High-Pressure Transcritical Atomization and Combustion

CTR Summer Program
Tutorial Seminar

07/08/2016

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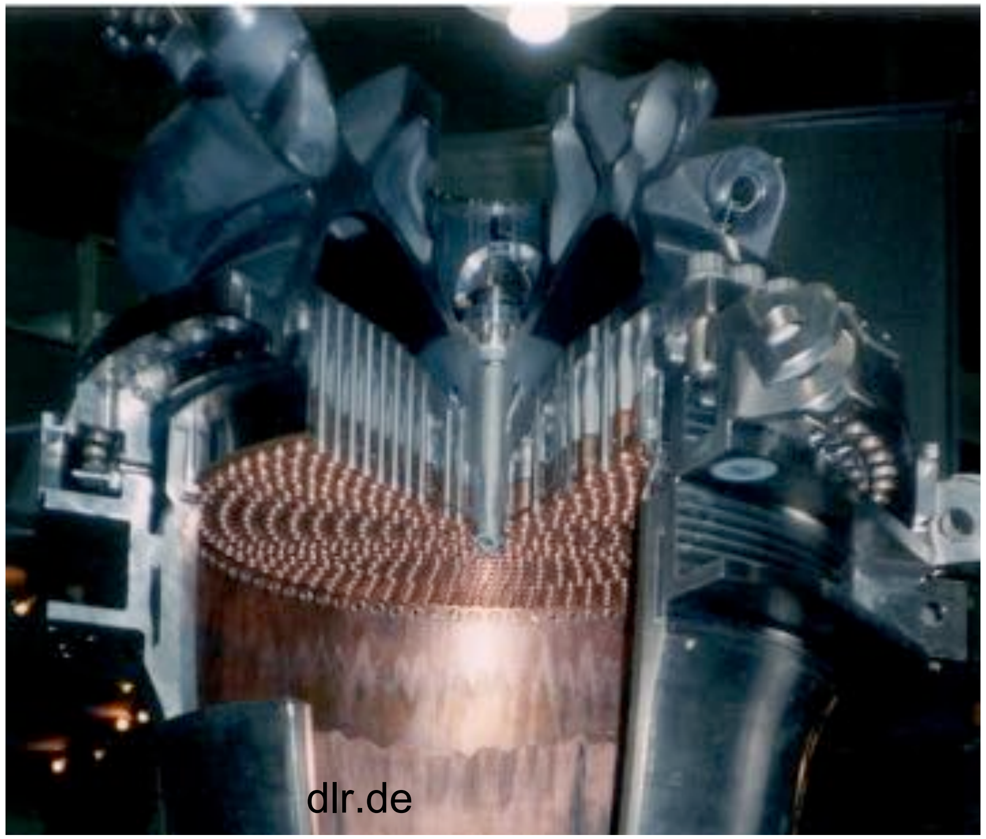
Rocket engines


dlr.de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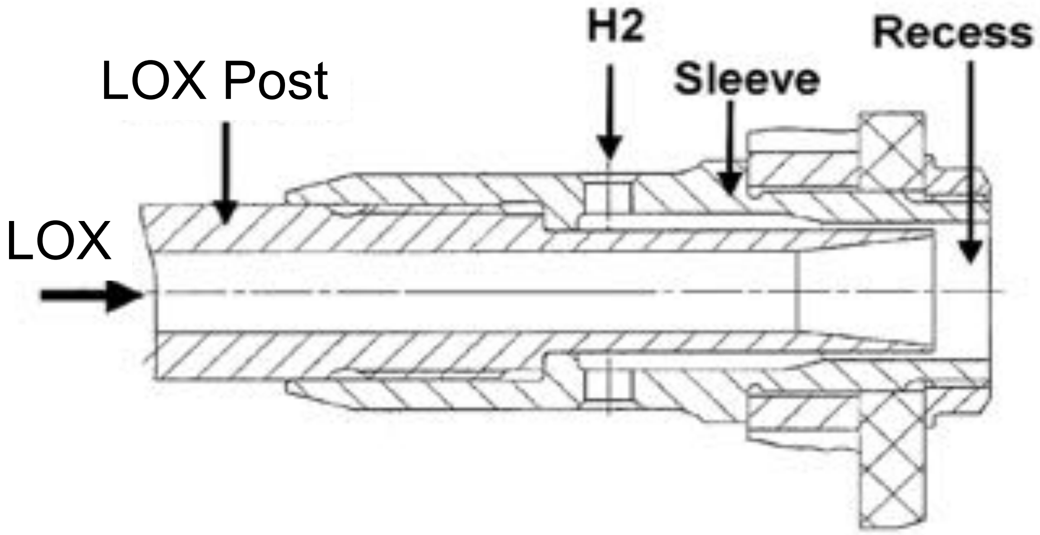

Rocket engines

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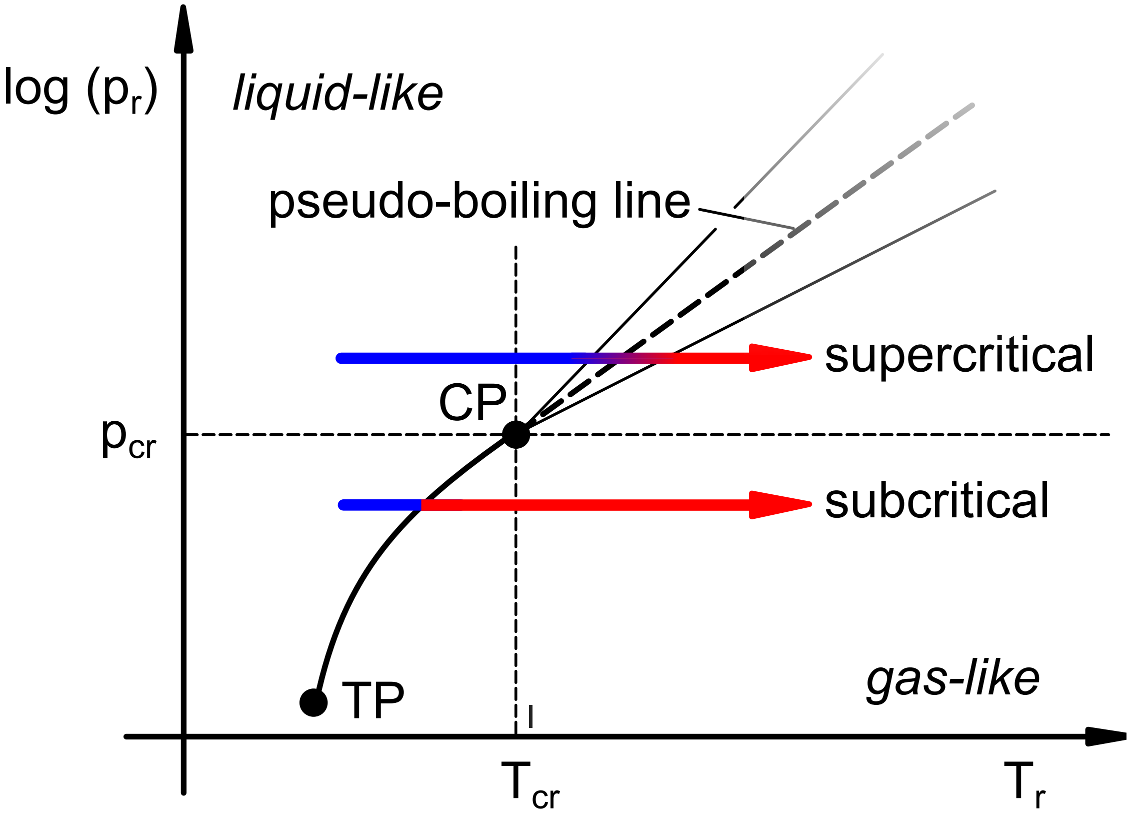
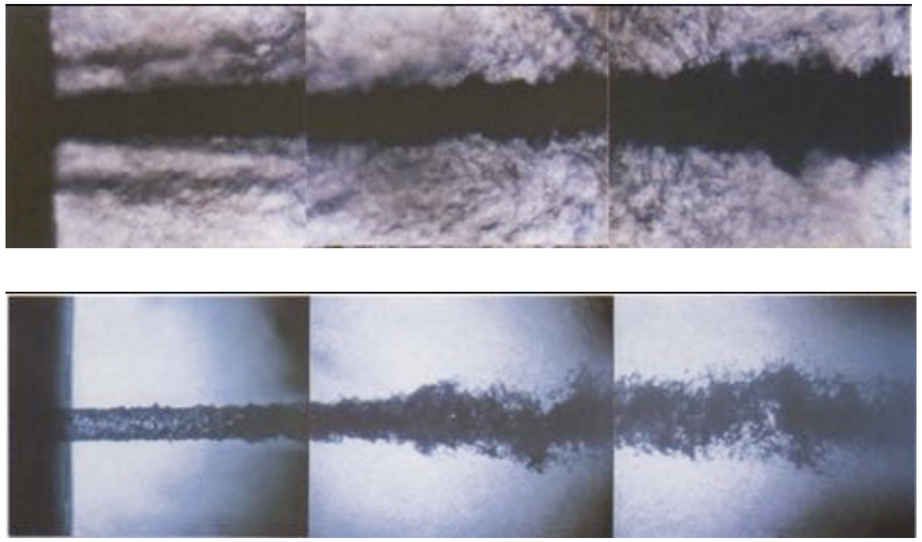
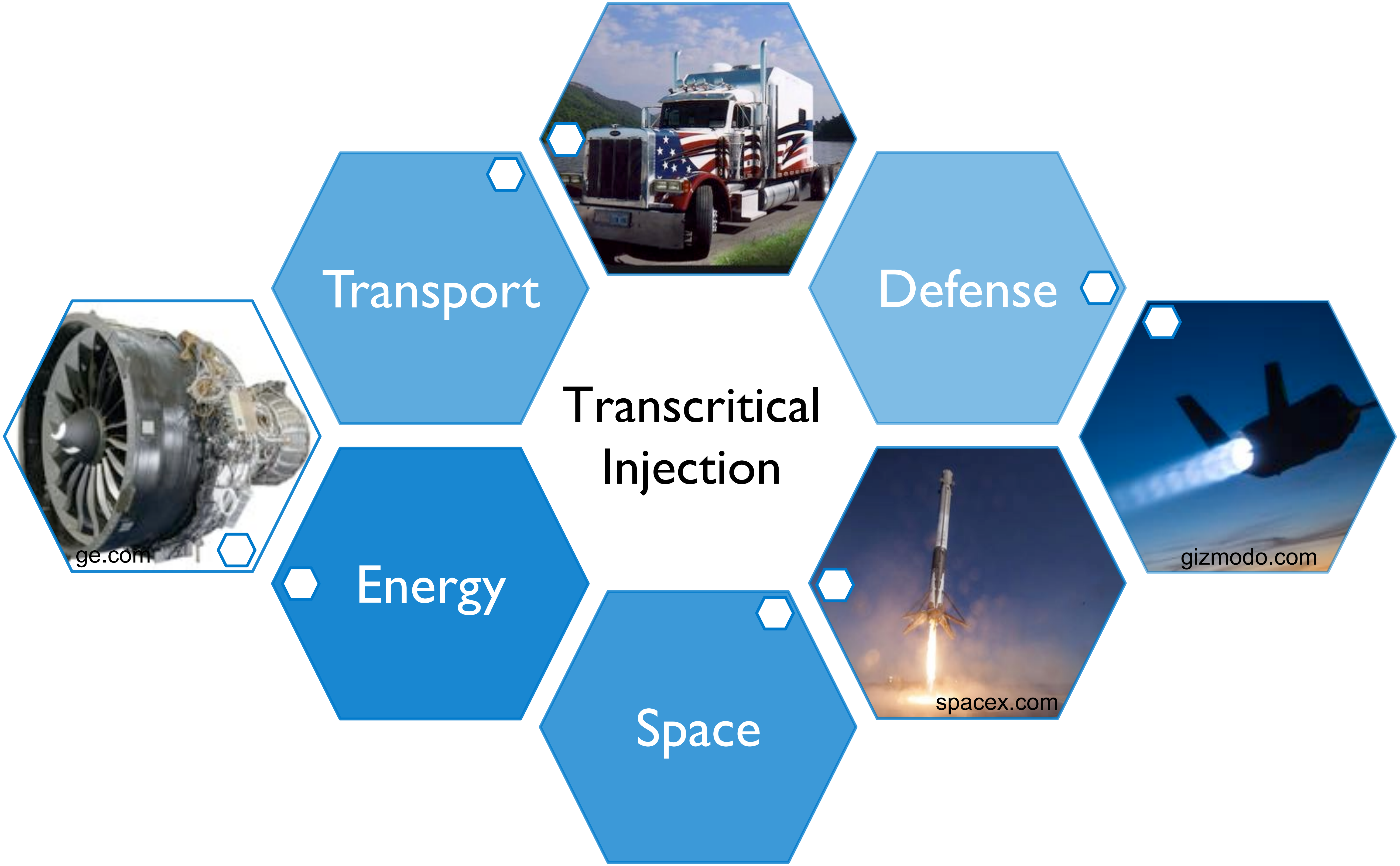




Mayer and Tamura *J. Propulsion Power* 1996

Transcritical injection is ubiquitous!



