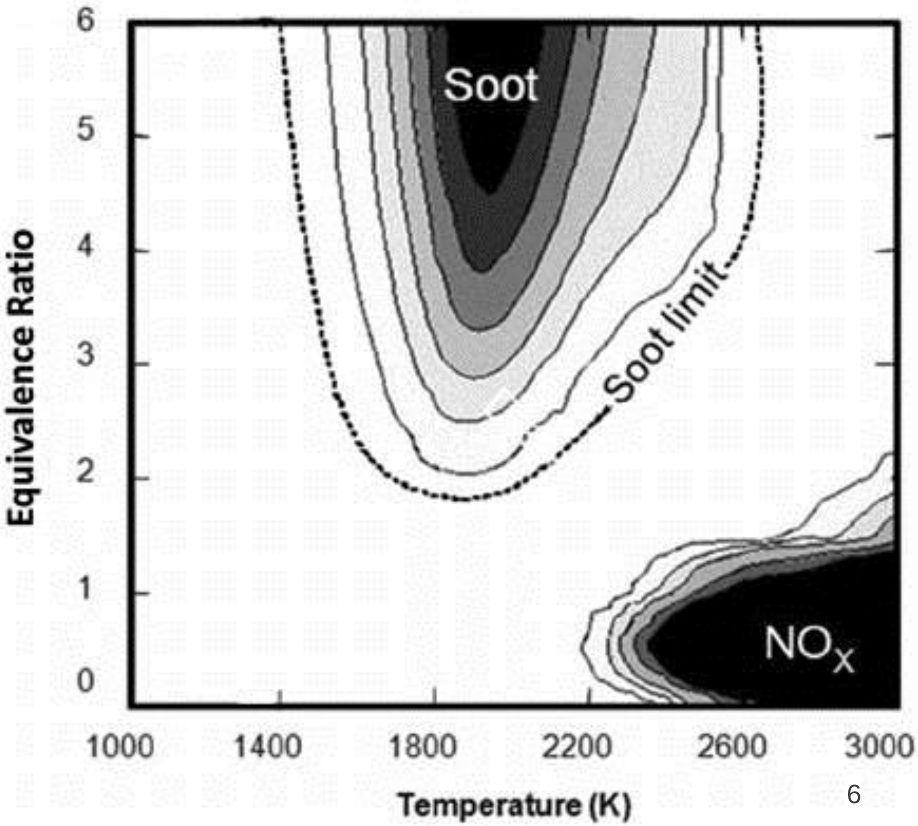

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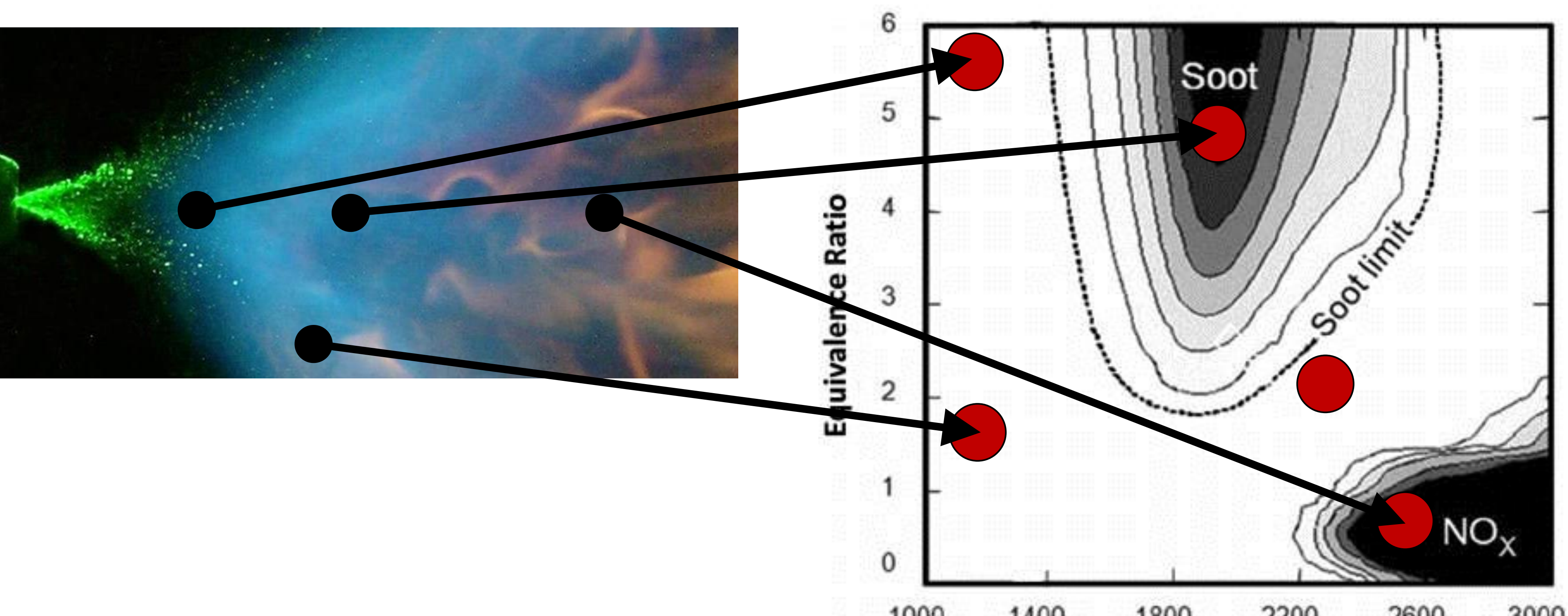

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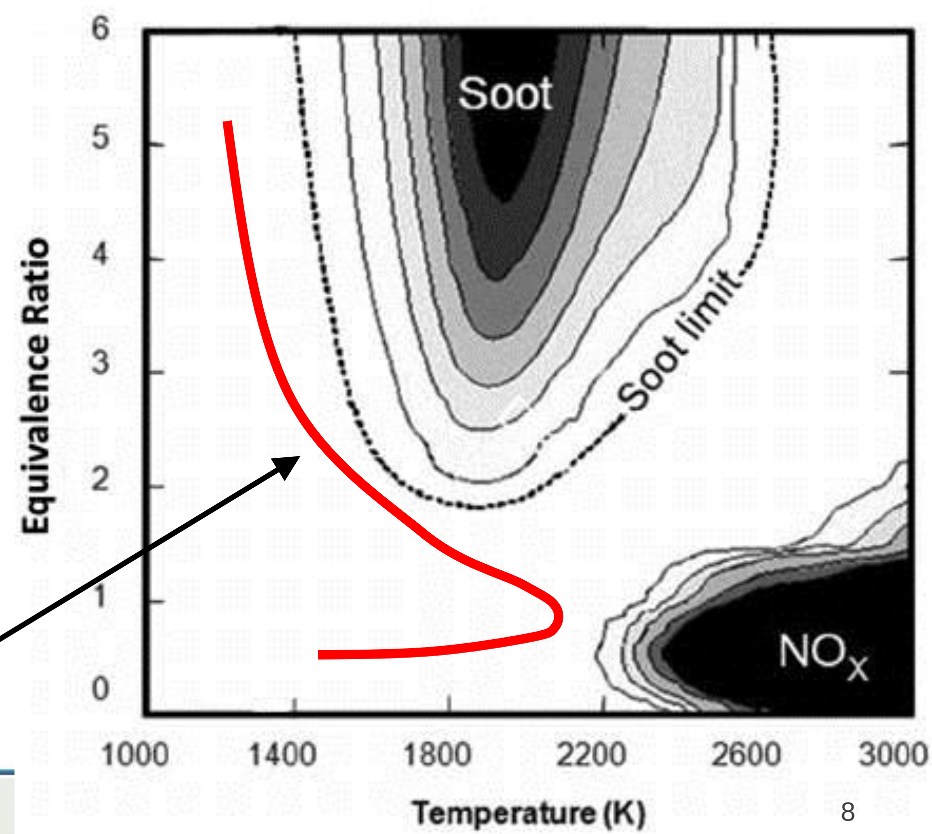


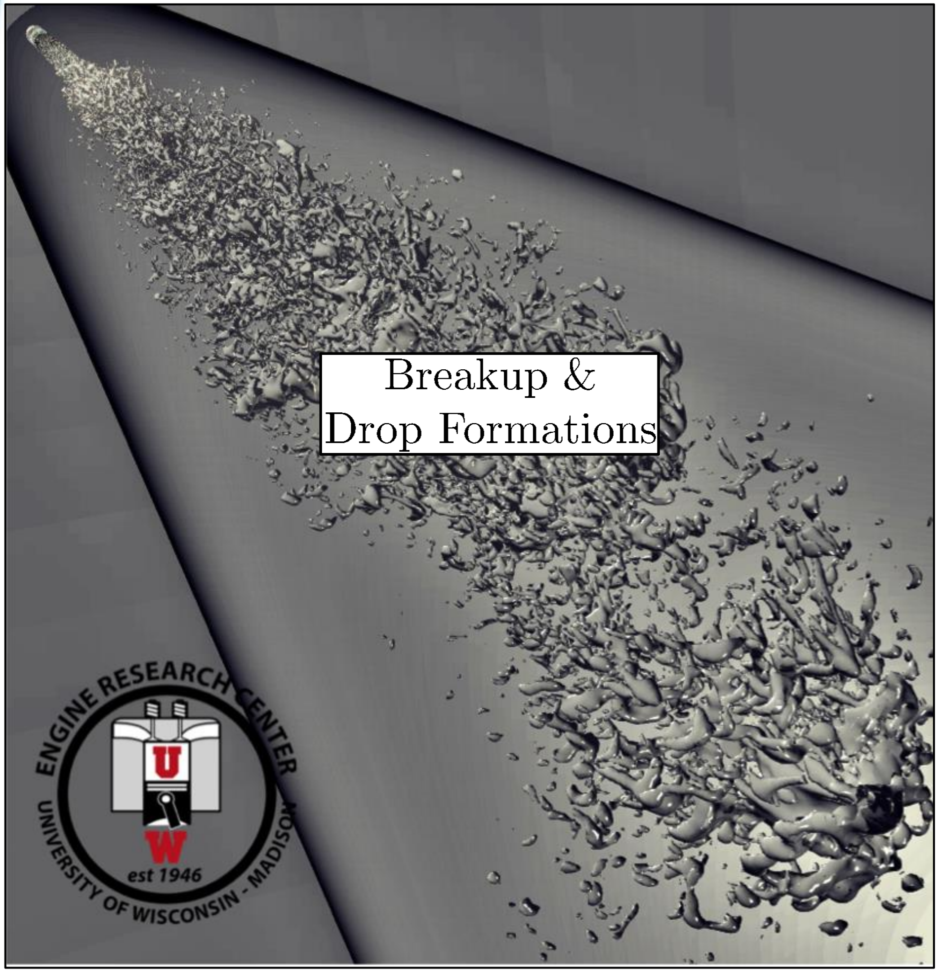
- Injection determines temporal progression of mixing
- Control of mixture preparation key to advanced combustion

Emerging “trans-critical” conditions in advanced devices

Requirement for new a capability for future engine design

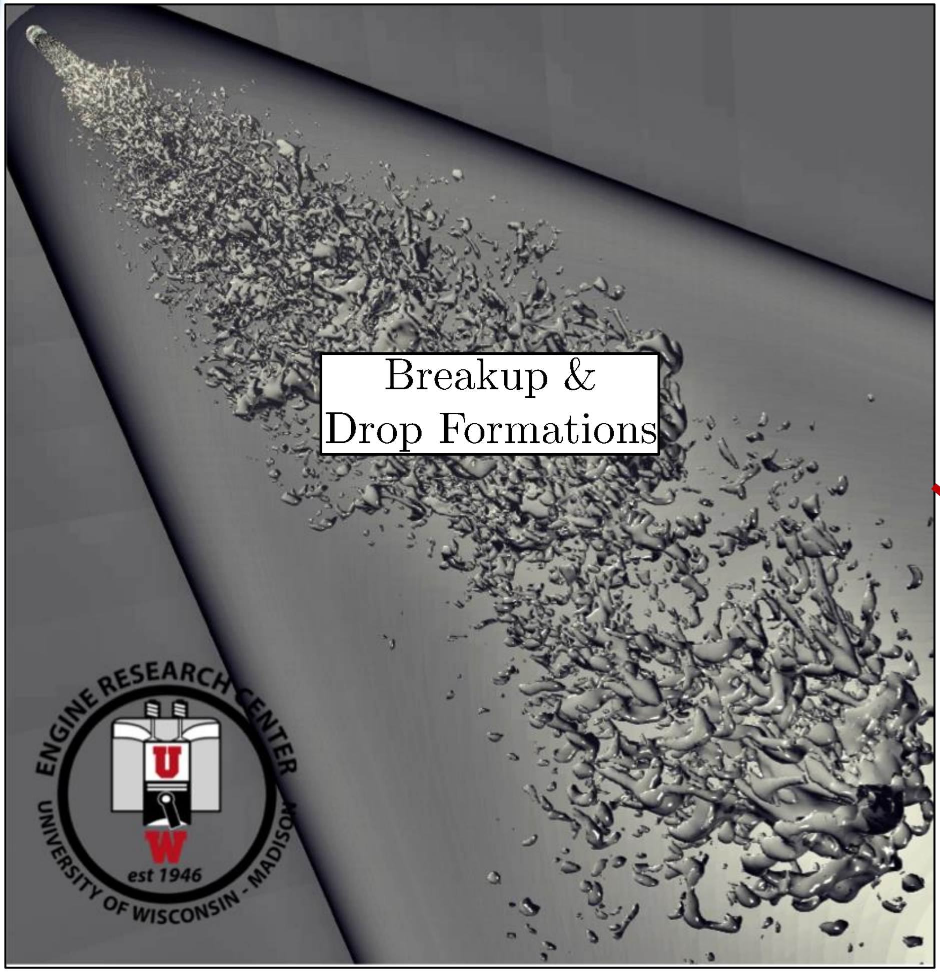
Emerging “trans-critical” conditions in modern combustion