Transcritical Injection

Transport

Defense

Energy

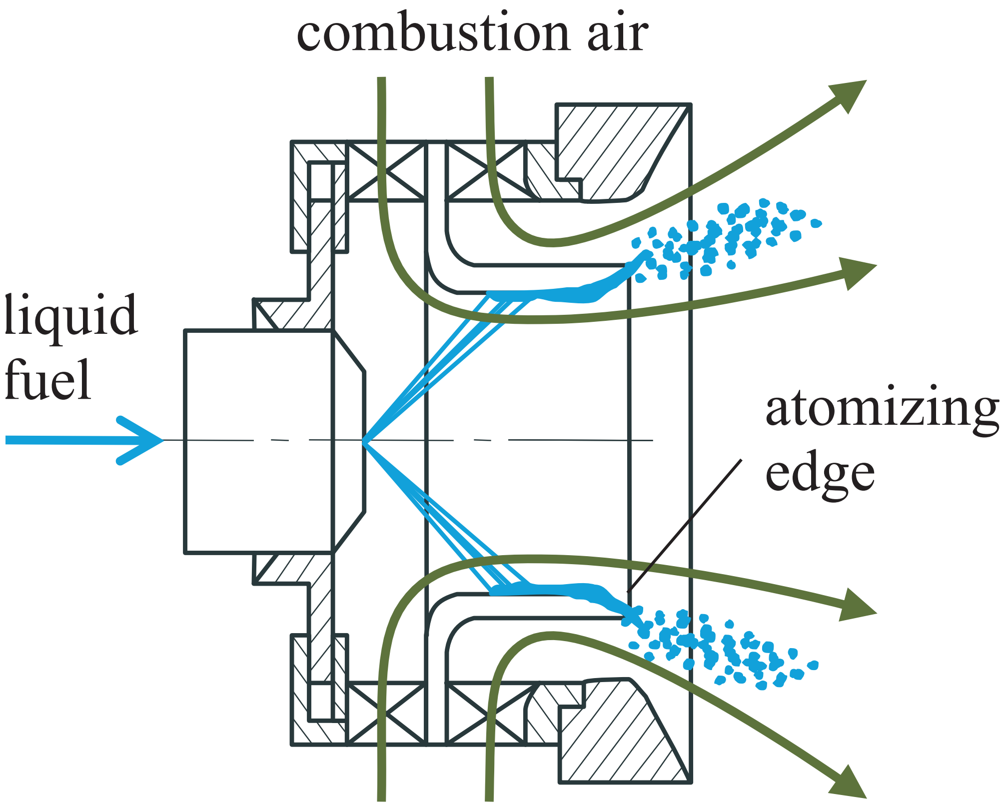
Space

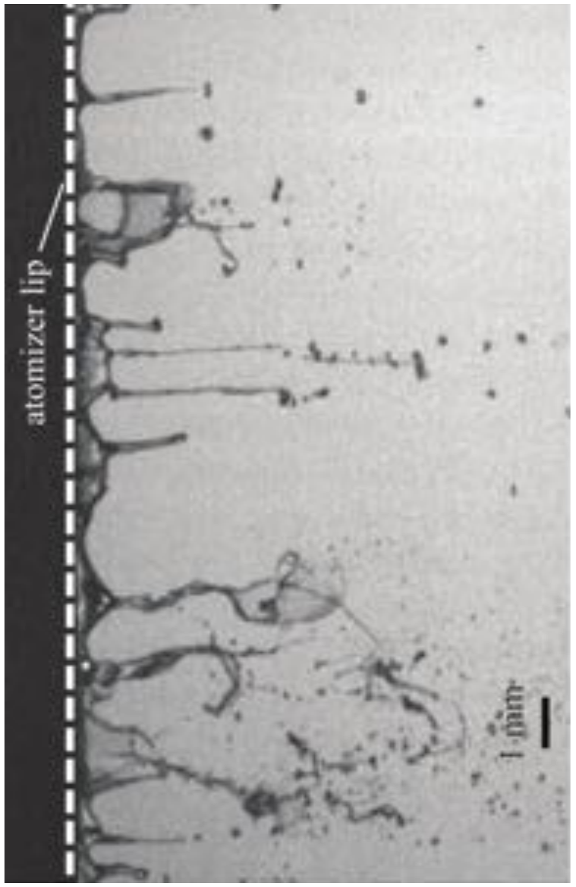
ge.com

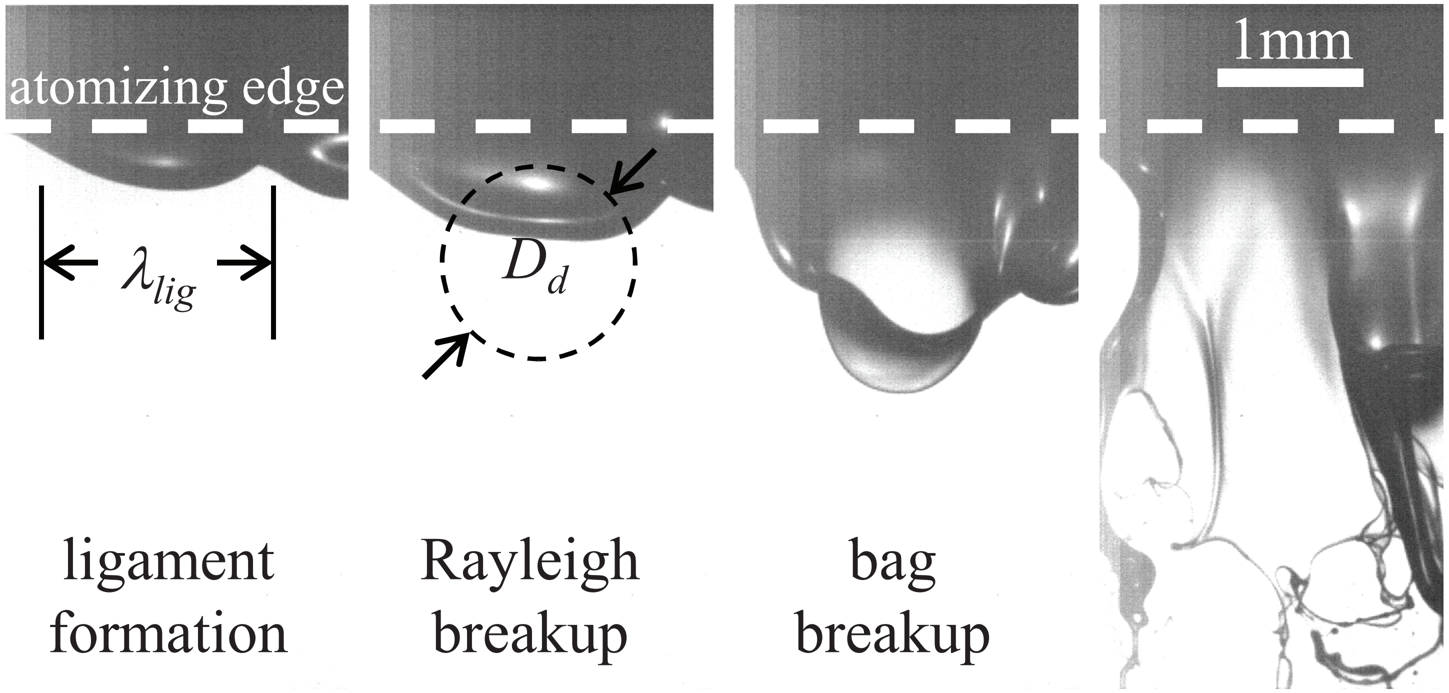
gizmodo.com

spacex.com

Gas turbines – prefilm atomizers







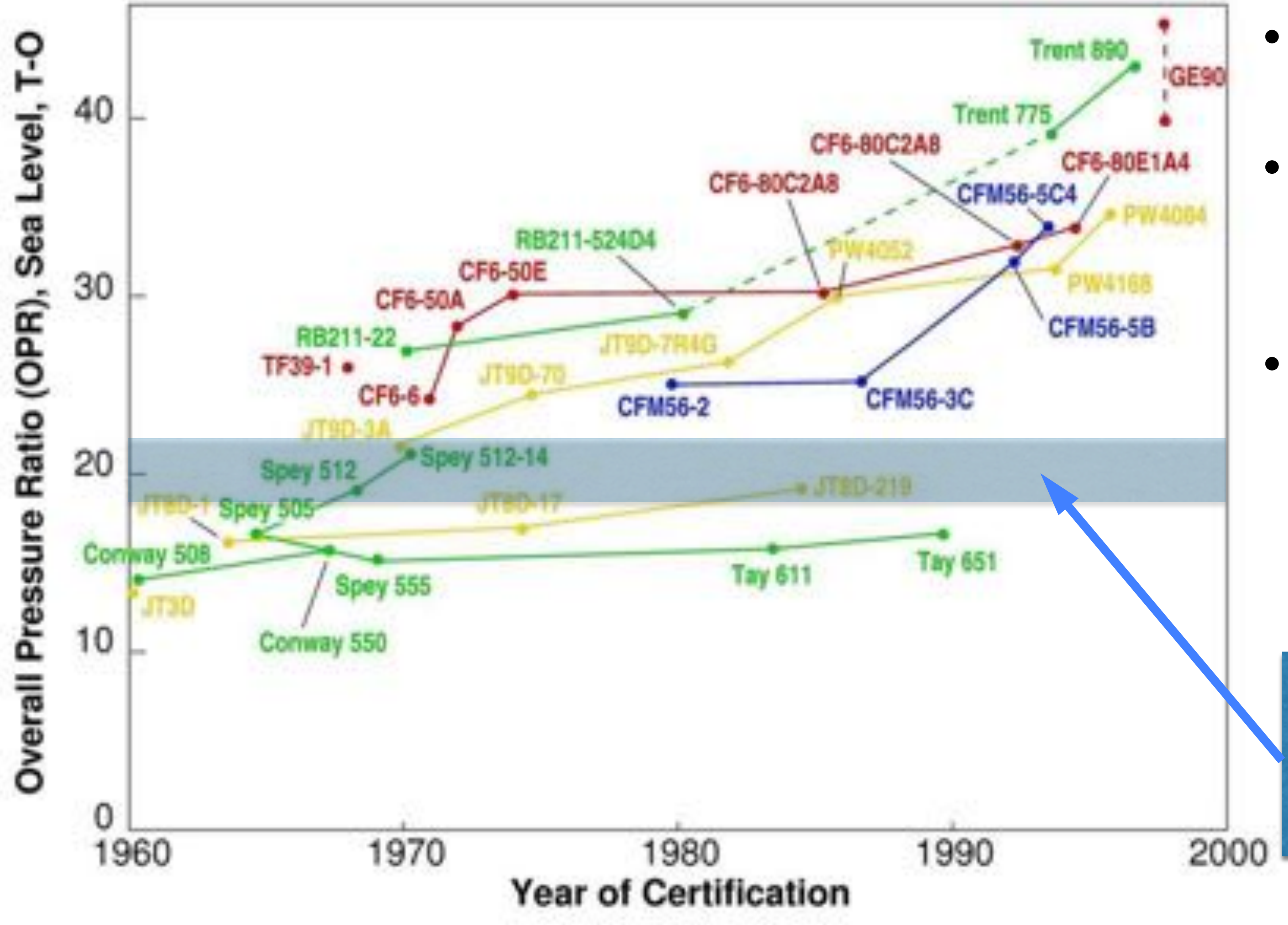
ligament formation

Rayleigh breakup

bag breakup

Gepperth et al. (2012)

Gas turbines – increase in pressure ratio

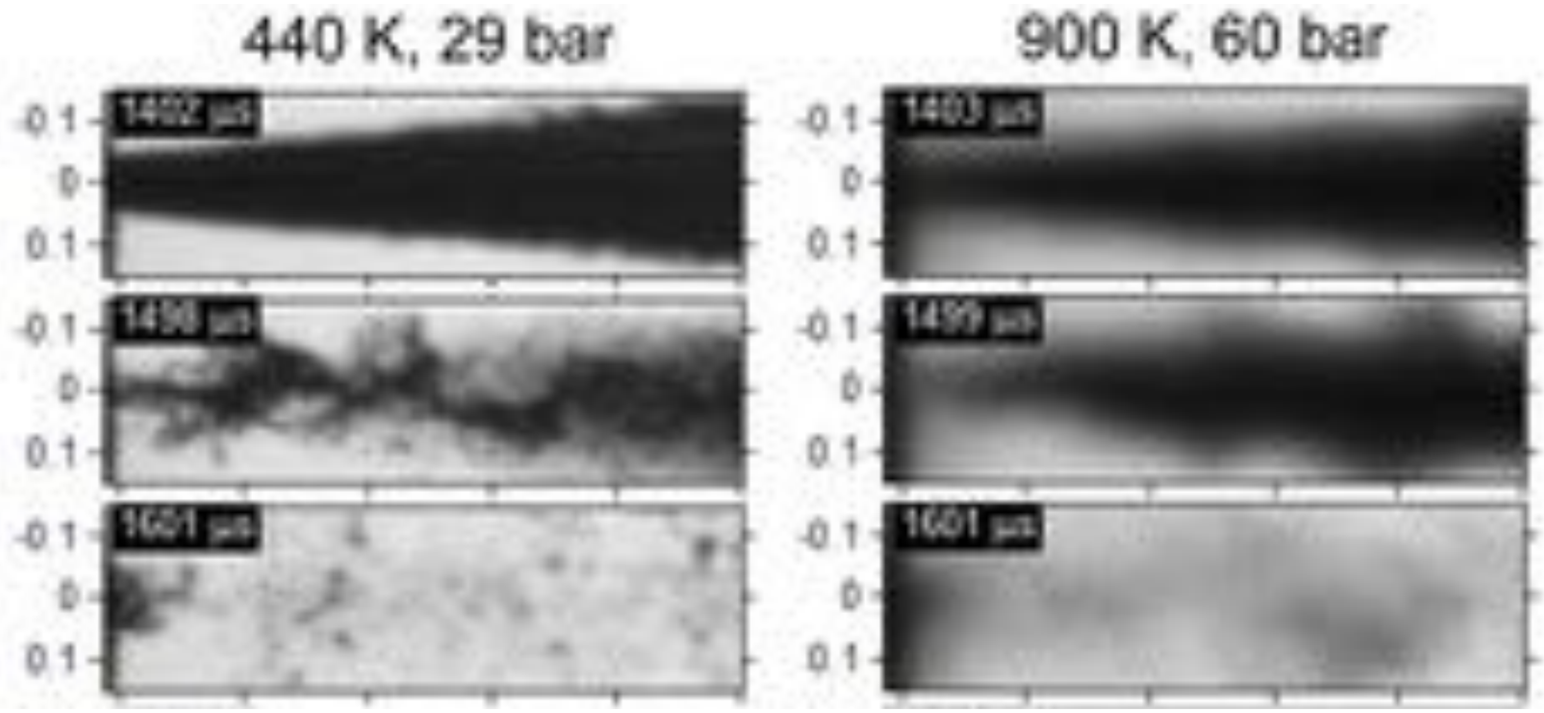


- OPR is rising!
- Switching super- / subcritical during climb
- Critical phase in take-off not designed with focus on transcritical injection

P_{cr} of kerosene ~20 bar

Jane's Aeroengines (1998)

Diesel injection – n–Dodecane – N_2



At supercritical conditions, (p_{cr} = 1.8 MPa, T_{cr} = 658 K) surface tension **and** mixing dominated injection is observed

Oefelein et al. (2012), Dahms et al. (2013), Manin et al. (2014)

Outline

I. Thermodynamics

II. Transcritical injection

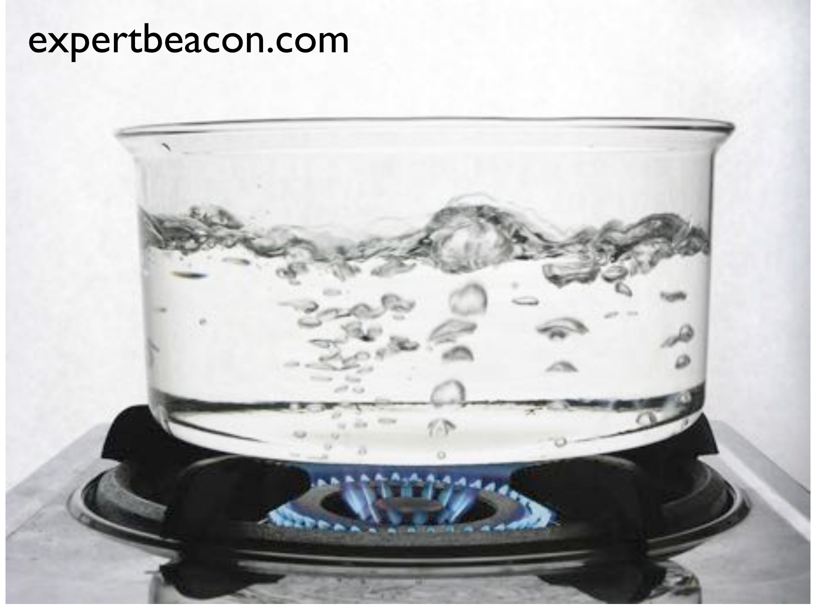
III. Combustion

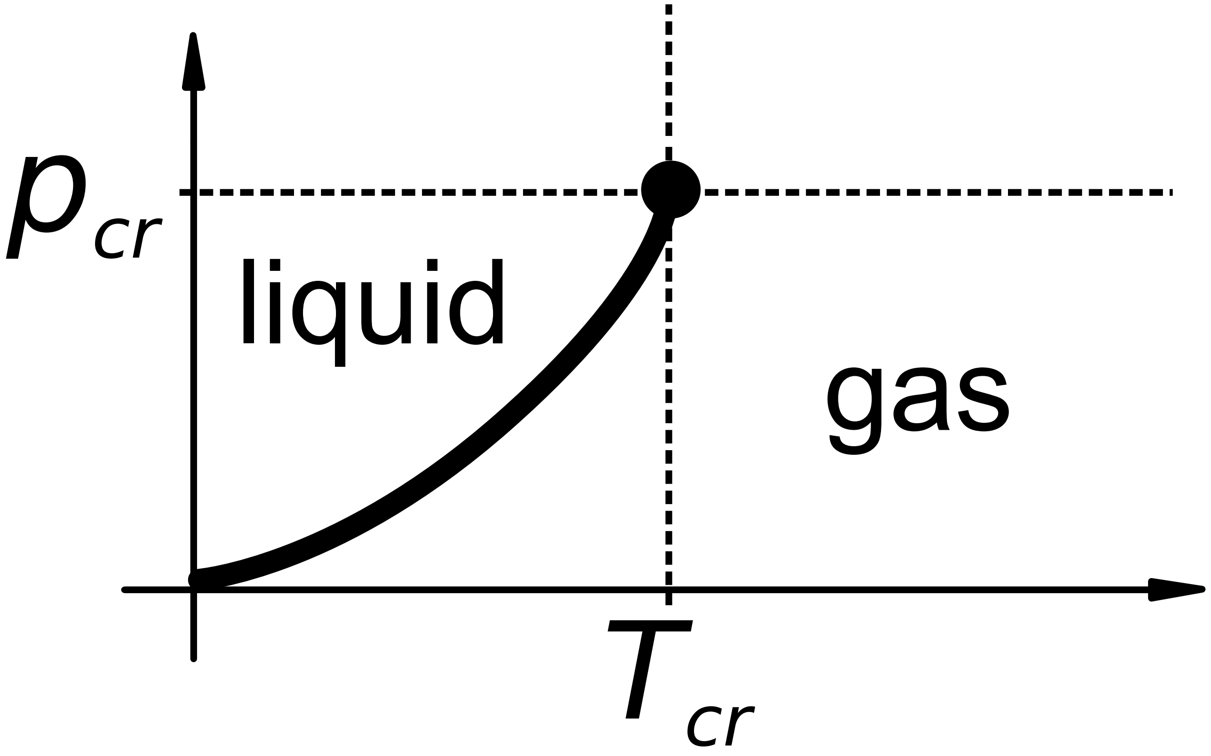
IV. Transcritical atomization

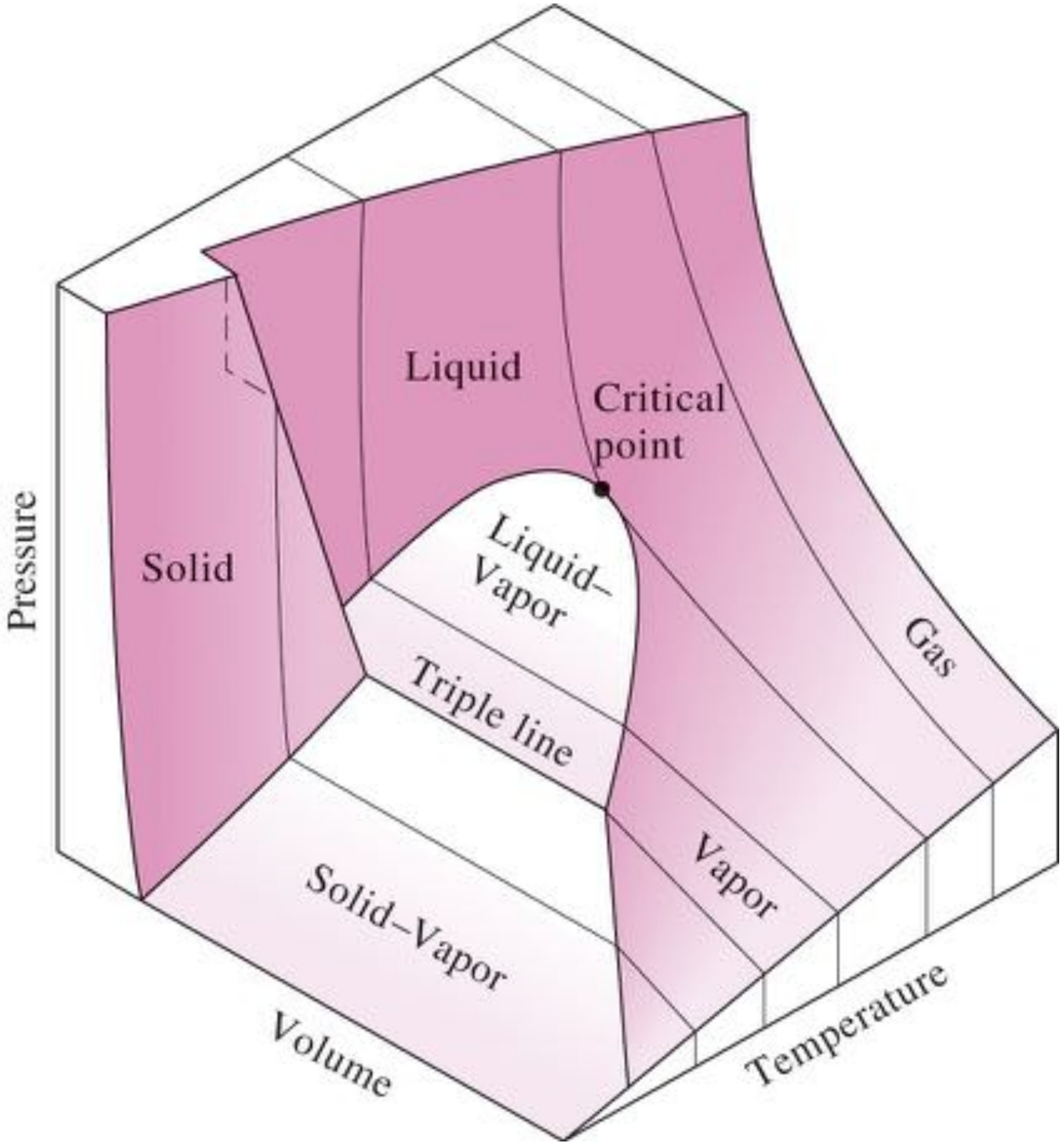
V. Open Challenges / Summary

1. What is a supercritical fluid?

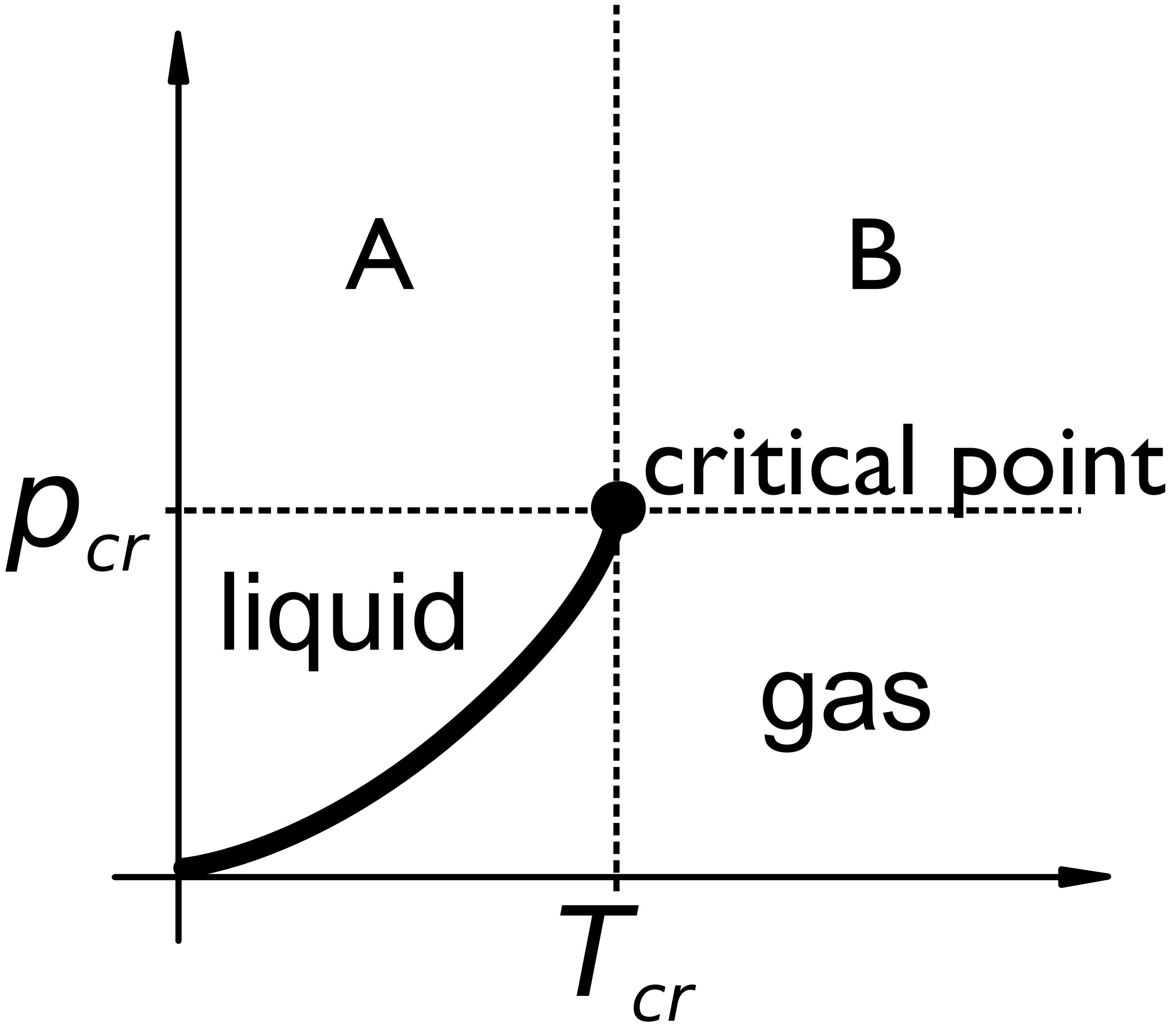
Fluid behavior can be described as a surface in pvT