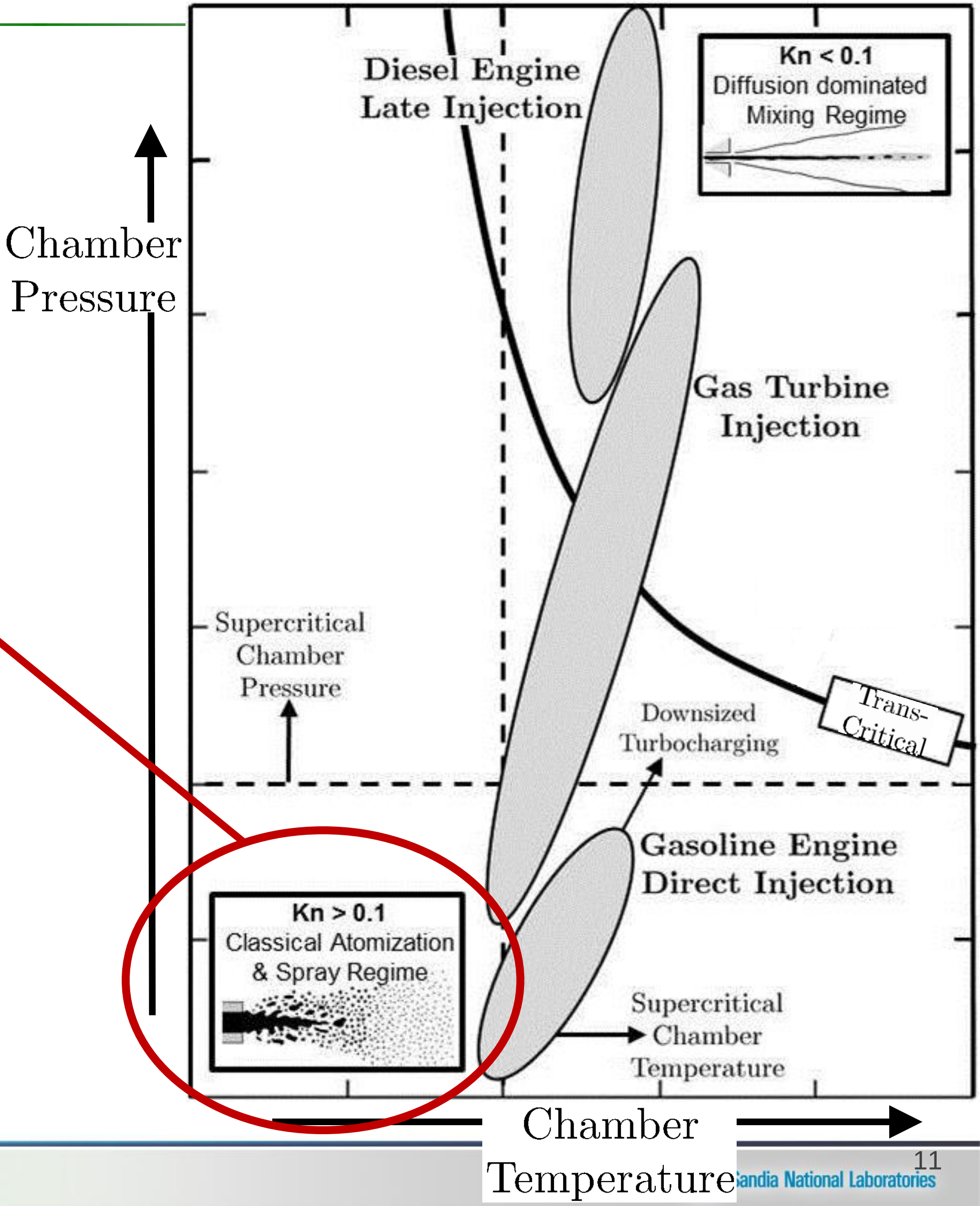
Classic engine ***spray*** *injection:*



Emerging "trans-critical" conditions in modern combustion

Classic engine ***spray*** *injection*

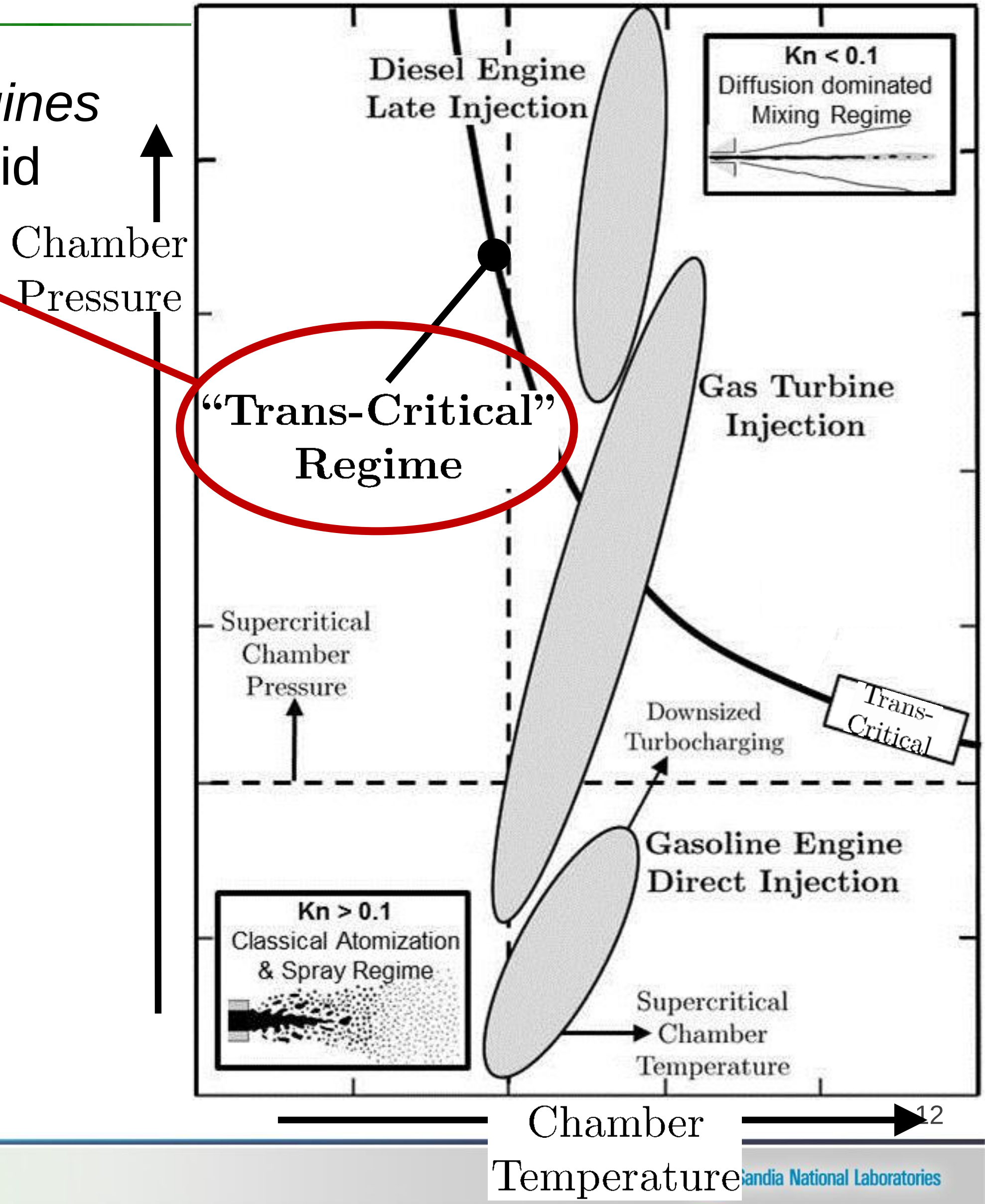




Emerging "trans-critical" conditions in modern combustion

*"**Trans-Critical**" injection in future engines*

- Discovery that spray injection not valid



Emerging "trans-critical" conditions in modern combustion

***"Trans-Critical"** injection in future engines*
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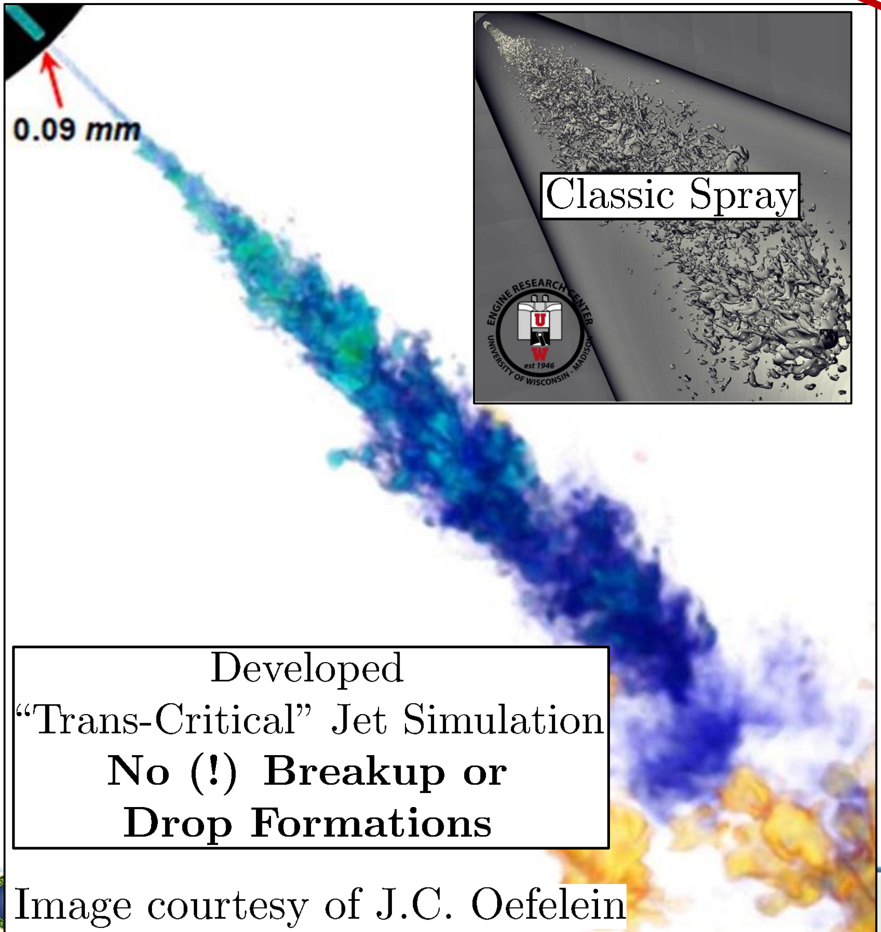
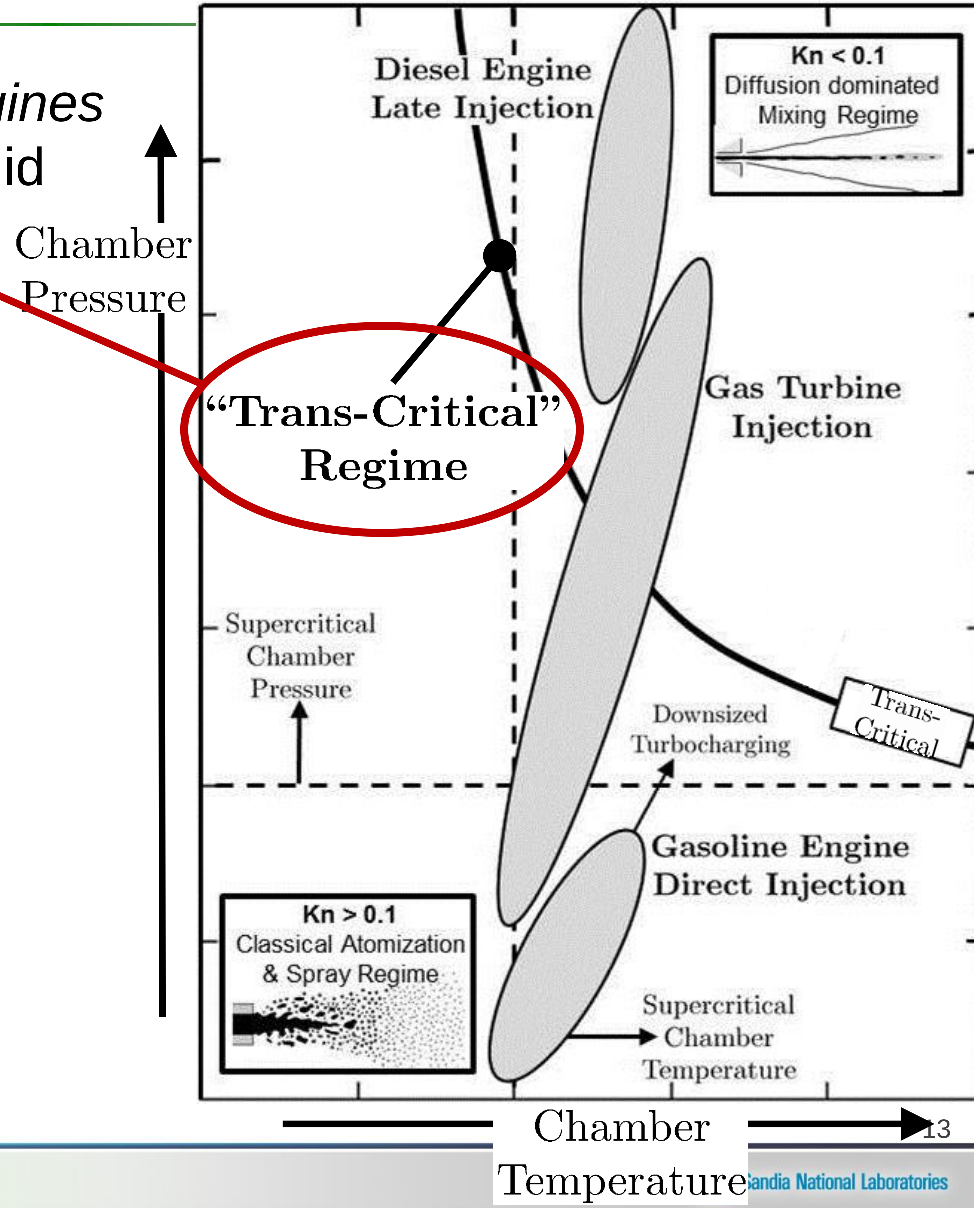


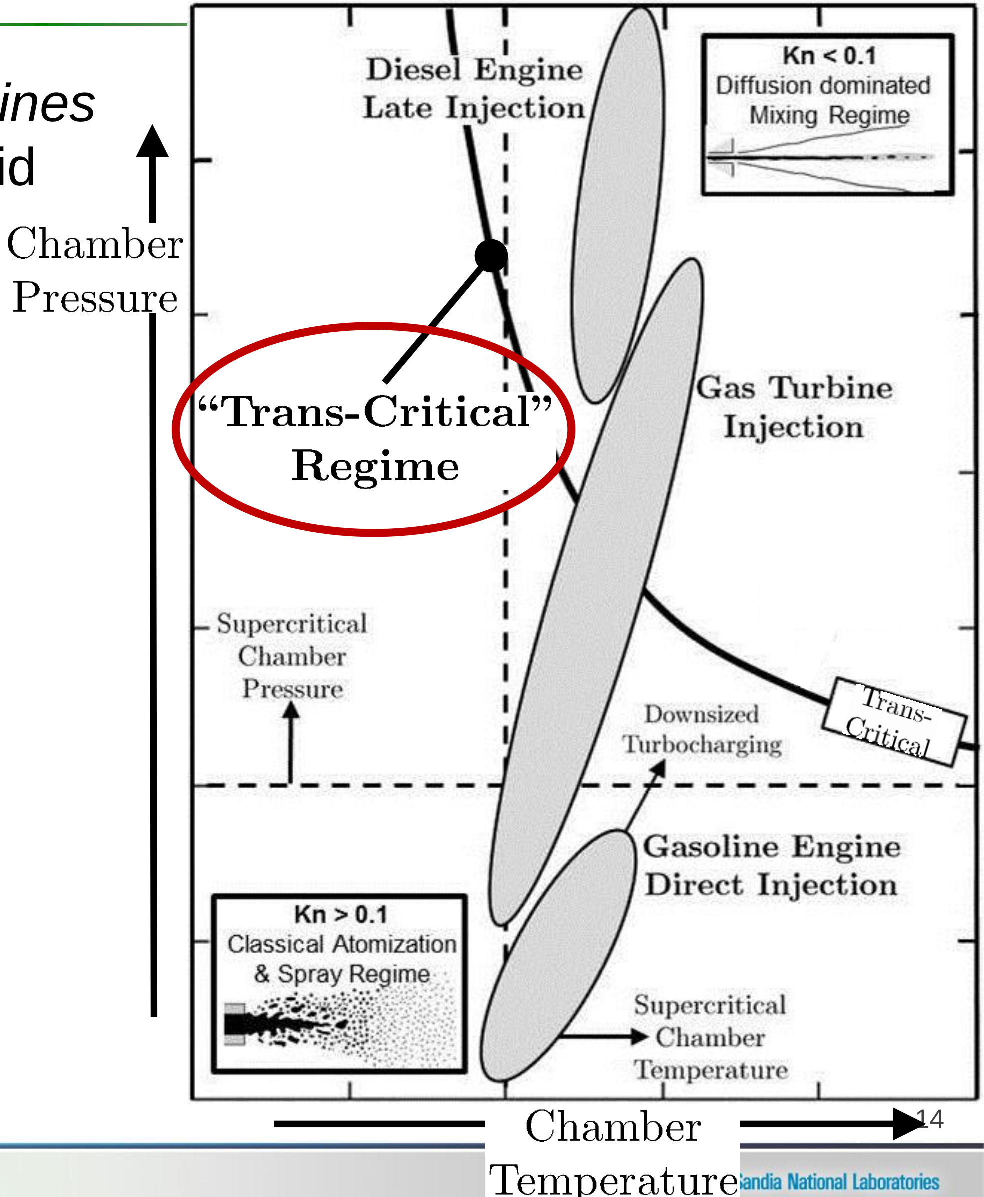
Image courtesy of J.C. Oefelein



Emerging "trans-critical" conditions in modern combustion

***"Trans-Critical"** injection in future engines*

- Discovery that spray injection not valid
- Spray models become questionable in efficient virtual engine design



Emerging "trans-critical" conditions in modern combustion

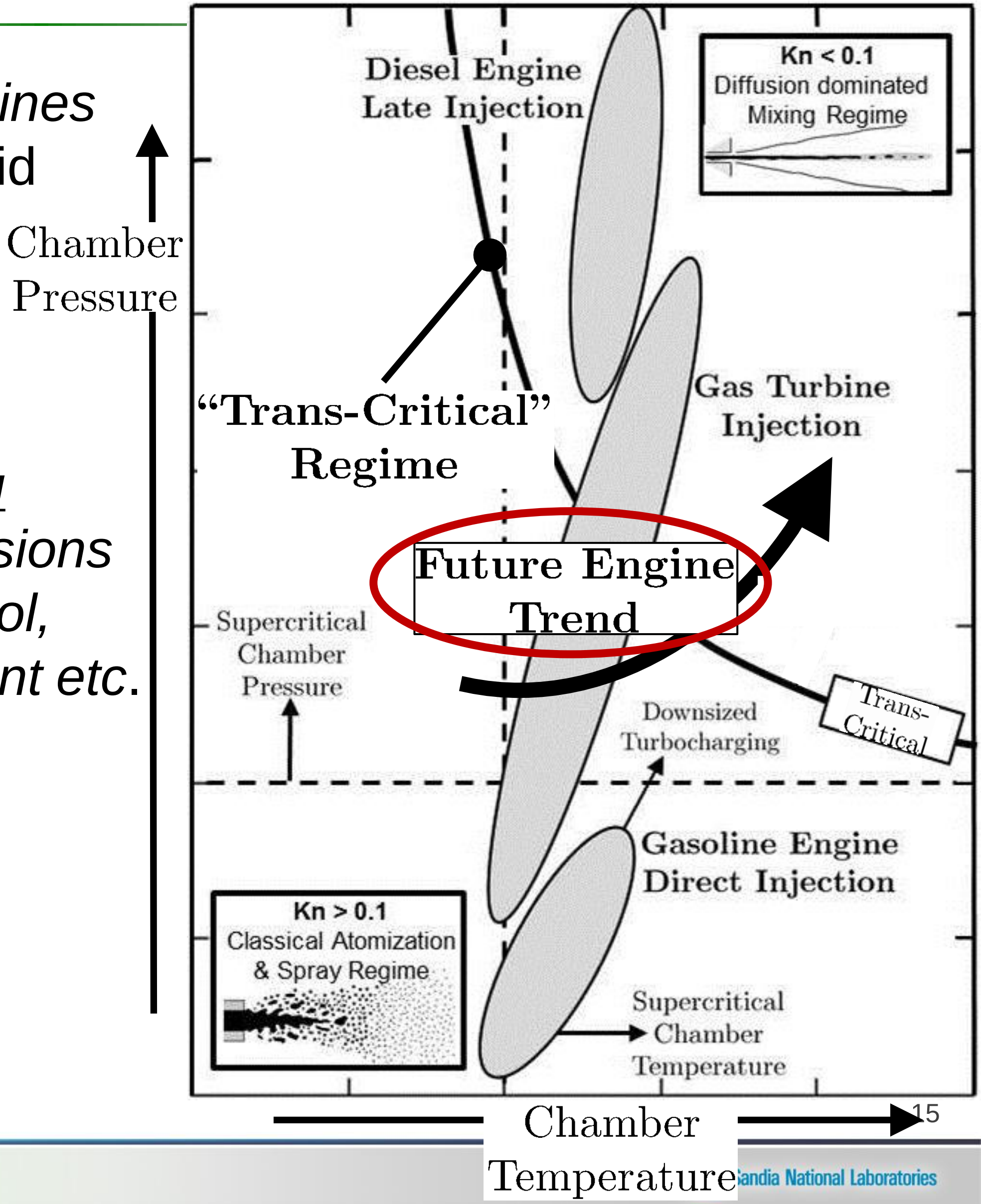
***"Trans-Critical"** injection in future engines*

- Discovery that spray injection not valid
- Spray models become questionable in efficient virtual engine design
- Future engine design trends **toward** trans-critical conditions

→ *higher pressures allow* ***downsizing***

→ *more fuel efficient, less (soot) emissions*

→ *smaller lighter engines, better to cool, better to package with after-treatment etc.*



Emerging "trans-critical" conditions in modern combustion

***"Trans-Critical"** injection in future engines*

- Discovery that spray injection not valid
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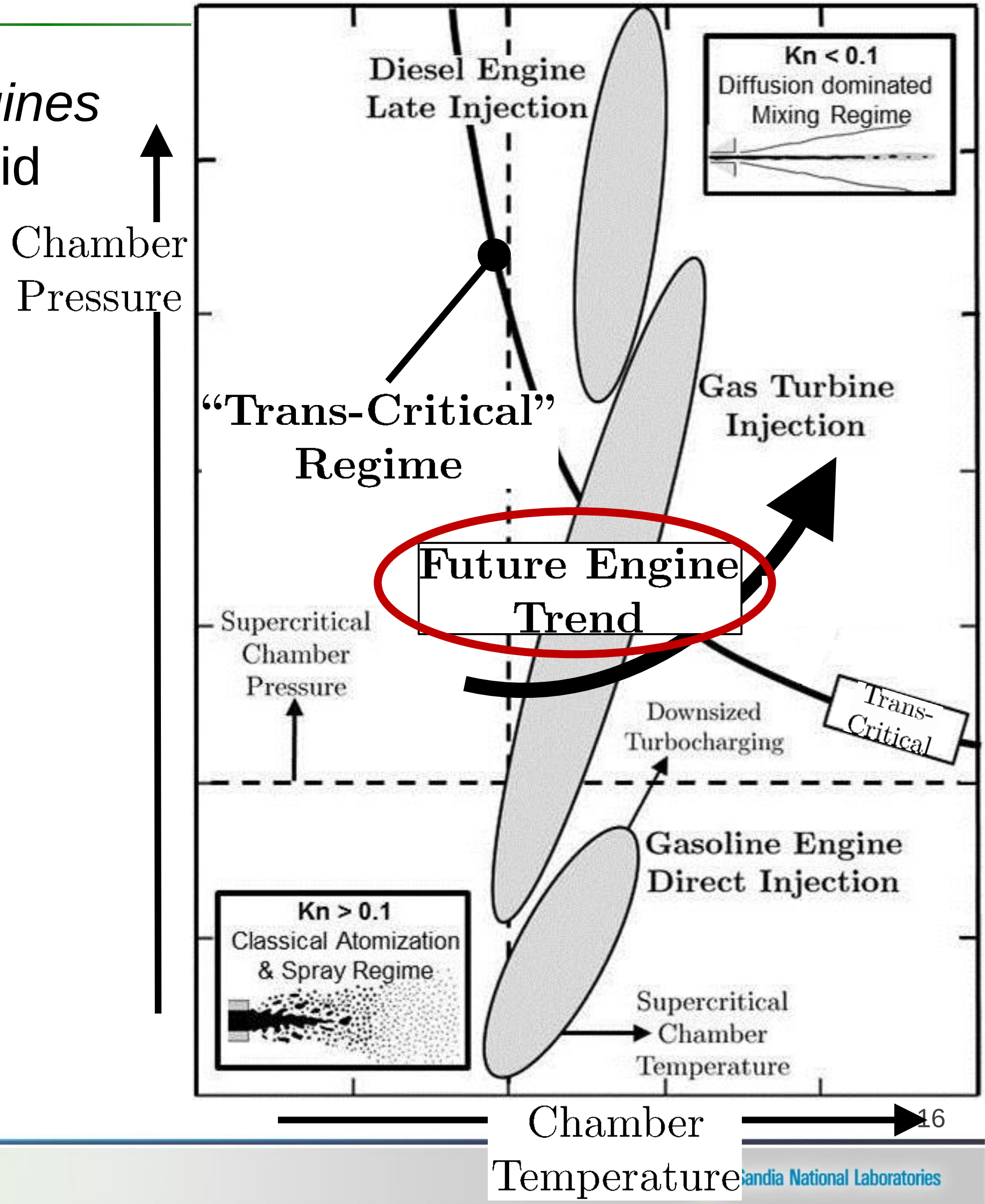
Research challenge:

(a) Understanding & predicting trans-critical conditions

(b) Development of high-speed & high-fidelity imaging for validation

(c) Development of suitable injection simulations



Collaborative theoretical & experimental research

Theory: Understanding trans-critical fuel injections using meso-scale science techniques

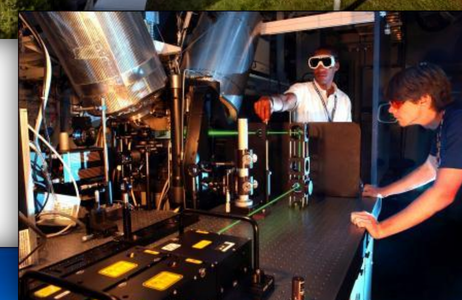
Imaging: Developing microscopic high-speed imaging for validation

Combustion Research Facility

CRF

A DOE Collaborative Research Facility dedicated to energy science and technology for the twenty-first century

- Leadership in combustion research since 1980
- 8200-m^2 office and laboratory facility
- 36 highly specialized labs
  - Laser-based diagnostics
  - Combustible and toxic gas handling
  - Computer-controlled safety system
- Dedicated computational facility



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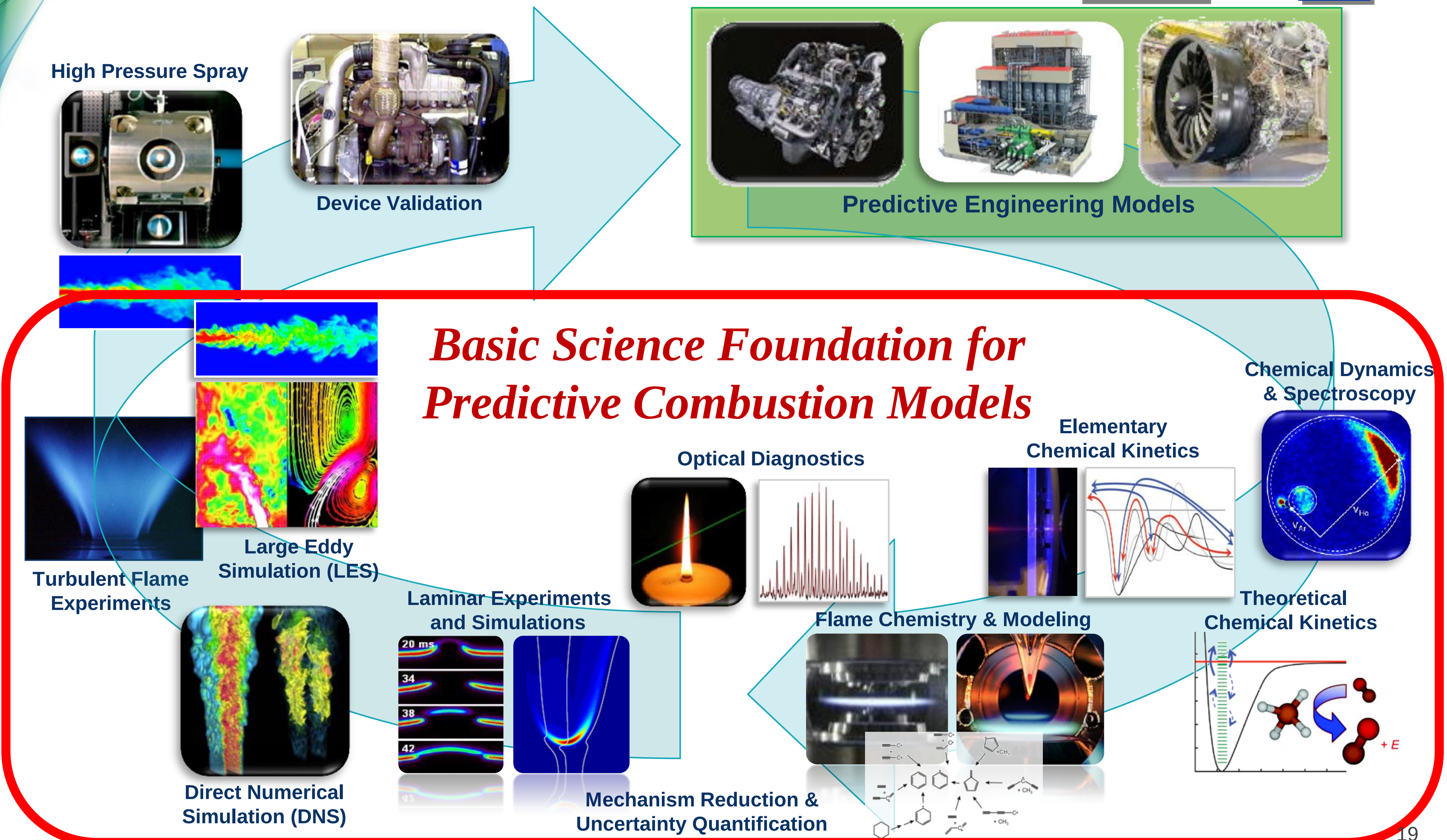
Fundamental Combustion Science Research at the CRF



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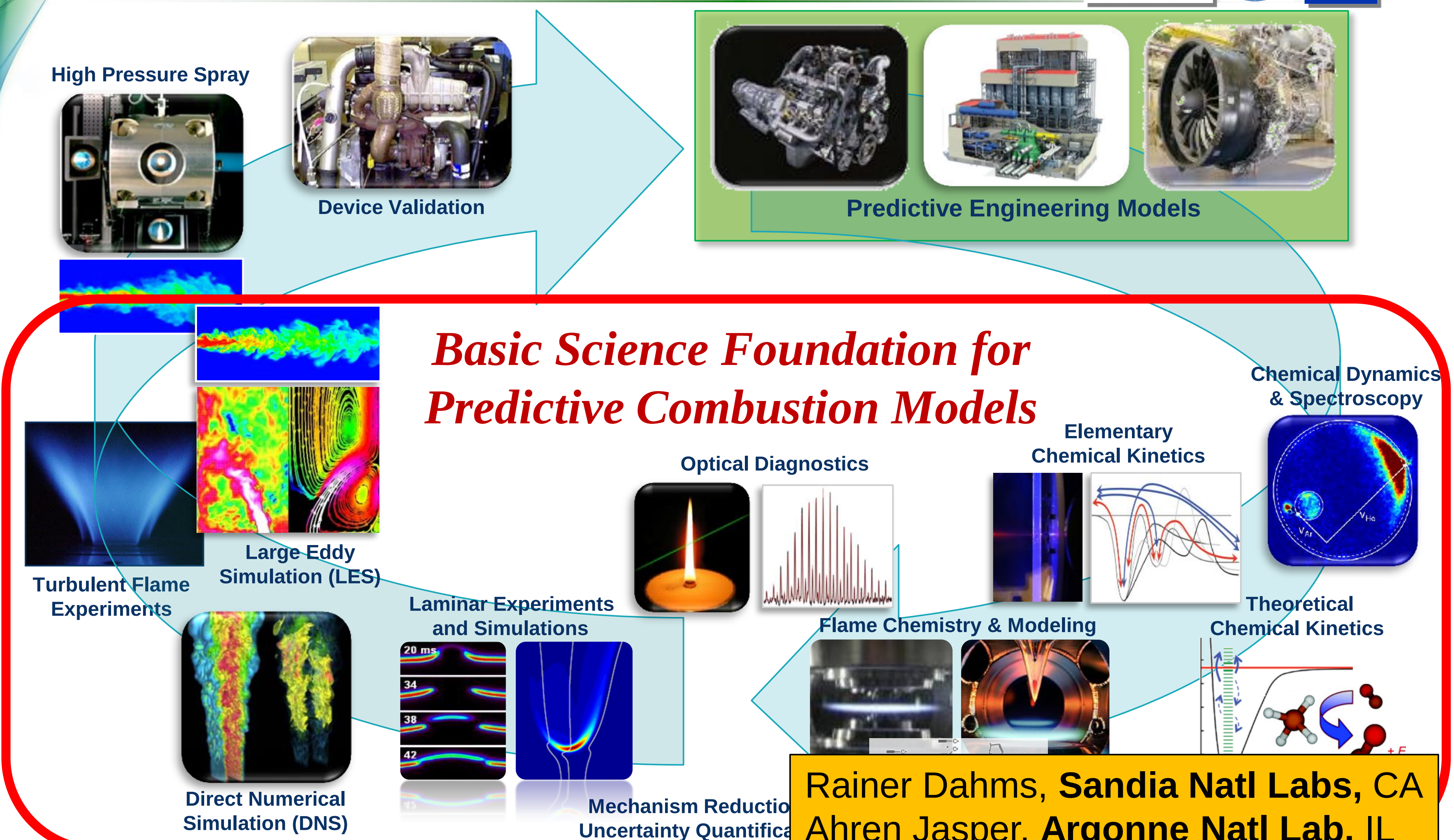

Rainer Dahms, **Sandia Natl Labs,** CA
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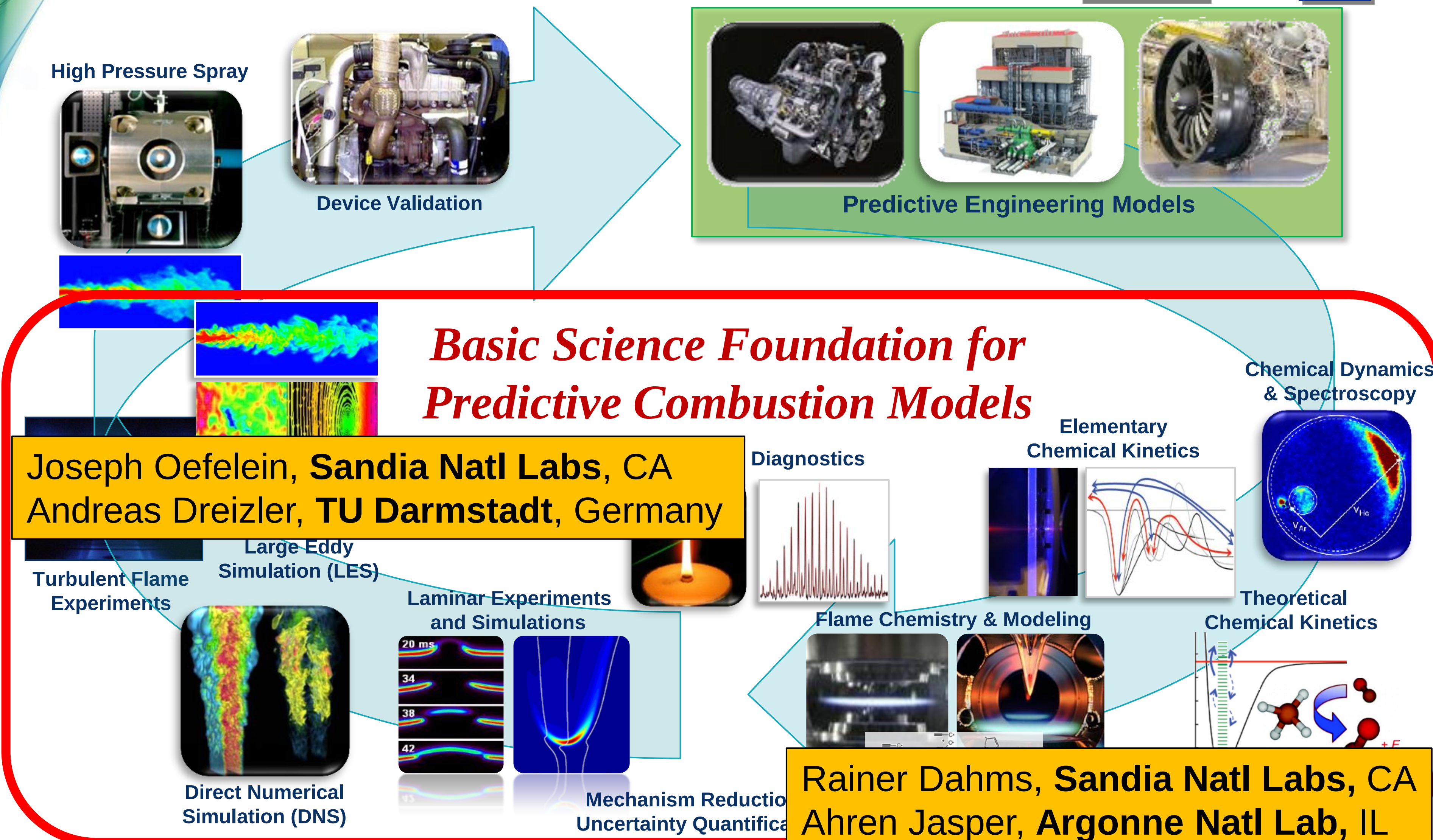
Fundamental Combustion Science Research at the CRF