expertbeacon.com





Nomenclature

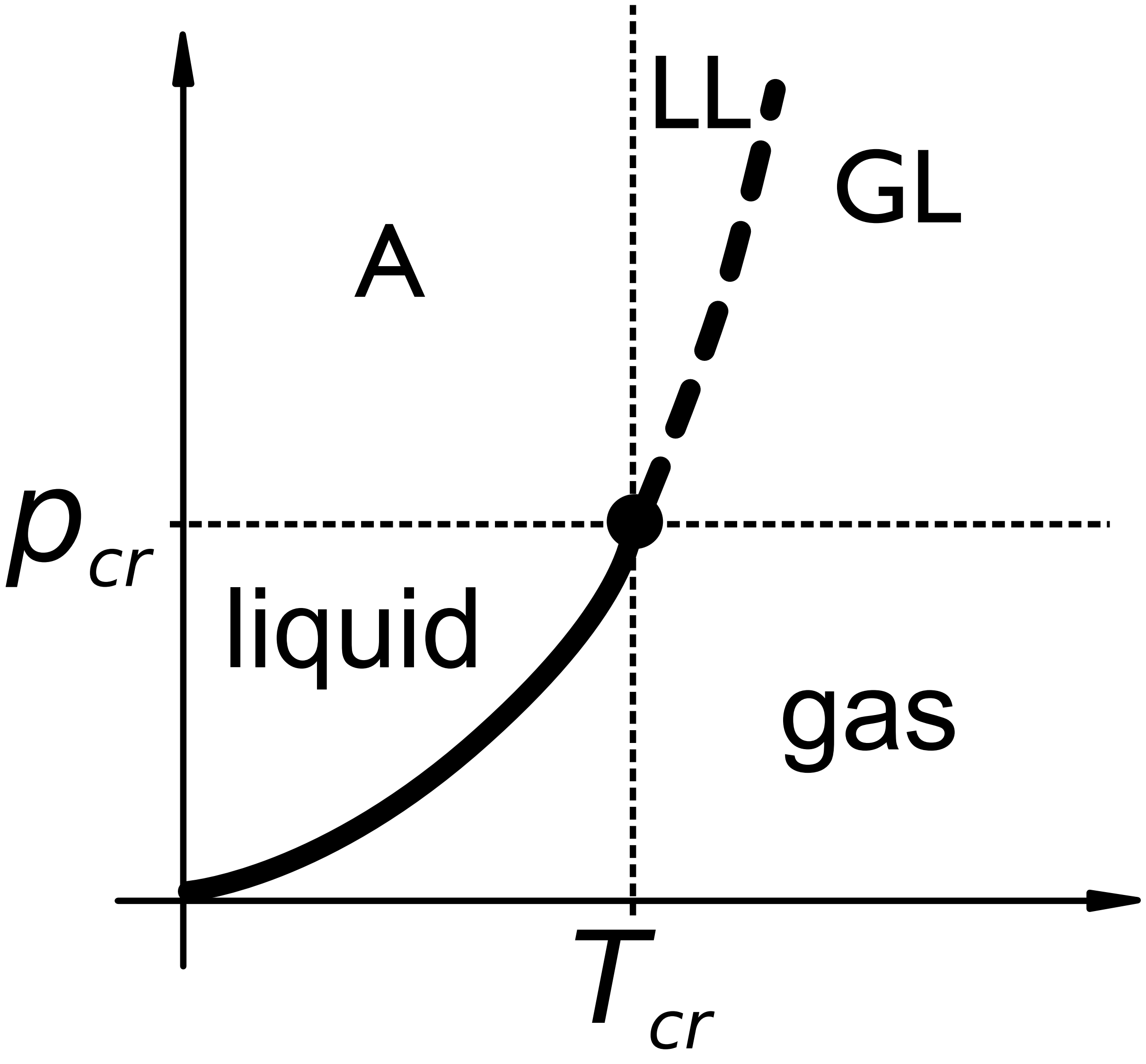


No consensus on naming

- Supercritical
    - B: Oschwald, Candel, etc.
    - A, B, gas: Bellan
    - Gas, B: Tucker, Younglove

- A
    - Transcritical
    - Compressed liquid
    - Compressible liquid
    - Supercritical

Different supercritical fluids

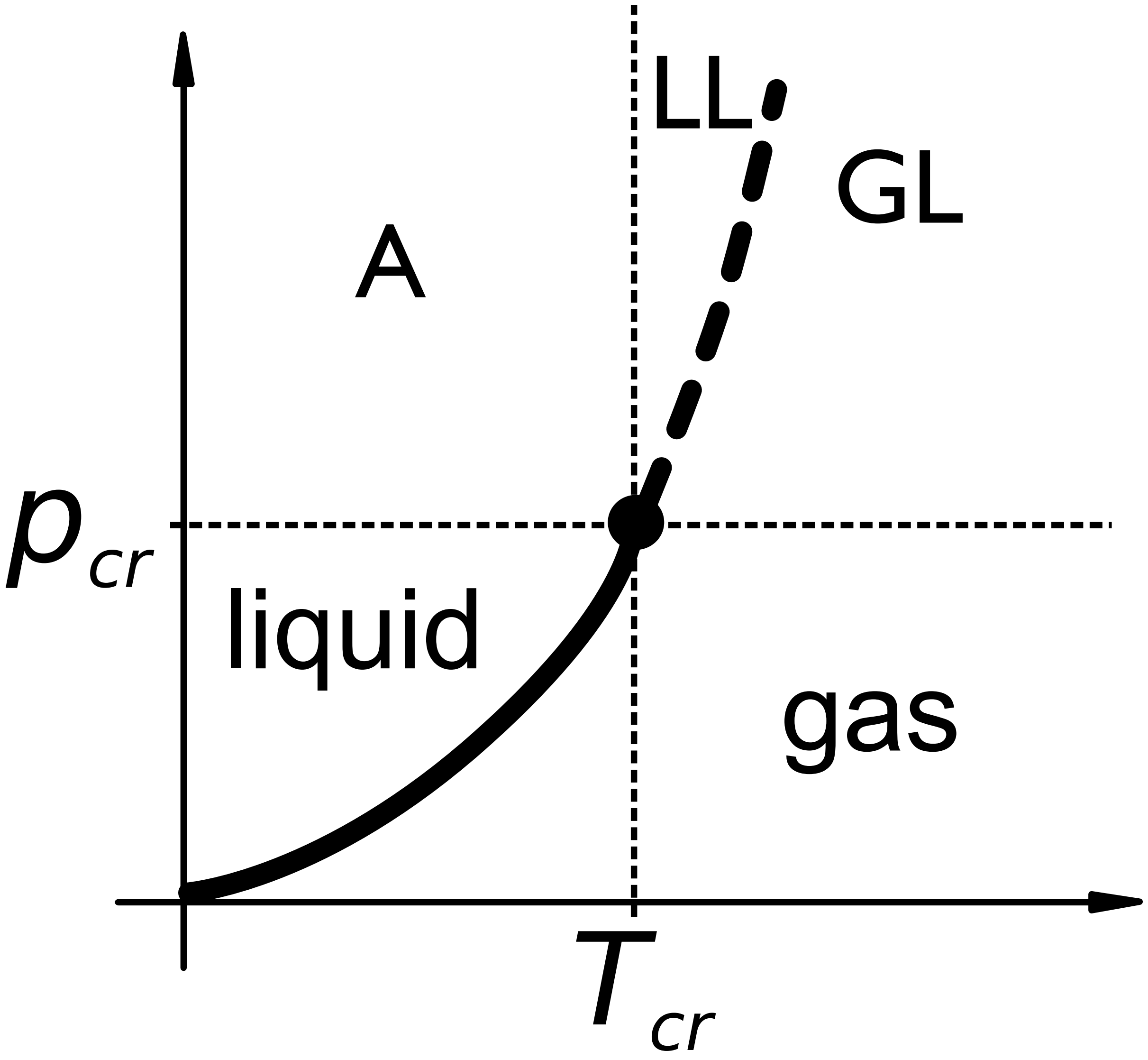


"Recently":

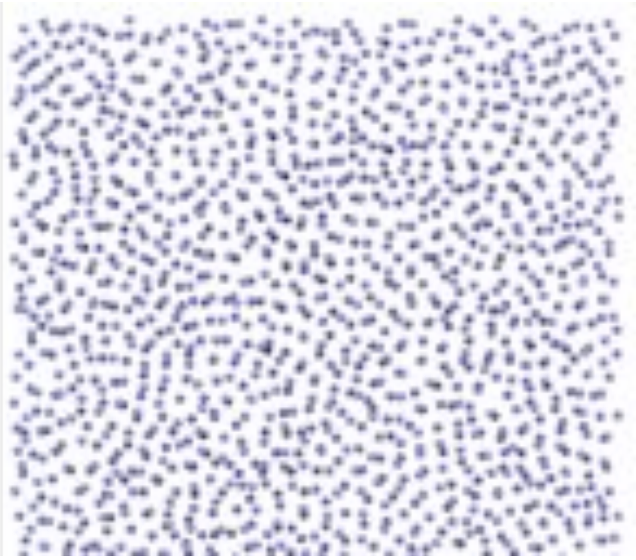
- **Liquid-like (LL)** and **gas-like (GL)** supercritical fluids (Nishikawa & Tanaka 1995, Gorelli et al. 2006)
- Divided by "ridge", characterized by peaks in isothermal compressibility and heat capacity ('pseudoboiling line' Oschwald et al. 2006)
- Doesn't make naming easier!

Molecular structure of state diagram

Molecular dynamics computations reveal the similarities and differences between the states



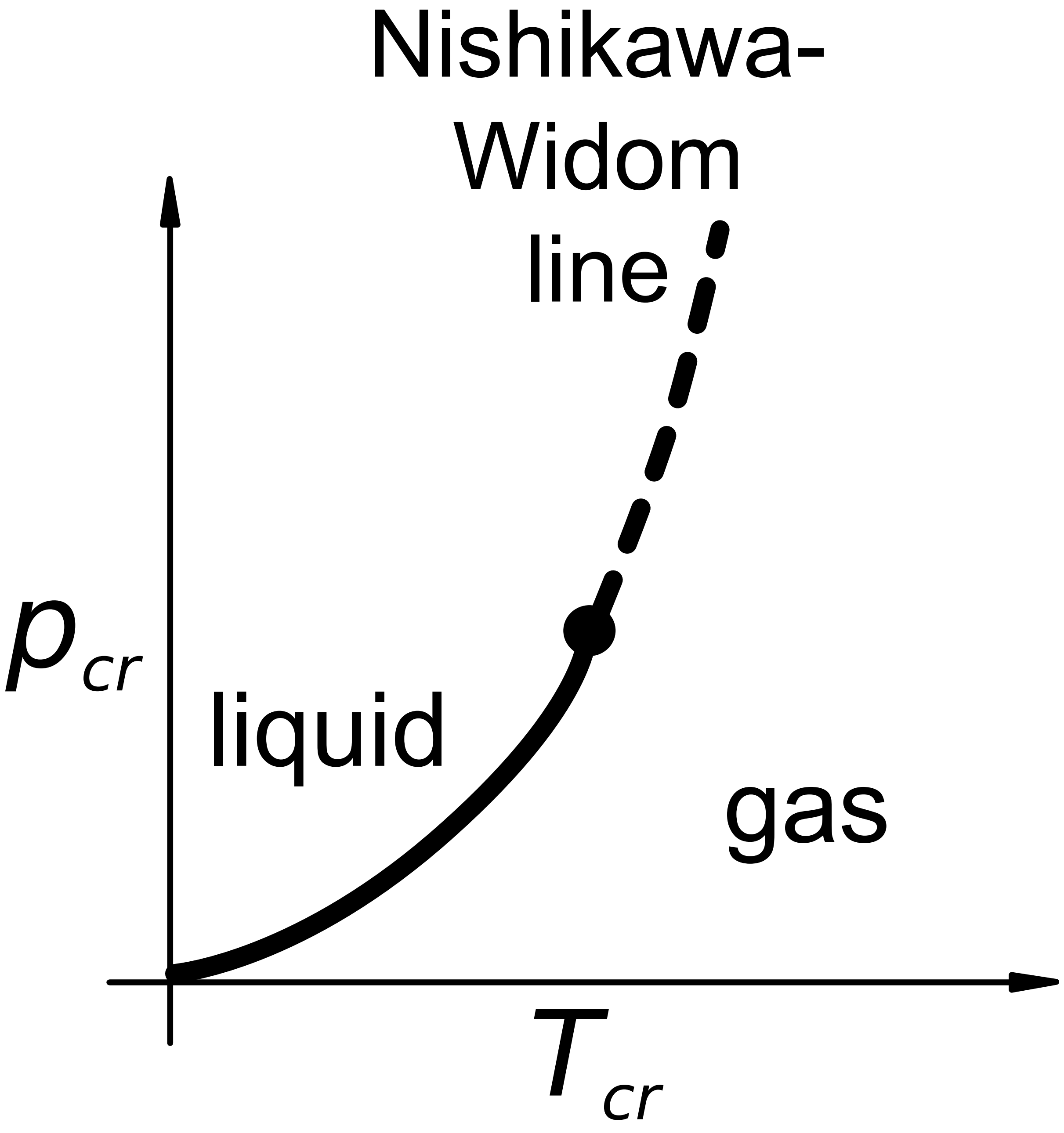
liquid, A, LL:



gas, GL:

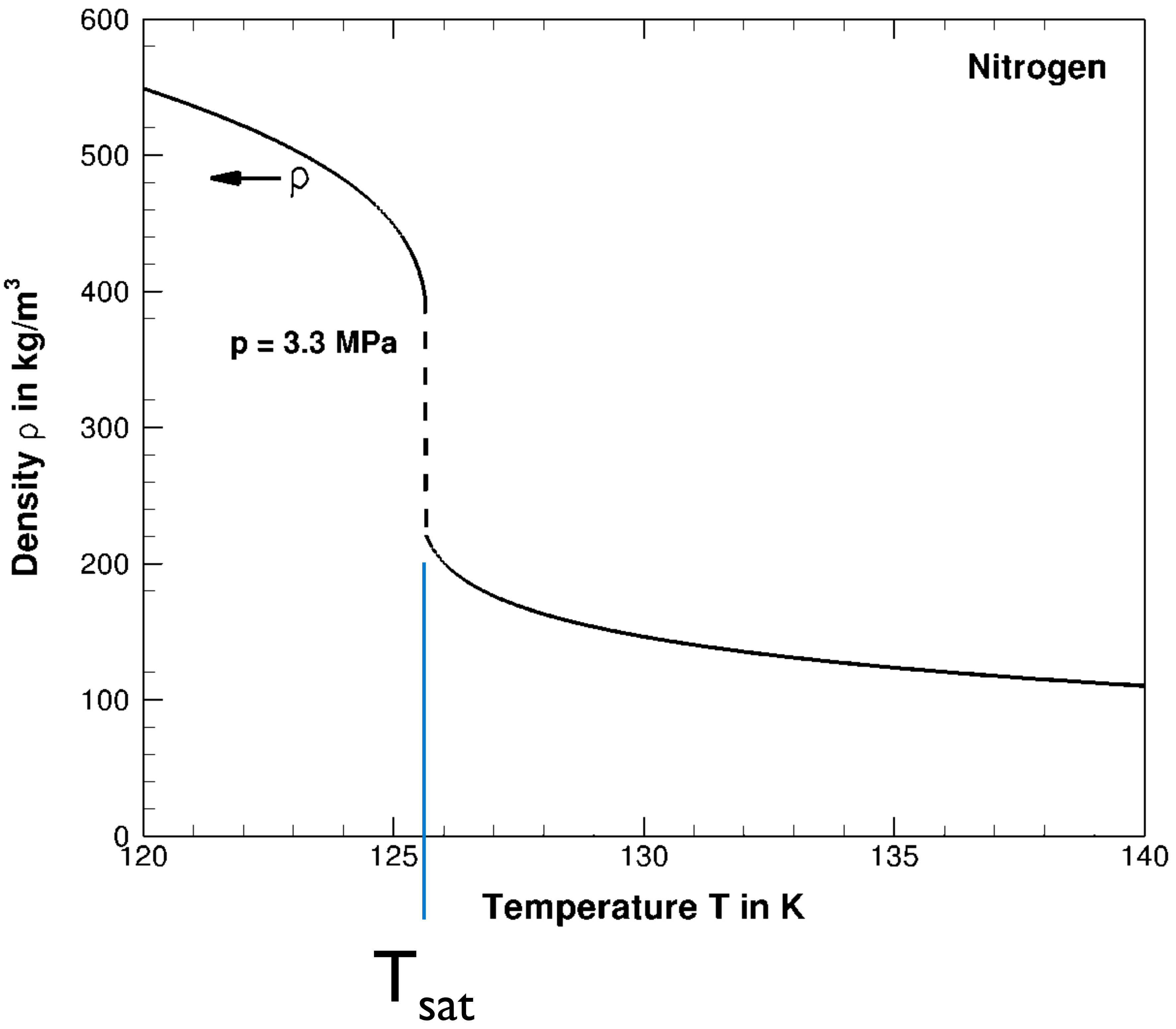
Molecular dynamics courtesy of Muralikrishna Raju

Molecular structure of state diagram



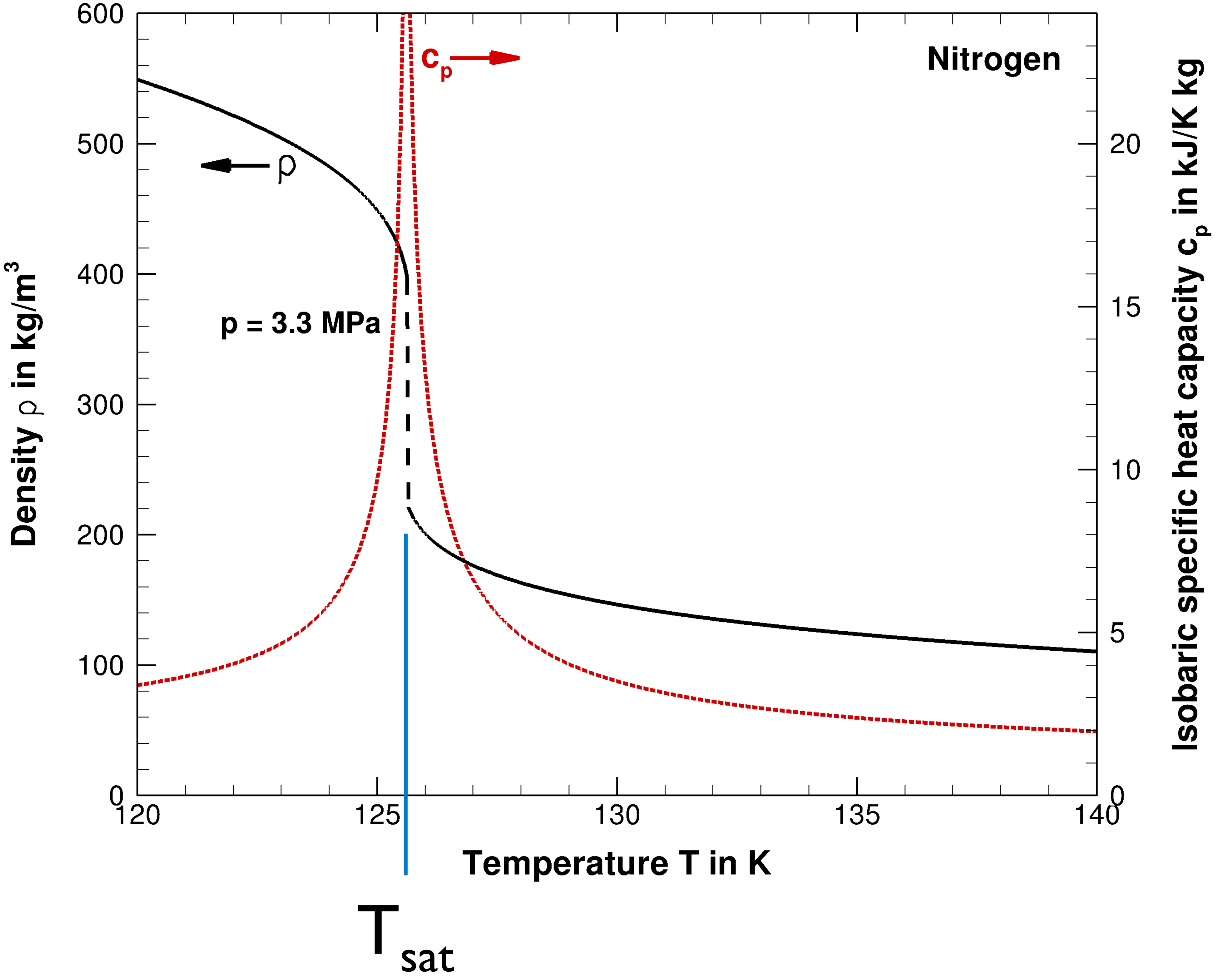
- Supercritical fluids are liquid, gaseous, or transitional
- There is no qualitative difference between a) the liquid states, and b) the gaseous states, regardless of pressure
- Transition is marked with Nishikawa-Widom / pseudoboiling line
- Peaks in heat capacity

Vaporization and pseudoboiling



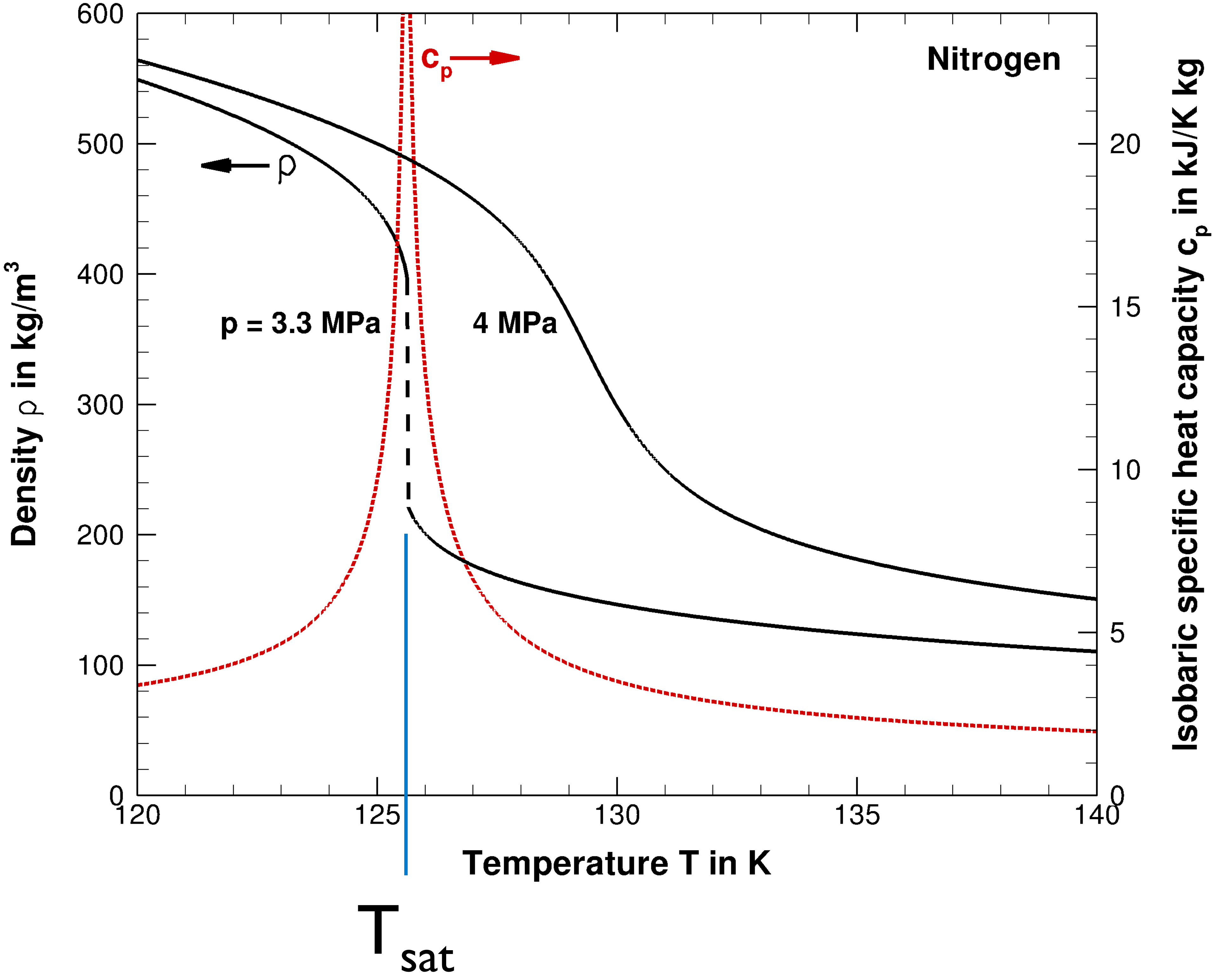
Vaporization is a first order phase transition from liquid to gaseous states at $\mathbf{T_{sat}}$

Vaporization and pseudoboiling



Vaporization
is a first order phase transition from liquid to gaseous states at
$\mathbf{T_{sat}}$