CHRYSLER Ford GE GM



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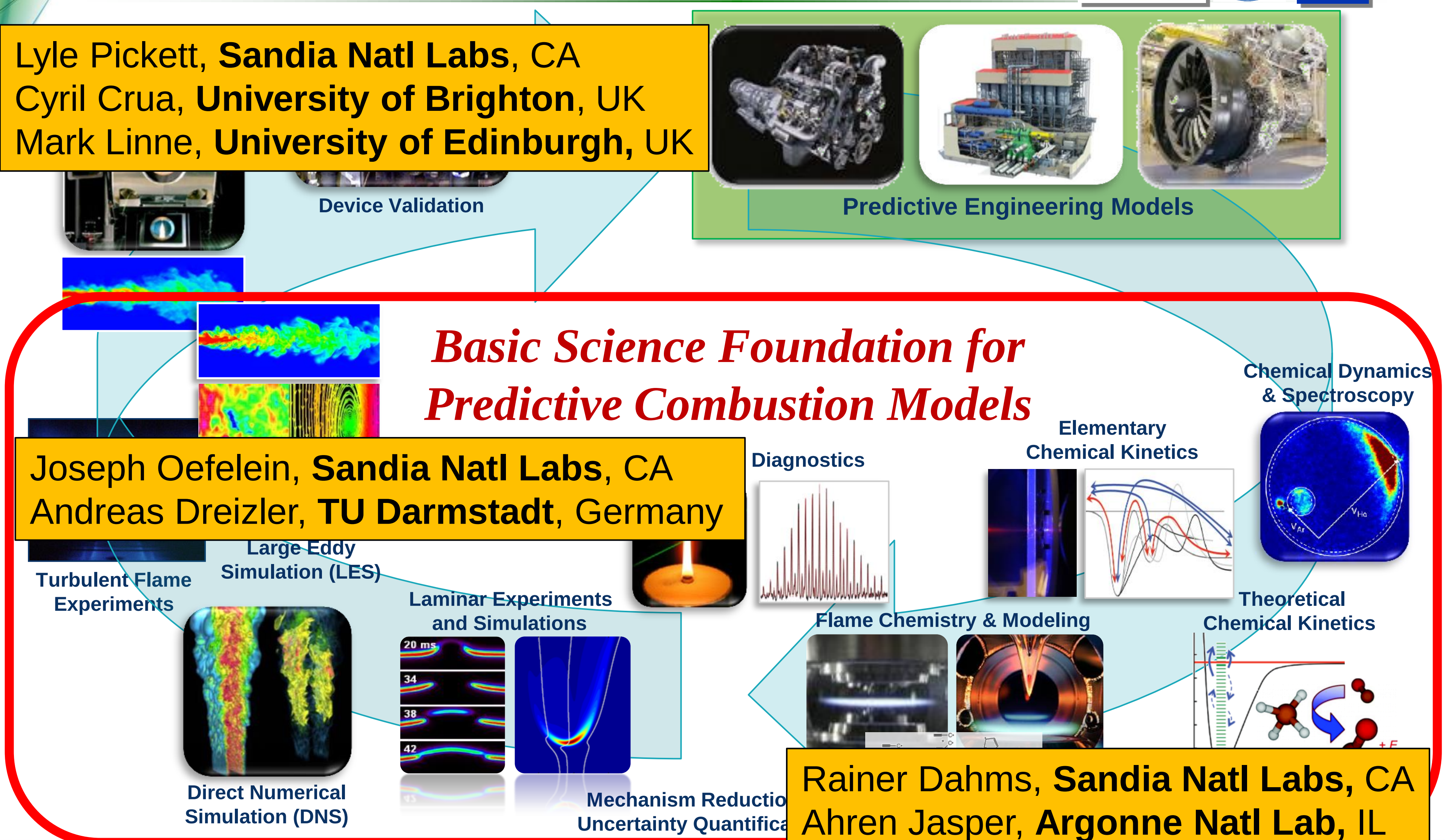
Lyle Pickett, **Sandia Natl Labs**, CA
Cyril Crua, **University of Brighton**, UK
Mark Linne, **University of Edinburgh,** UK



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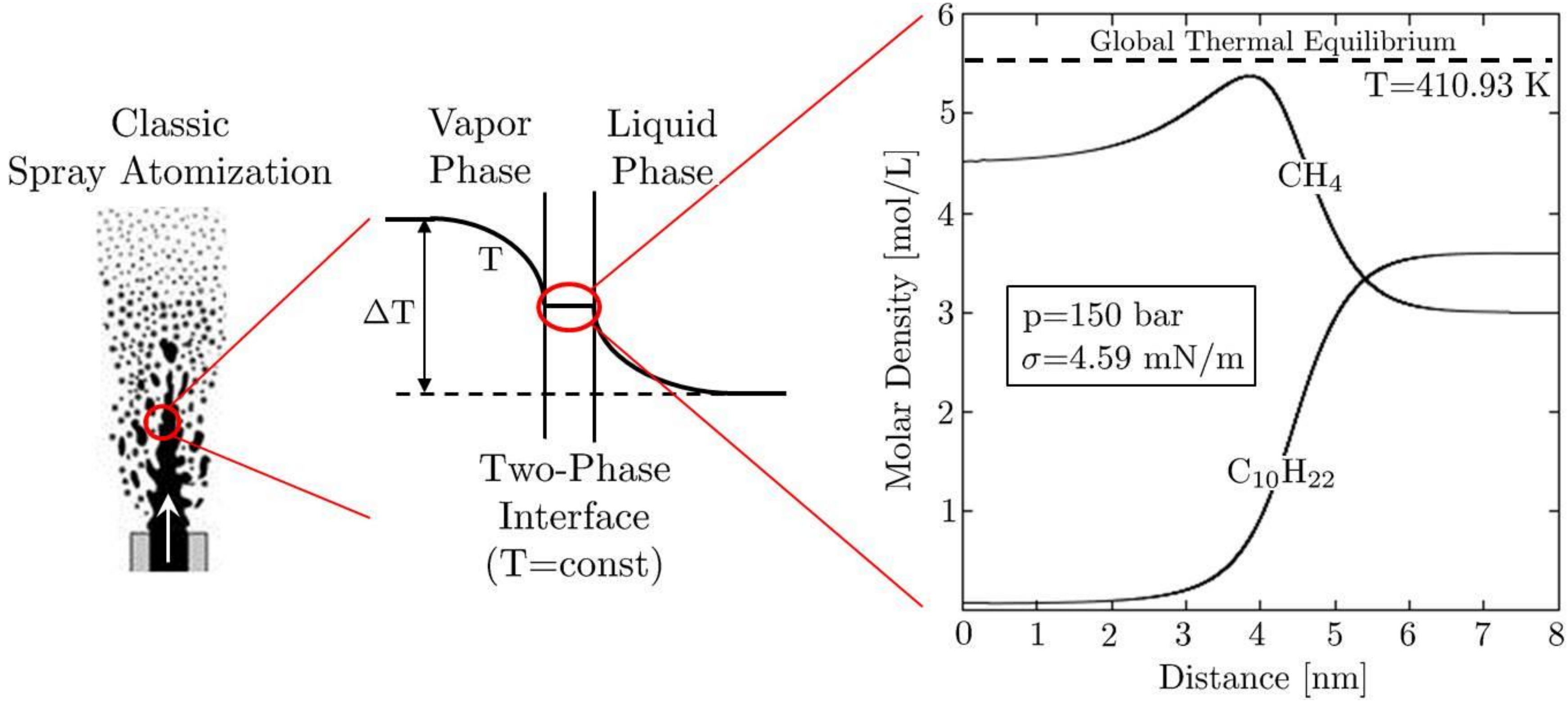
Meso-scale capillary theory for molecular gas-liquid interfaces

Basic Energy Sciences



Meso-scale capillary theory:

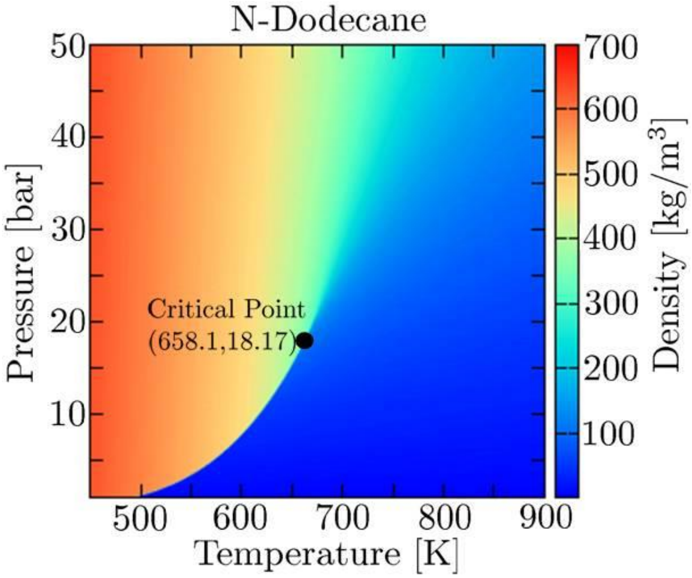
- Consistent with high-fidelity Monte Carlo & Molecular Dynamics simulations!
- Efficiency instrumental in developed engineering tool

Real-fluid multi-component thermodynamics & transport
Eric Lemmon, NIST, Boulder

- **Helmholtz energy (A) equation of state**

$$\frac{A}{RT} = \alpha^0(\delta,\tau) + \alpha^r(\delta,\tau)$$

All thermodynamic properties derivable from A

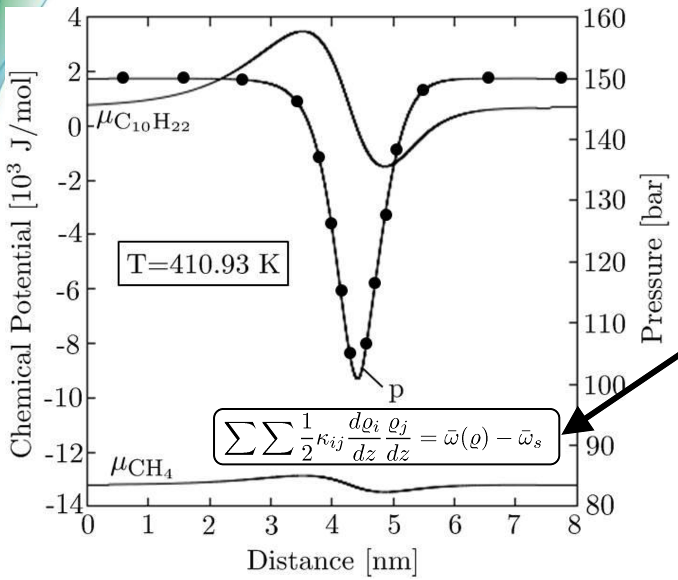


- **Applies to (arbitrary) liquid & gas mixtures at all relevant pressures and temperatures** (incl. near-critical and supercritical)

- **Contrast to previous frameworks:** Exhibits unique & desirable behavior over entire two-phase regime of fluid densities (including meta-stable, unstable regions)

From molecular dynamics to classic two-phase theory & spray atomization

Basic Energy Sciences



- **Isothermal interface regardless of temperature difference**
- **Interface: State of global thermal equilibrium → Helmholtz free energy is minimal !**
  - *Mean-field equation only valid for minimal free energy!*

From molecular dynamics to classic two-phase theory & spray atomization

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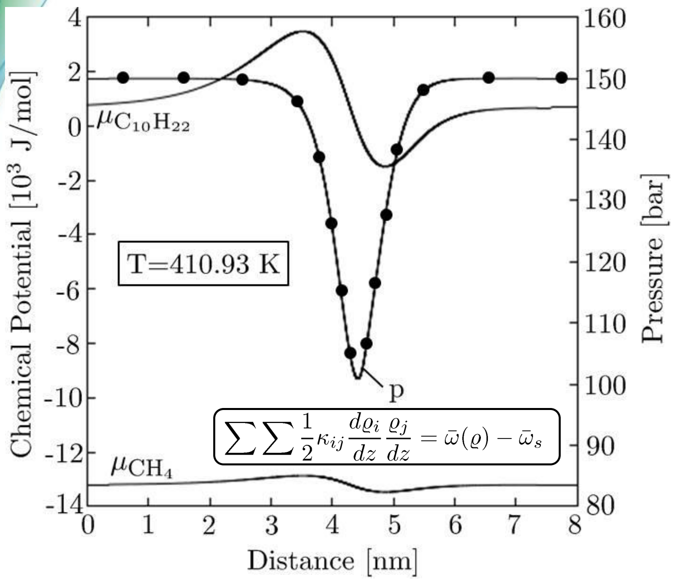

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Justifies assumptions in two-phase theory:

- Calculations of true critical points of mixtures
- Evaporation & heating laws
- Surface tension forces

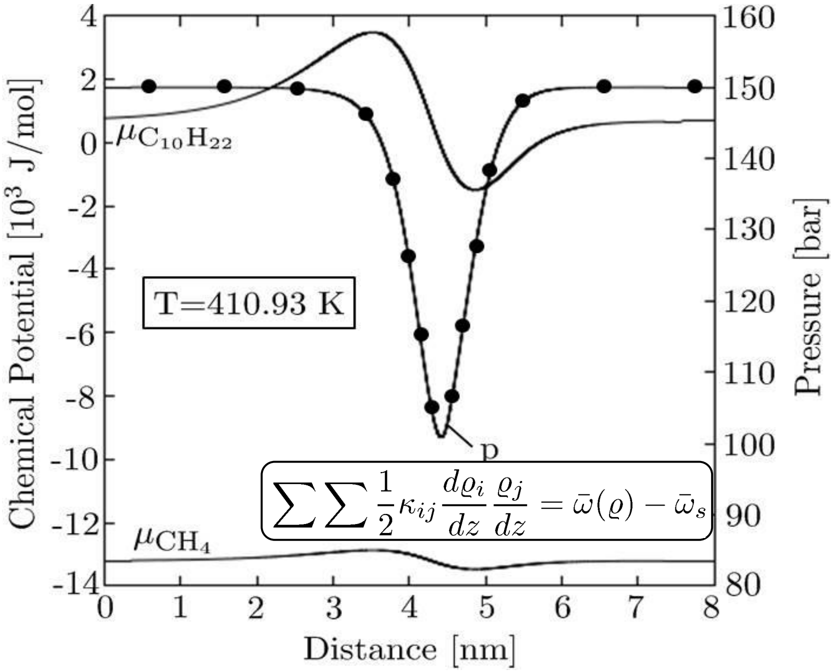
➢ Atomization & evaporation

Fundamental changes in interfacial molecular dynamics

Basic Energy Sciences

- **Helmholtz energy only minimized in isothermal systems**

$$dF \leq -SdT - pdV$$



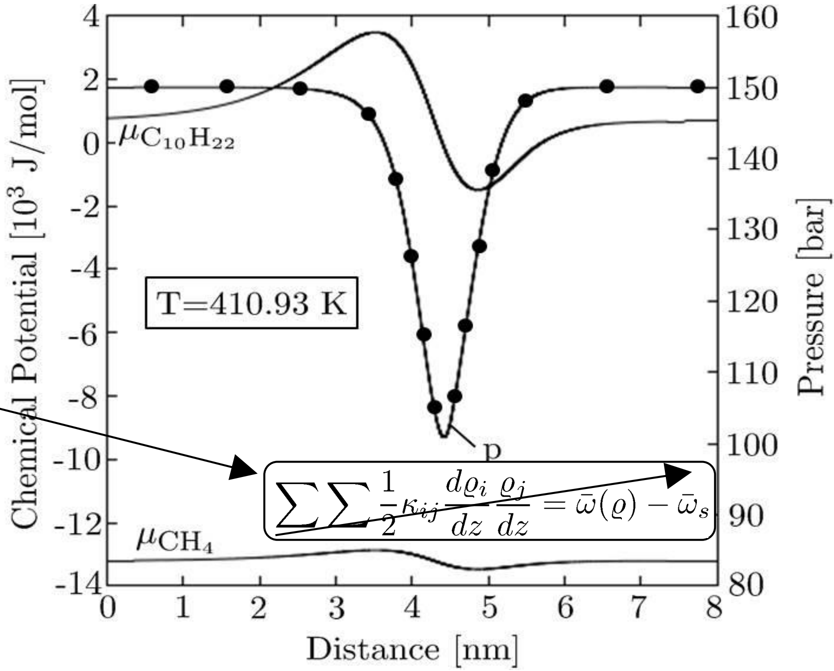
Fundamental changes in interfacial molecular dynamics

Basic Energy Sciences

- **Helmholtz energy only minimized in isothermal systems**

$$dF \leq -SdT - pdV$$

- **With interfacial temperature profile: Helmholtz energy no longer be minimized!**
  1. Fundamental eqn. becomes invalid
  2. Breakdown of classic two-phase relations
  3. Spray & drop dynamics no longer apply



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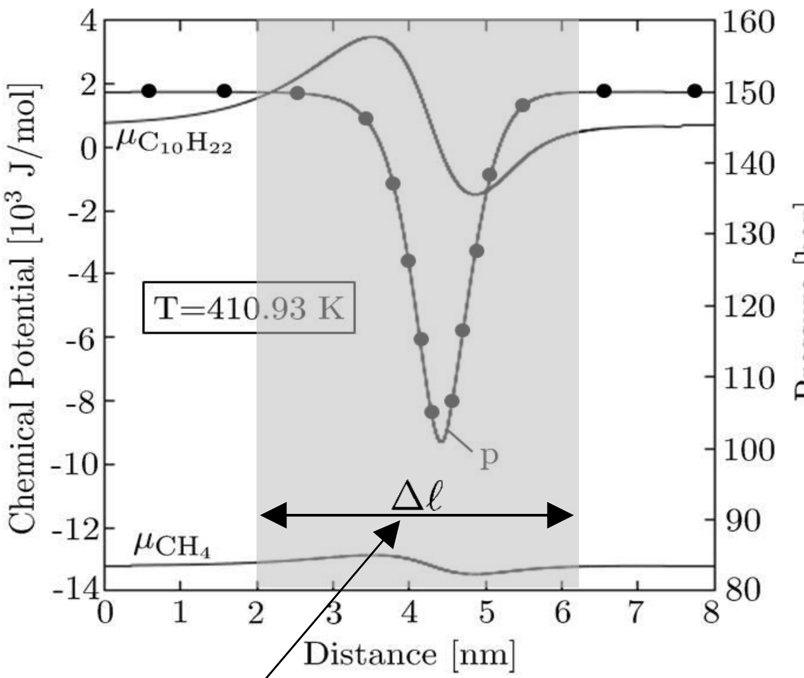
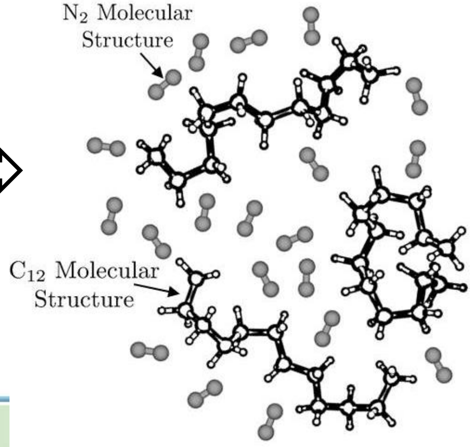


- **Temperature profile over length scale derivable from theory & ab-initio simulation**

$$\frac{\partial T}{\partial t} = \frac{k}{\varrho c_p}\nabla^2 T$$



$$\Delta\ell \geq 5 \cdot \frac{k}{\varrho c_p \bar{v}}$$

***If interface thicker than ΔL, interface disrupts*!**

→ "Trans-Critical" Condition

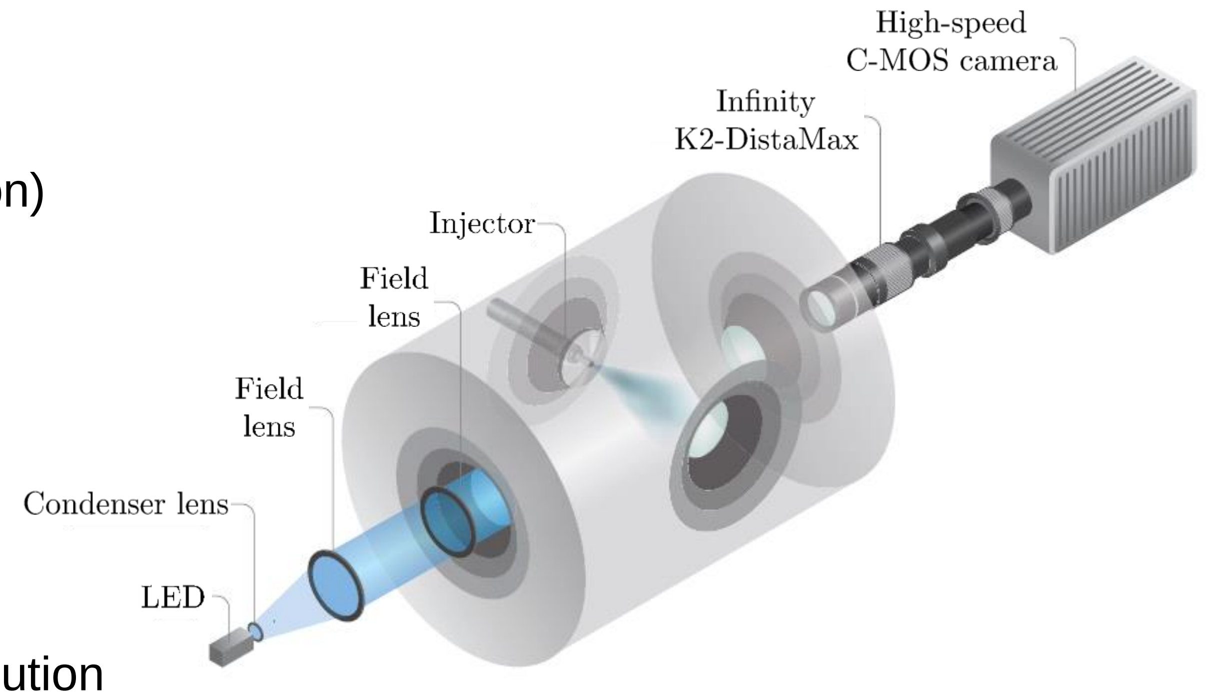
Imaging: Microscopic high-speed imaging for validation

C. Crua (**University of Brighton**) & L.M. Pickett (**Sandia CRF**)

Vehicle Technologies Office

- Long-distance microscopic imaging system

a) High-speed camera
b) Microscope (8x magnification)
c) Blue light emitting LED for background illumination

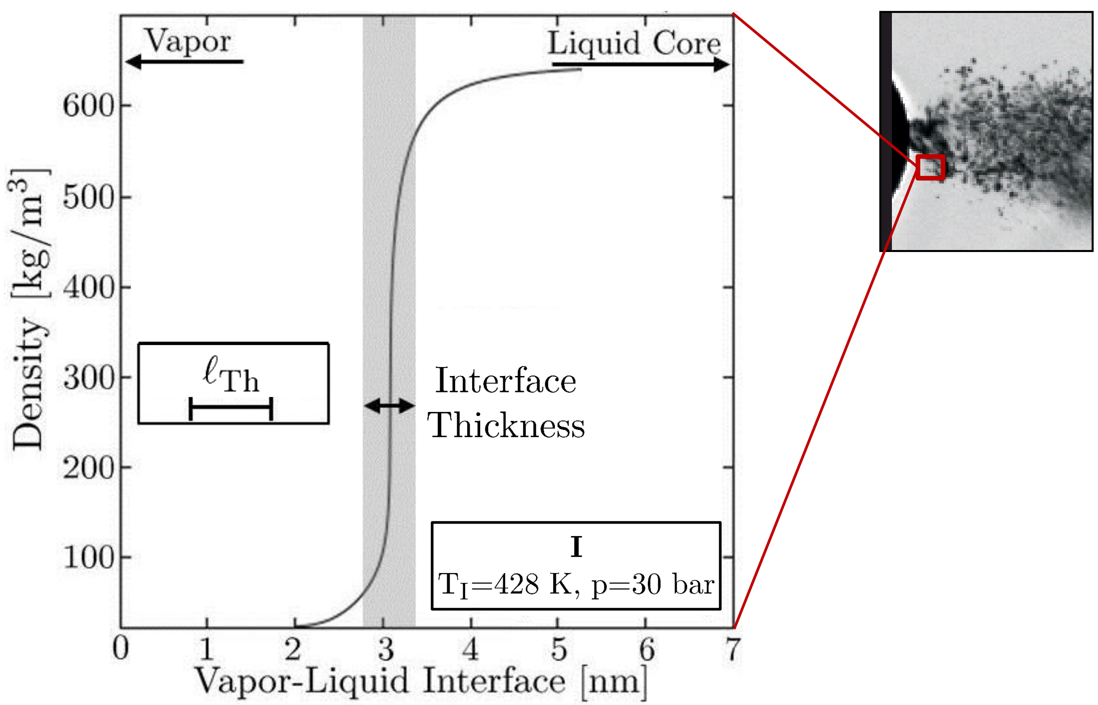


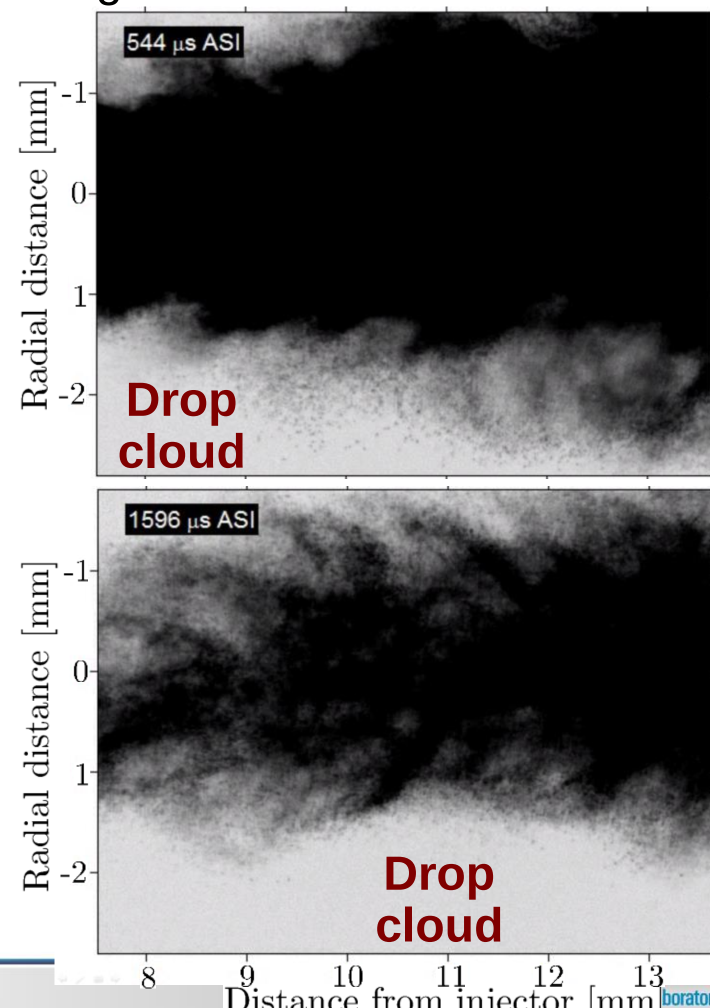
- 2.5 um/pixel resolution
- 15,000 frames/sec time resolution