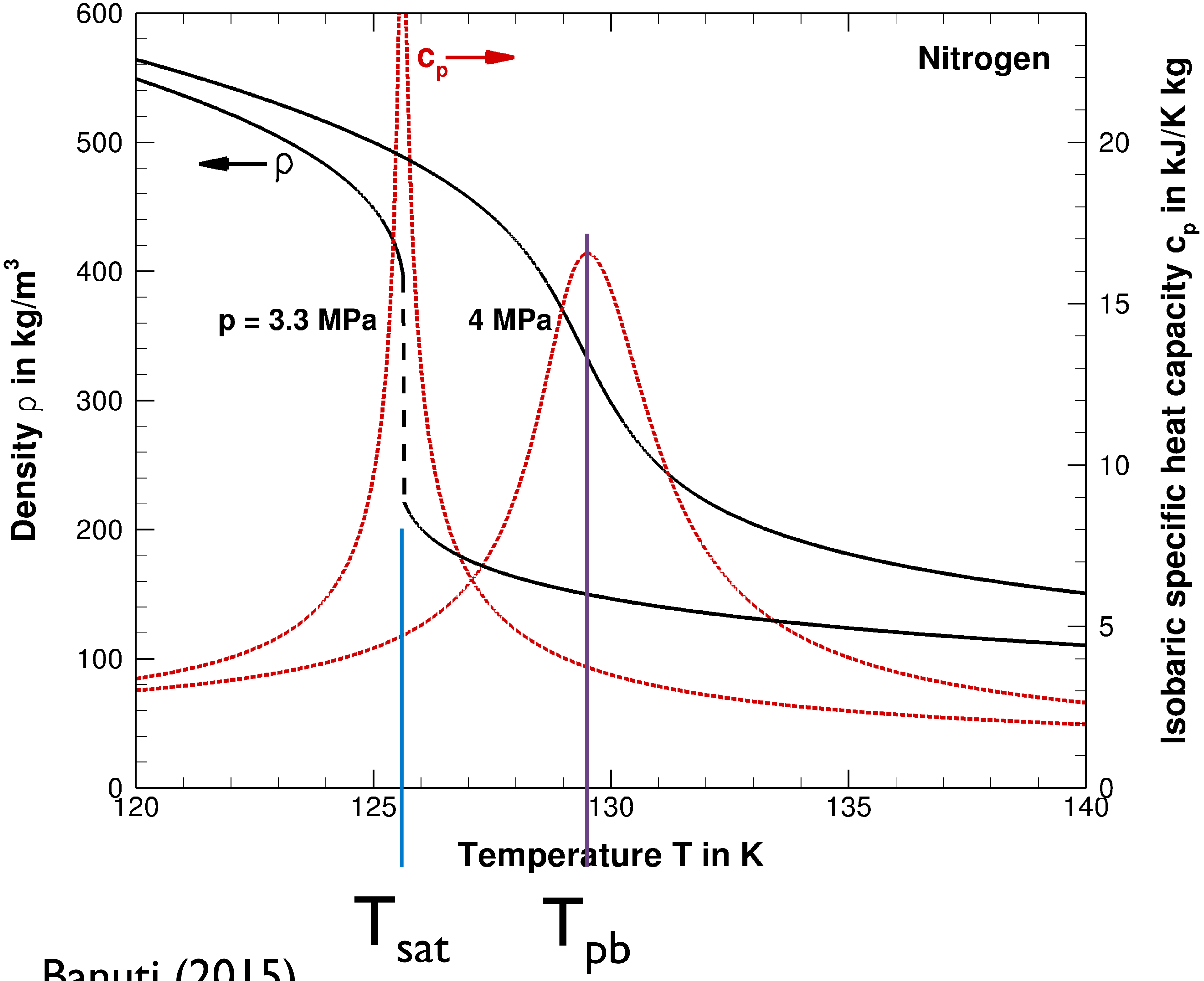
Vaporization and pseudoboiling



Vaporization is a first order phase transition from liquid to gaseous states at $\mathbf{T_{sat}}$

Pseudoboiling is a higher order phase transition from liquid-like to gas-like supercritical states around $\mathbf{T_{pb}}$

Vaporization and pseudoboiling

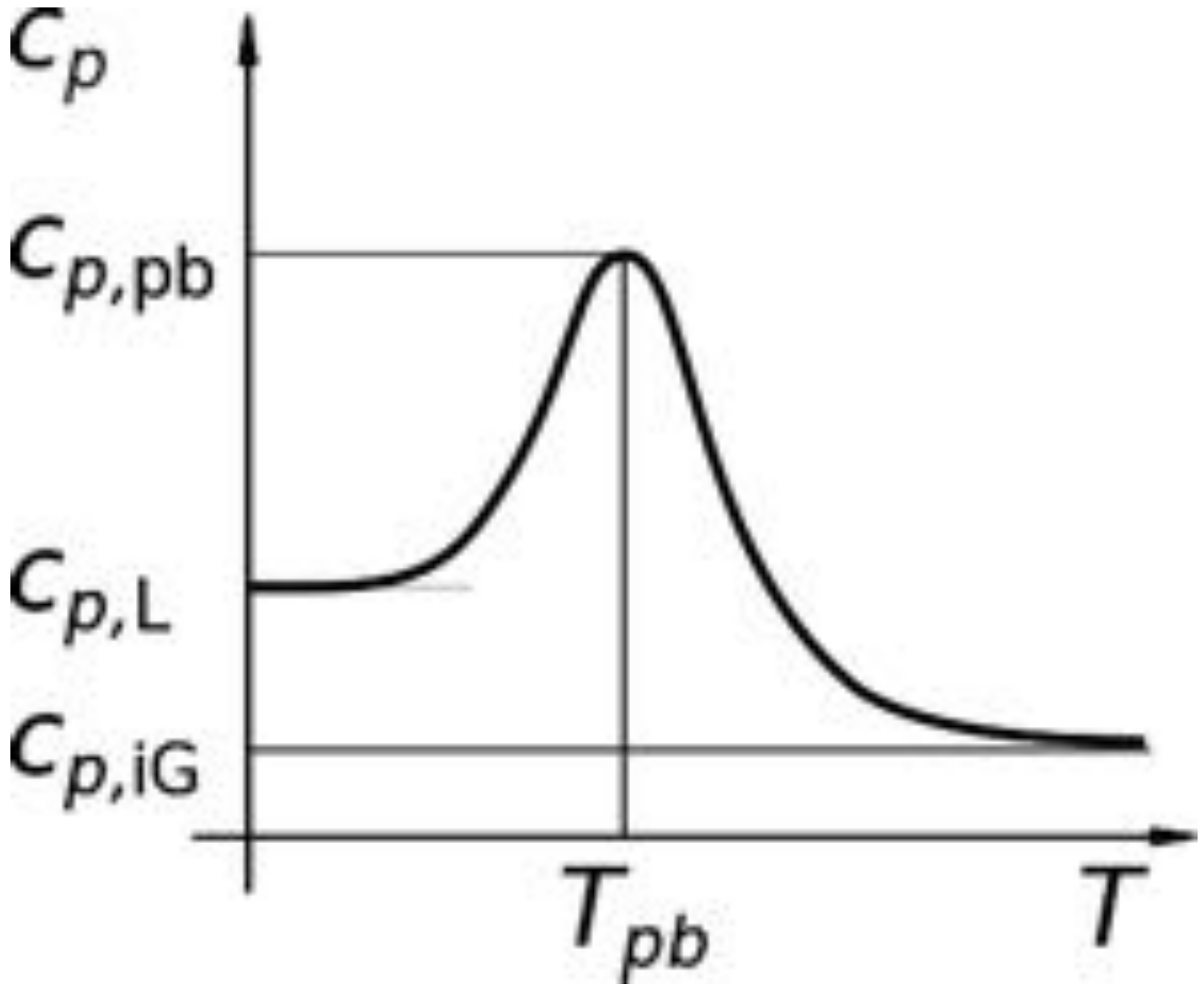


Banuti (2015)

Vaporization is a first order phase transition from liquid to gaseous states at $\mathbf{T_{sat}}$

Pseudoboiling is a higher order phase transition from liquid-like to gas-like supercritical states around $\mathbf{T_{pb}}$

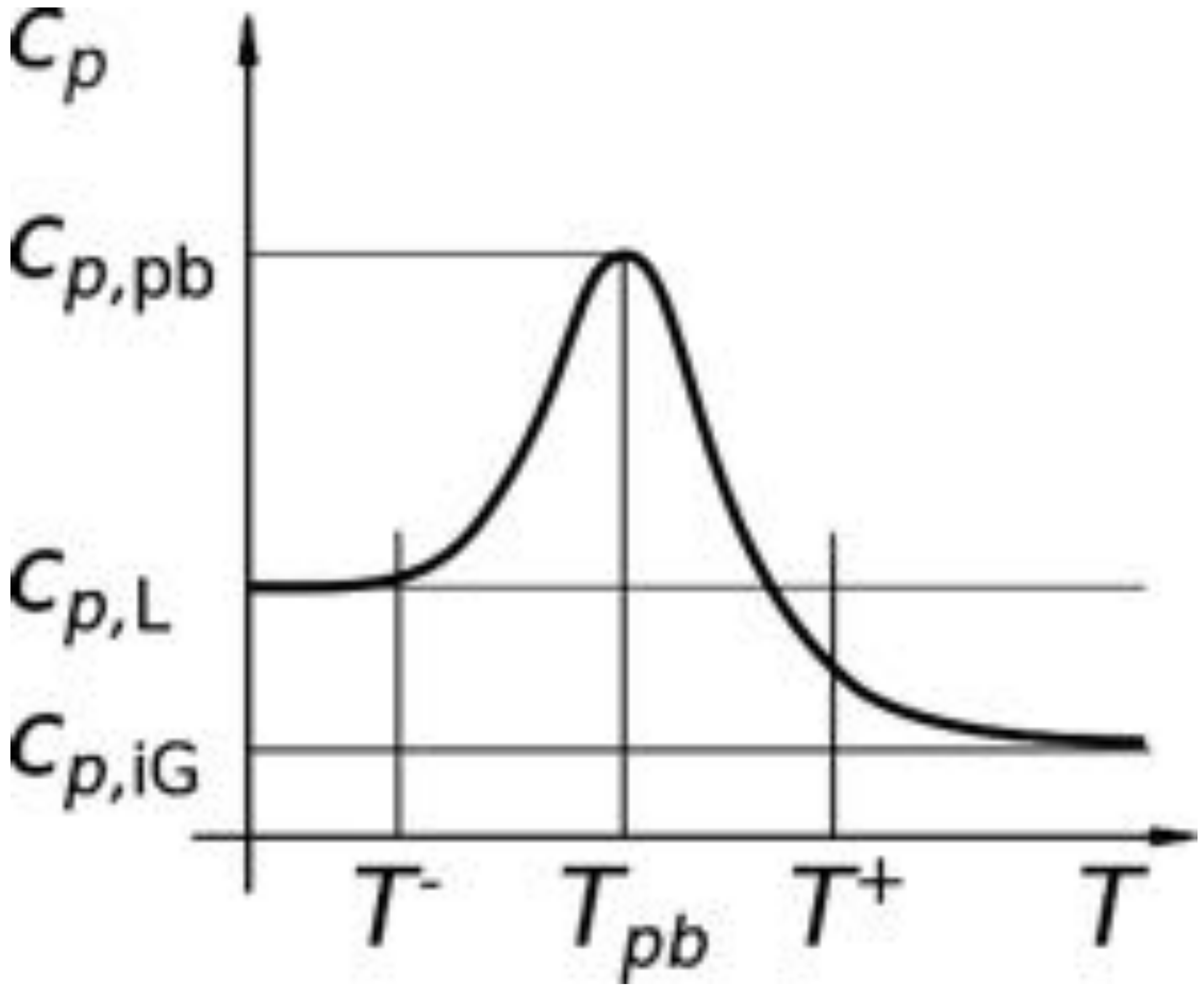
Energy budget during pseudoboiling



- Pseudoboiling temperature T_{pb} at maximum c_p

Banuti (2015)