Two-phase interface calculations & experimental validation

- ❑ Careful comparison of imaging & simulation
- ❑ Liquid n-dodecane C_{12} (T=363 K) into gaseous nitrogen at different conditions

"Low" Pressure (30 bar)





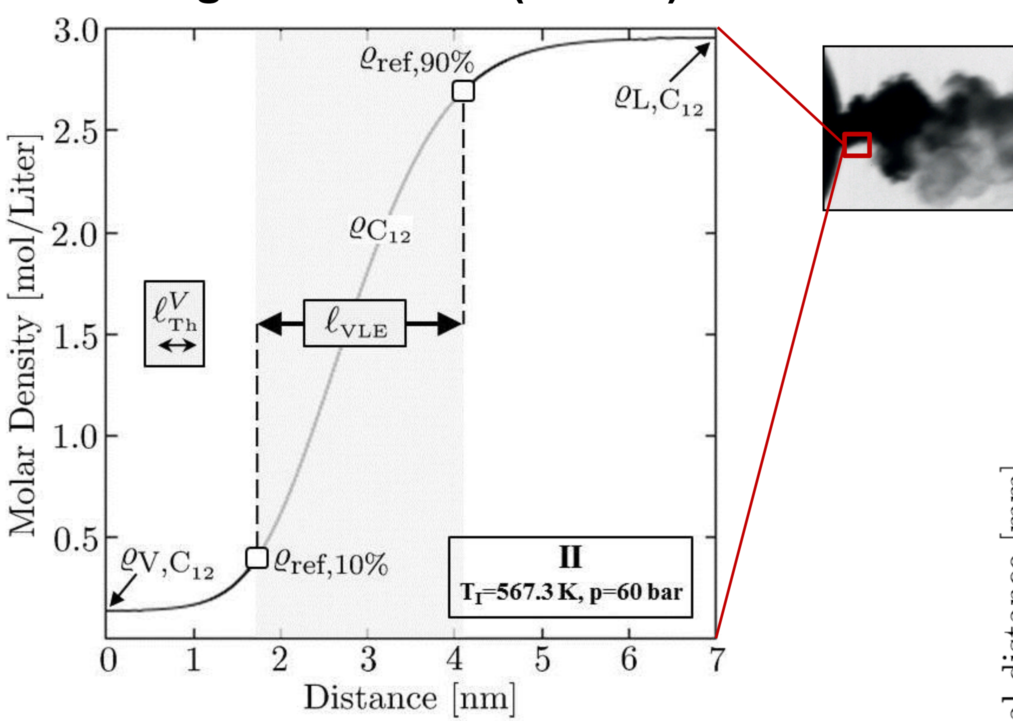
→Isothermal Interface

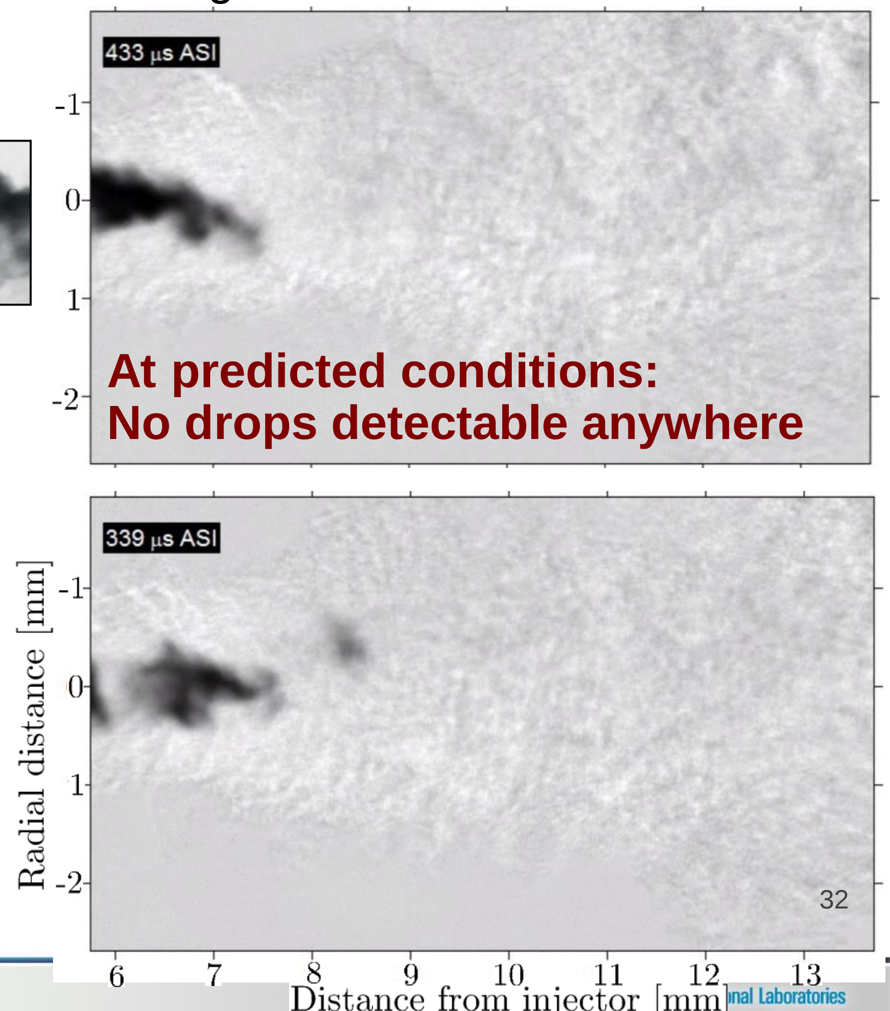
Classic two-phase theory valid

Two-phase interface calculations & experimental validation

- ❑ Careful comparison of imaging & simulation
- ❑ Liquid n-dodecane C_{12} (T=363 K) into gaseous nitrogen at different conditions

“High” Pressure (60 bar)





→Non-isothermal Interface

Two-phase theory invalid →Trans-critical jet

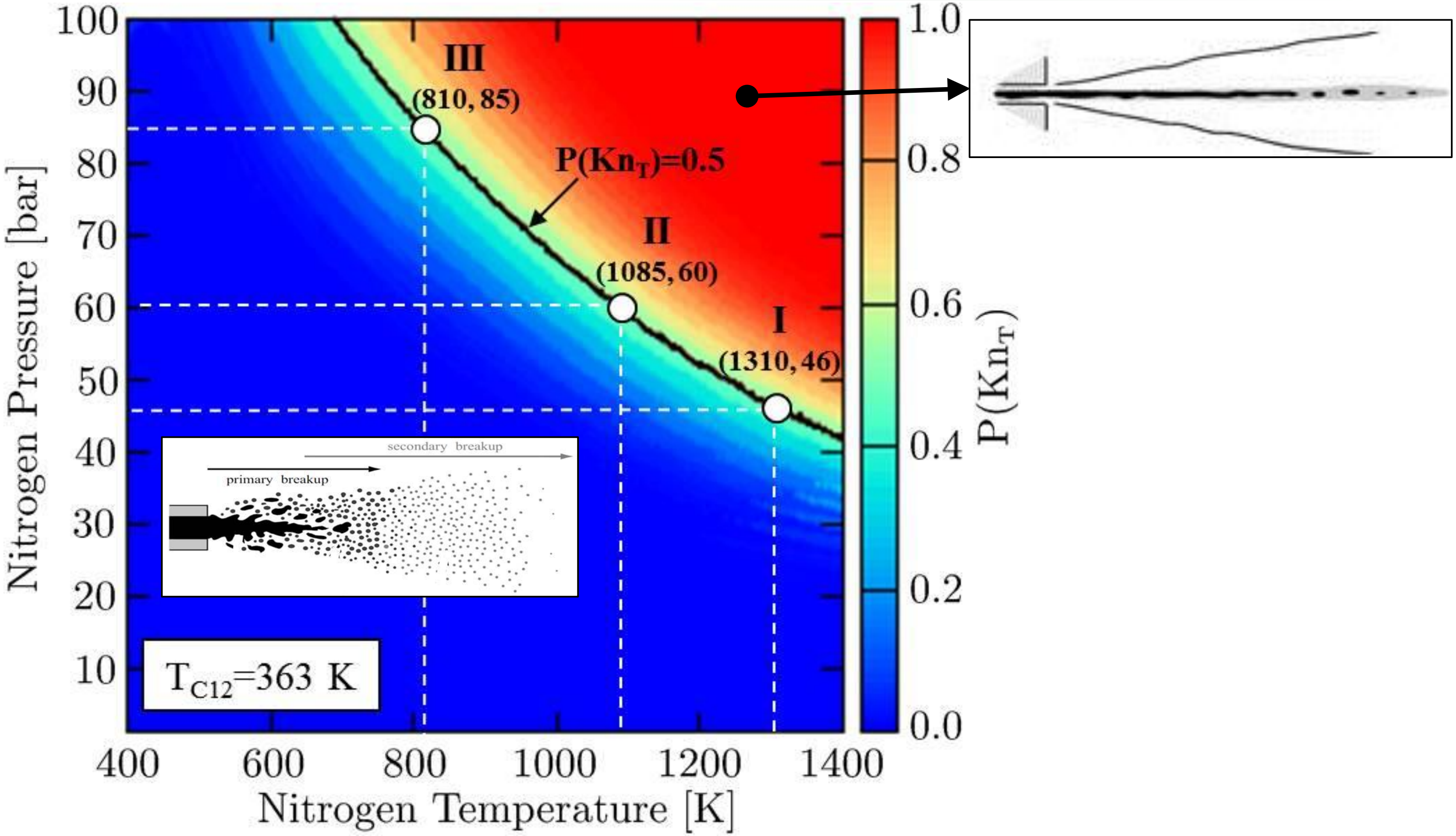
Results & outcome

(a) Predictive & affordable model for trans-critical fuel injections

(b) Paradigm change in gas turbines, liquid rockets & diesel engines

Regime diagram of liquid injection

Predictive & affordable model



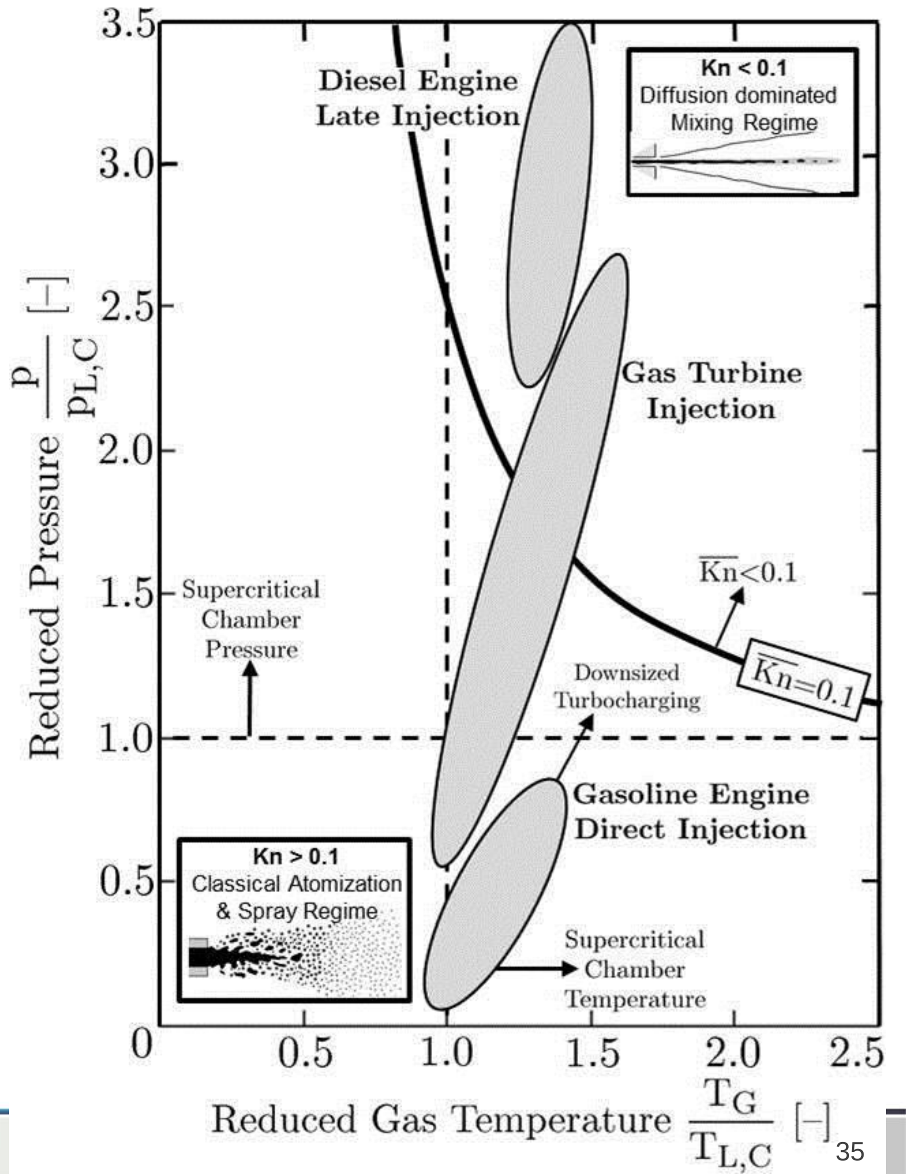
- ❑ **Meso-scale interface simulations predict transition conditions between classic sprays and trans-critical jets**