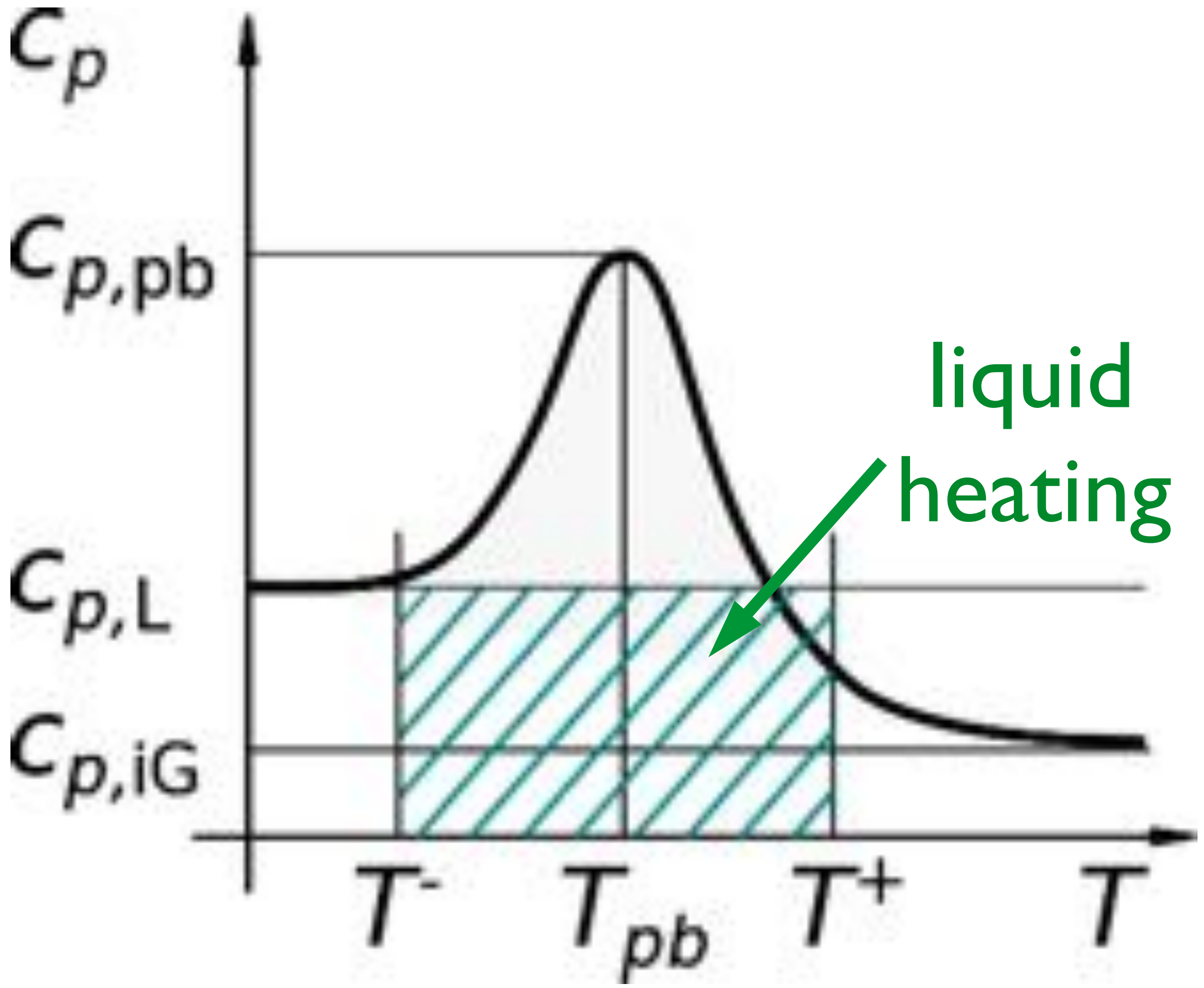
Energy budget during pseudoboiling



- Pseudoboiling temperature T_{pb} at maximum c_p
- Transition occurs over finite T interval

Banuti (2015)

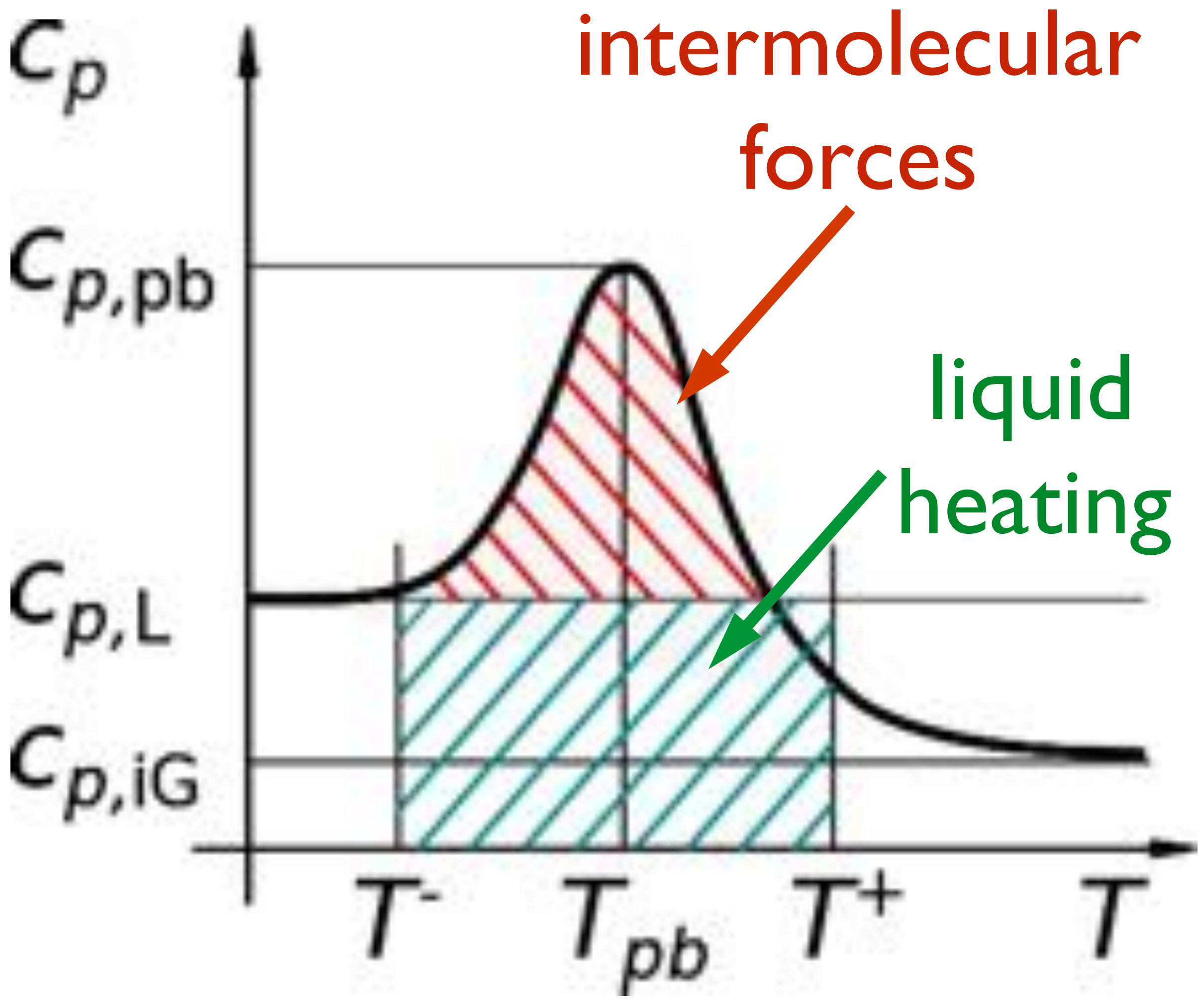
Energy budget during pseudoboiling



- Pseudoboiling temperature T_{pb} at maximum c_p
- Transition occurs over finite T interval
- Added heat leads to
  - Increase in temperature

Banuti (2015)

Energy budget during pseudoboiling



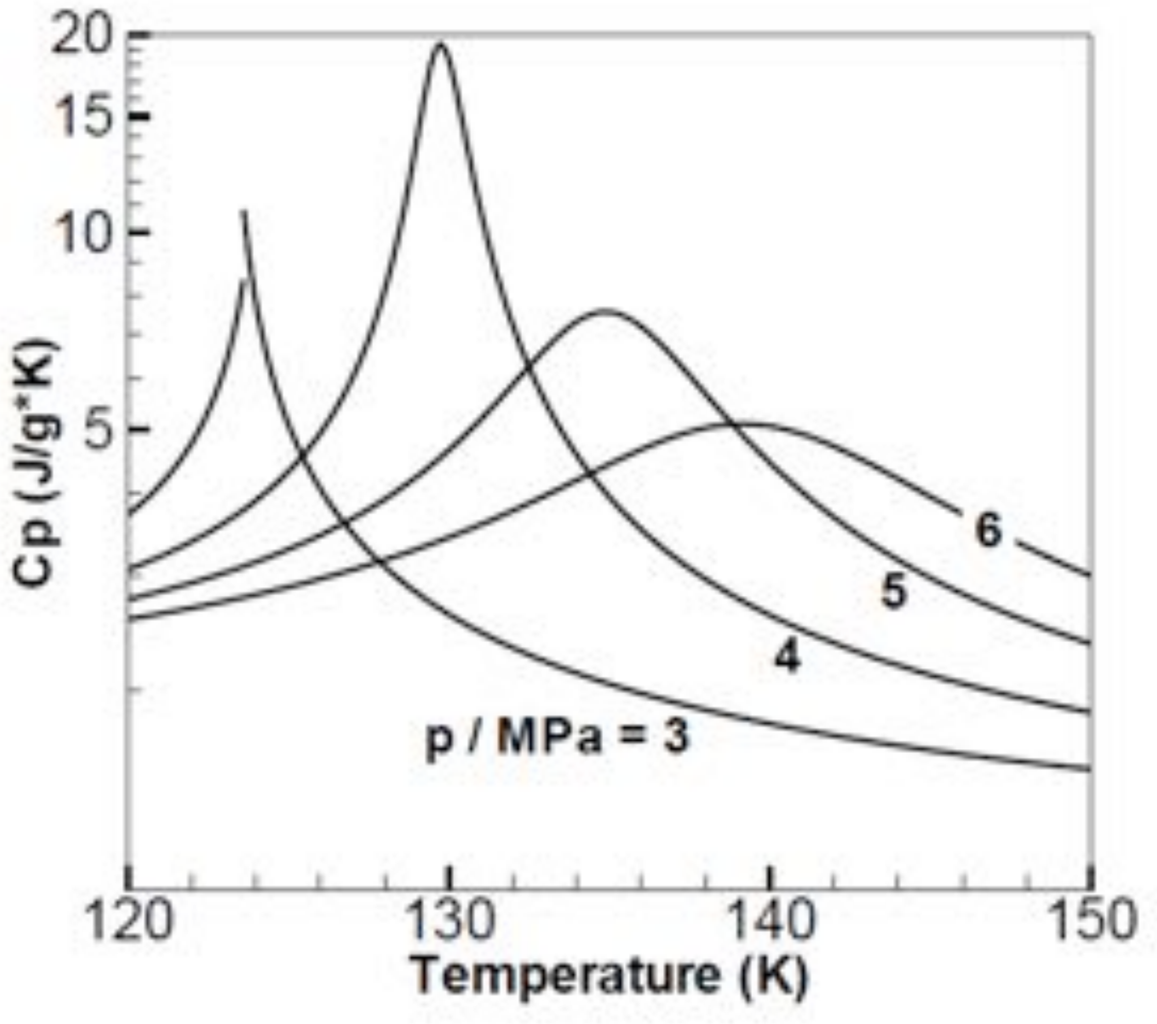
- Pseudoboiling temperature T_{pb} at maximum c_p
- Transition occurs over finite T interval
- Added heat leads to
  - Increase in temperature
  - Overcoming inter-molecular forces

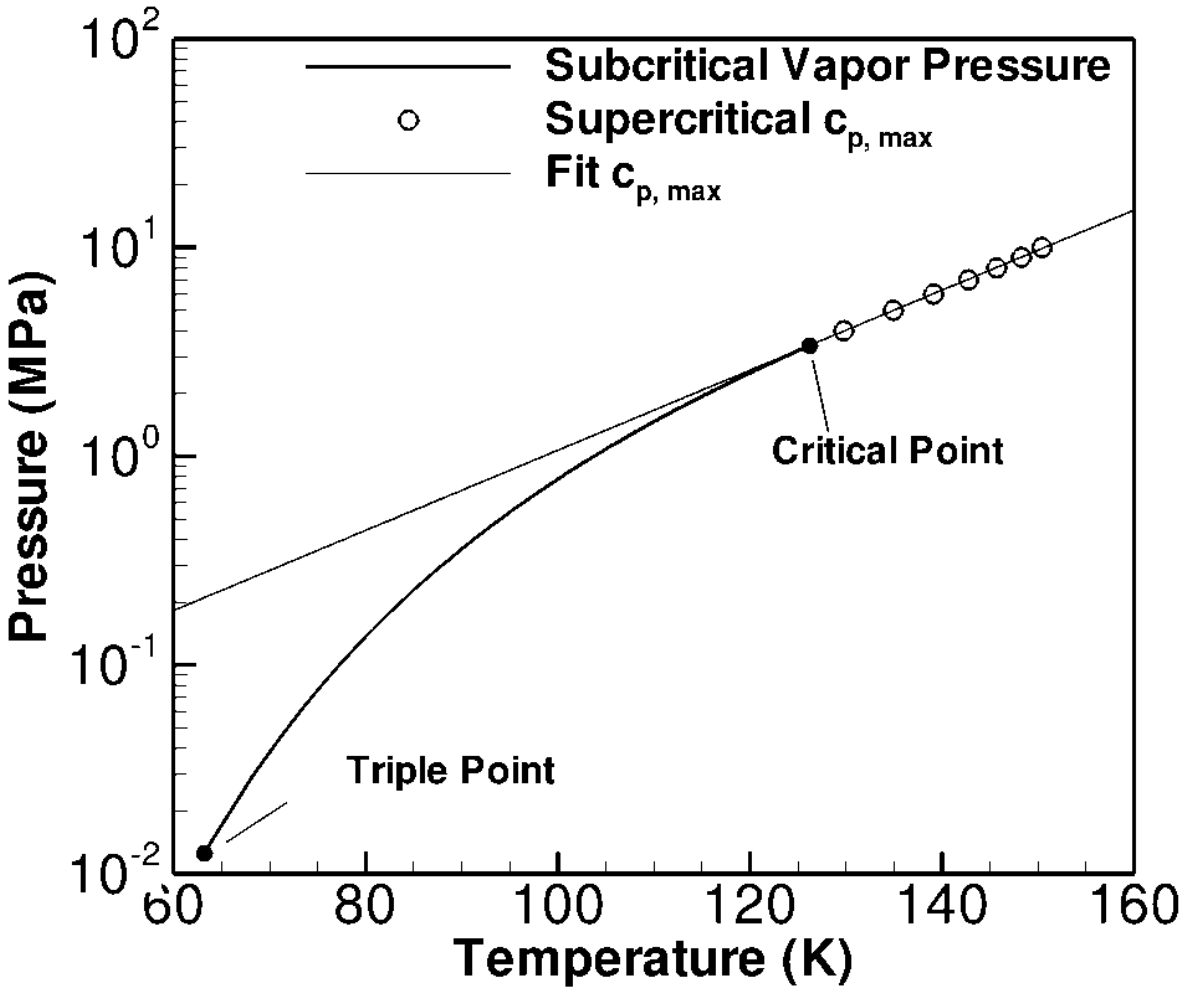
A latent heat needs to be overcome at supercritical pressures!