Consequences to IC engines & gas turbines

a) Gasoline injection develops as classic spray

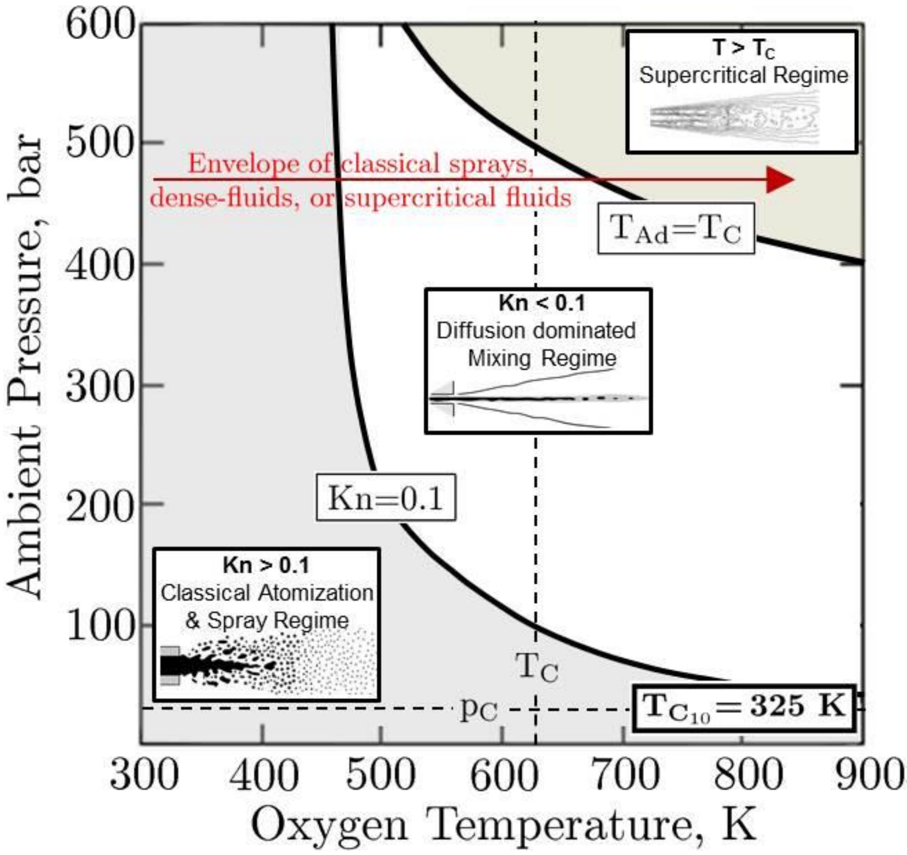
b) At relevant conditions & contrary to conventional wisdom

- Diesel engine & gas turbine injection <u>not</u> as classic spray but as "trans-critical" jet
- Classic industry modeling tools also become questionable



Consequences to liquid rockets

- Trans-critical jet for LOx-GH2 rockets
- **For new hydrocarbon systems & contrary to conventional wisdom**
- Liquid rocket injection as classic spray, <u>not</u> “trans-critical” jet
- Widely-applied modeling tools also become questionable



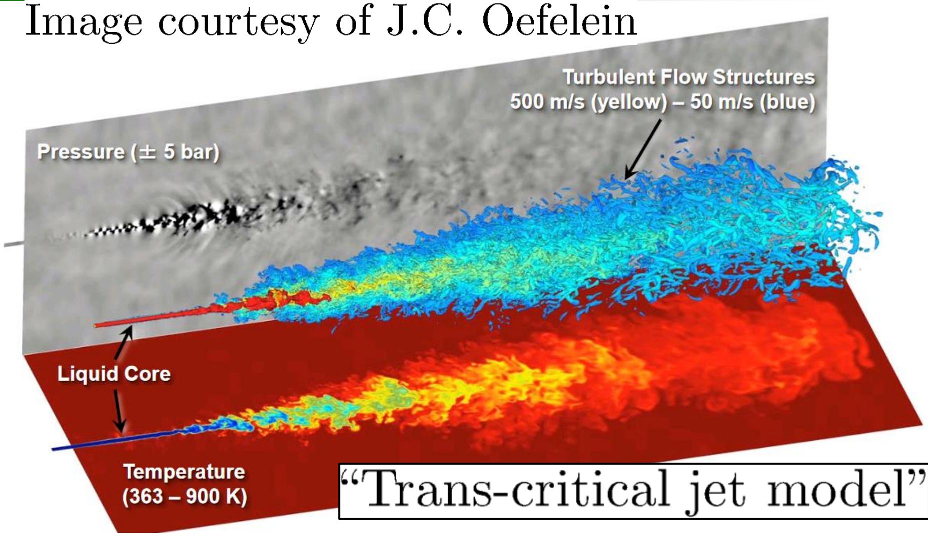
Perspectives & outlook

(a) Integration of advances into industry CFD

(b) Exert control over injections independent of "trans-critical" conditions

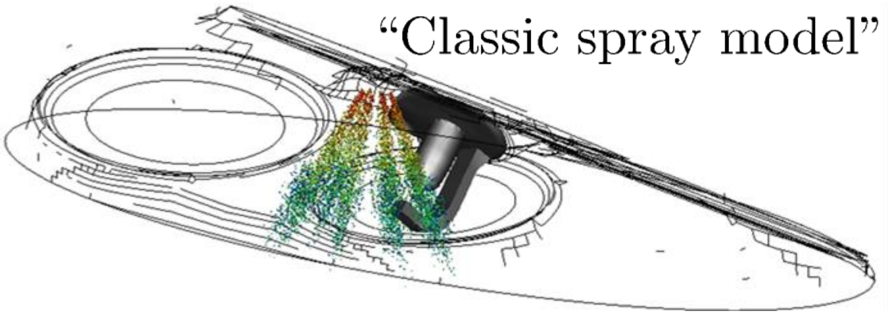
Development of industry simulation tools

Image courtesy of J.C. Oefelein



- ❑State-of-the-art simulation tools can treat both extremes of classic sprays & "trans-critical" jets
- ❑Such simulation methods differ greatly

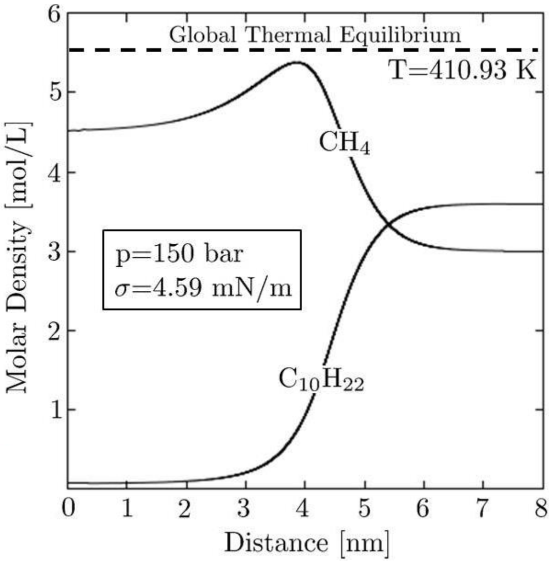
- ➢Future research:
  Develop simulation tools to seamlessly treat both extremes in unified framework



Utilizing our fundamental understanding:
Control injection regardless of “trans-critical conditions”

Fundamental molecular understanding of two-phase interfaces:

- Interfacial molecular dynamics “swarm” to minimize Helmholtz free energy
- Resulting density & species profile distributions manifest in spray atomization & evaporation



<u>Idea:</u> We aim to control which thermodynamic potential, besides Helmholtz energy, is minimized!

<u>Proof of concept at high pressures:</u>

High-pressure trans-critical jet

- Previously: High-pressure conditions lead to “trans-critical” jet dynamics

- Control with isothermal boundary layer: Dynamics “switch” to spray atomization

Utilizing our fundamental understanding:
Control injection regardless of "trans-critical conditions"

Fundamental molecular understanding of two-phase interfaces:

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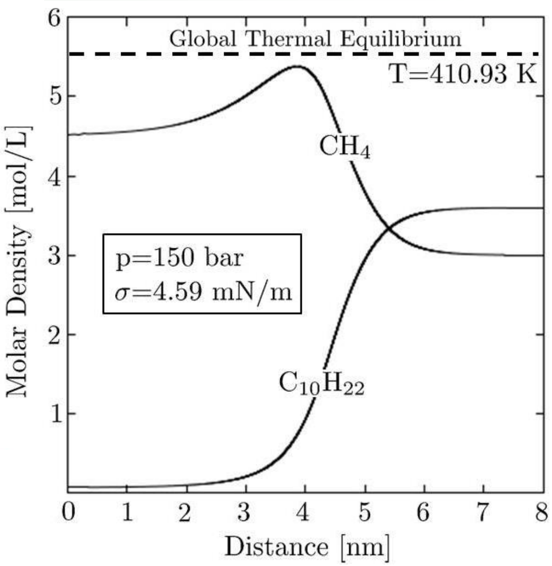

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<u>Proof of concept at high pressures:</u>

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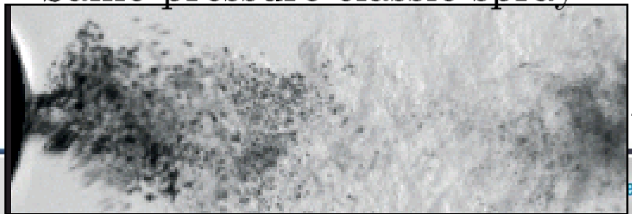
High-pressure trans-critical jet

Same pressure classic spray



Summary & Conclusions

I. Mixture preparation key element in future clean & efficient combustion technology

II. Advanced power & propulsion systems move toward "trans-critical" conditions where liquid injection is poorly understood

III. Gas-liquid interface dynamics revealed by meso-scale simulation & high-speed macroscopic imaging

IV. Capability developed to predict liquid injection dynamics

V. Under some relevant conditions, predictions led to paradigm change for IC engines, gas turbines & liquid rockets

VI. Future work seeks to develop advanced simulation models and, ultimately, aims to control injection dynamics

Recent Journal Publications

- Rainer N. Dahms, "Understanding the breakdown of classic two-phase theory and spray atomization at engine-relevant conditions," Phys. Fluids, **28**:042108, 2016
- Rainer N. Dahms, "Gradient Theory simulations of pure fluid interfaces using a generalized expression for influence parameters and a Helmholtz energy equation of state for fundamentally consistent two-phase calculations," *J. Colloid Interface Sci*., **445**:48-59, 2015.
- Rainer N. Dahms and Joseph C. Oefelein, "Liquid jet breakup regimes at supercritical pressures," *Combust. Flame*, **162**:3648-3657, 2015.
- Rainer N. Dahms and Joseph C. Oefelein, "Atomization and dense-fluid breakup regimes in liquid rocket engines," *Journal of Propulsion and Power*, **31**:1221-1231, 2015.
- Rainer N. Dahms and Joseph C. Oefelein, "Non-equilibrium gas-liquid interface dynamics in high-pressure liquid injection systems," *Proc. Combust. Inst*., **35**:1587-1594, 2015.
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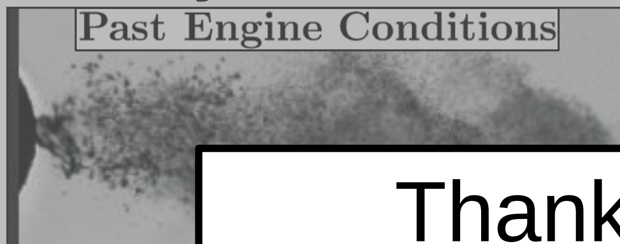
Fuel injection under trans-critical conditions



Thank you for your attention!

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