Banuti (2015)

Where does pseudoboiling occur?

- Pseudoboiling points (c_p max) can be added to p T diagram
- Line up nicely in log-linear plot

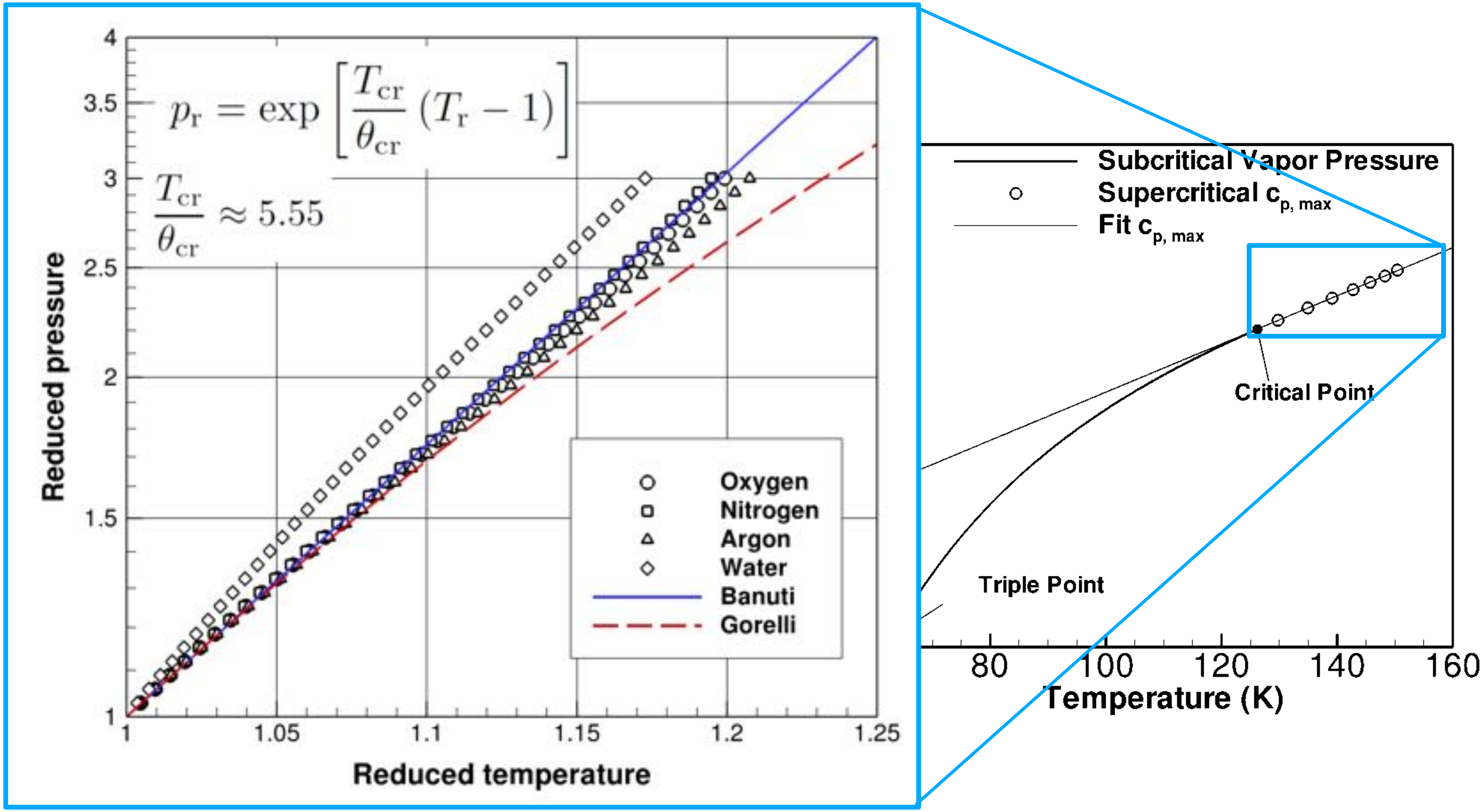




Banuti (2015)

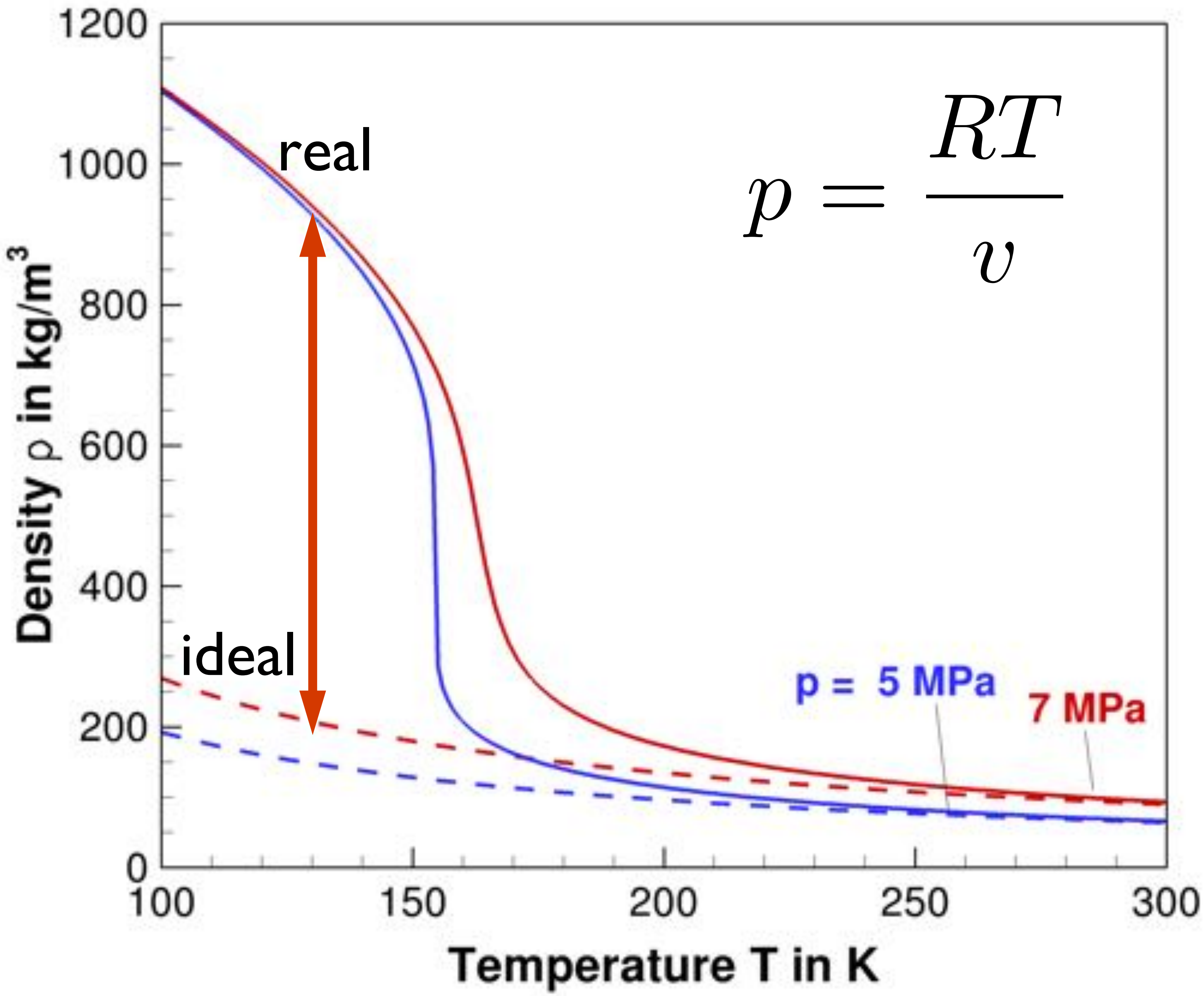
Where does pseudoboiling occur?

- Pseudoboiling points (c_p max) can be added to p T diagram
- Line up nicely in log-linear plot – for number of fluids!



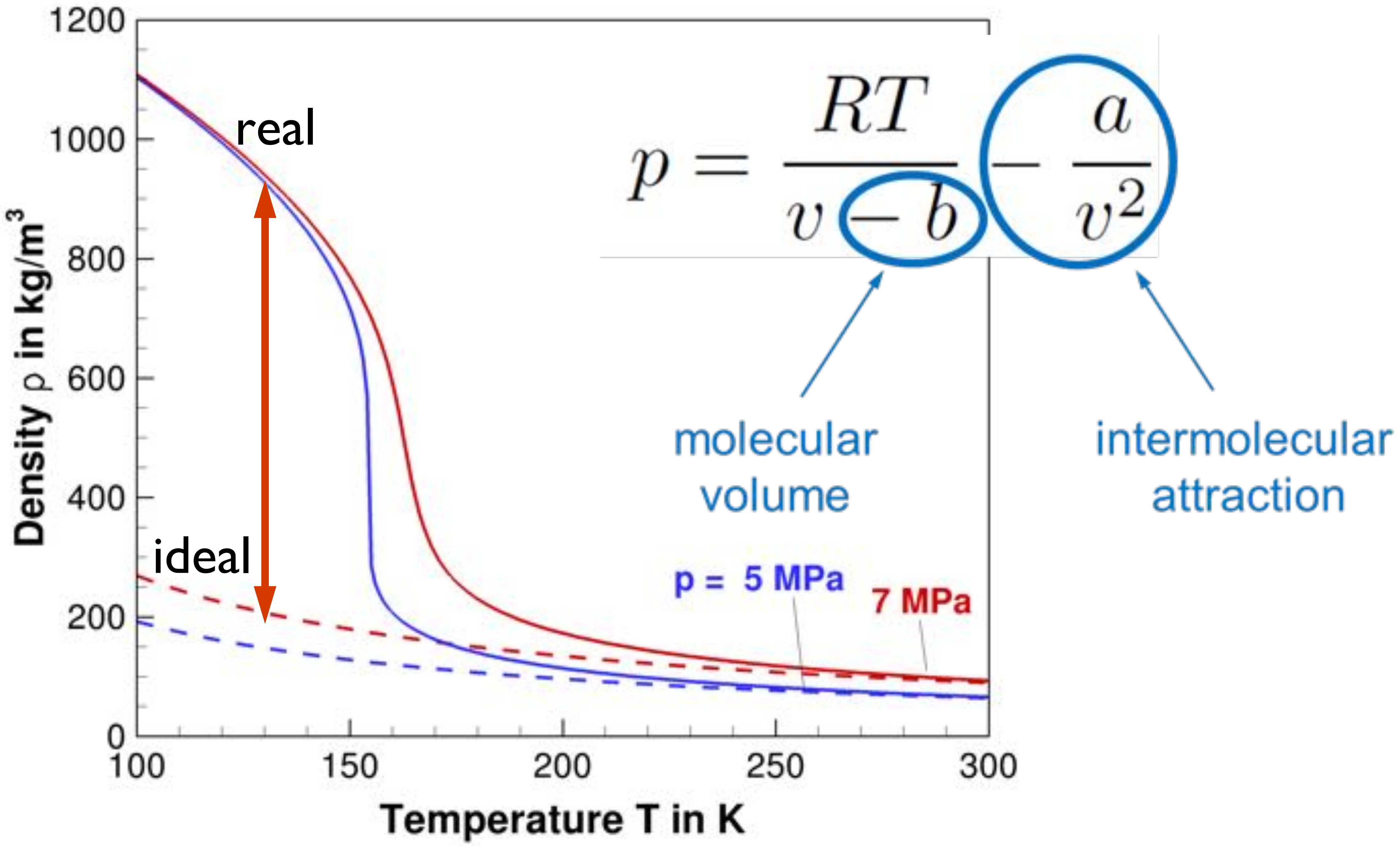
Banuti (2015)

What is the difference between a real and an ideal gas?



$$p = \frac{RT}{v}$$

What is the difference between a real and an ideal gas?



$$p = \frac{RT}{v - b} - \frac{a}{v^2}$$

molecular volume

intermolecular attraction

Real fluid equations of state

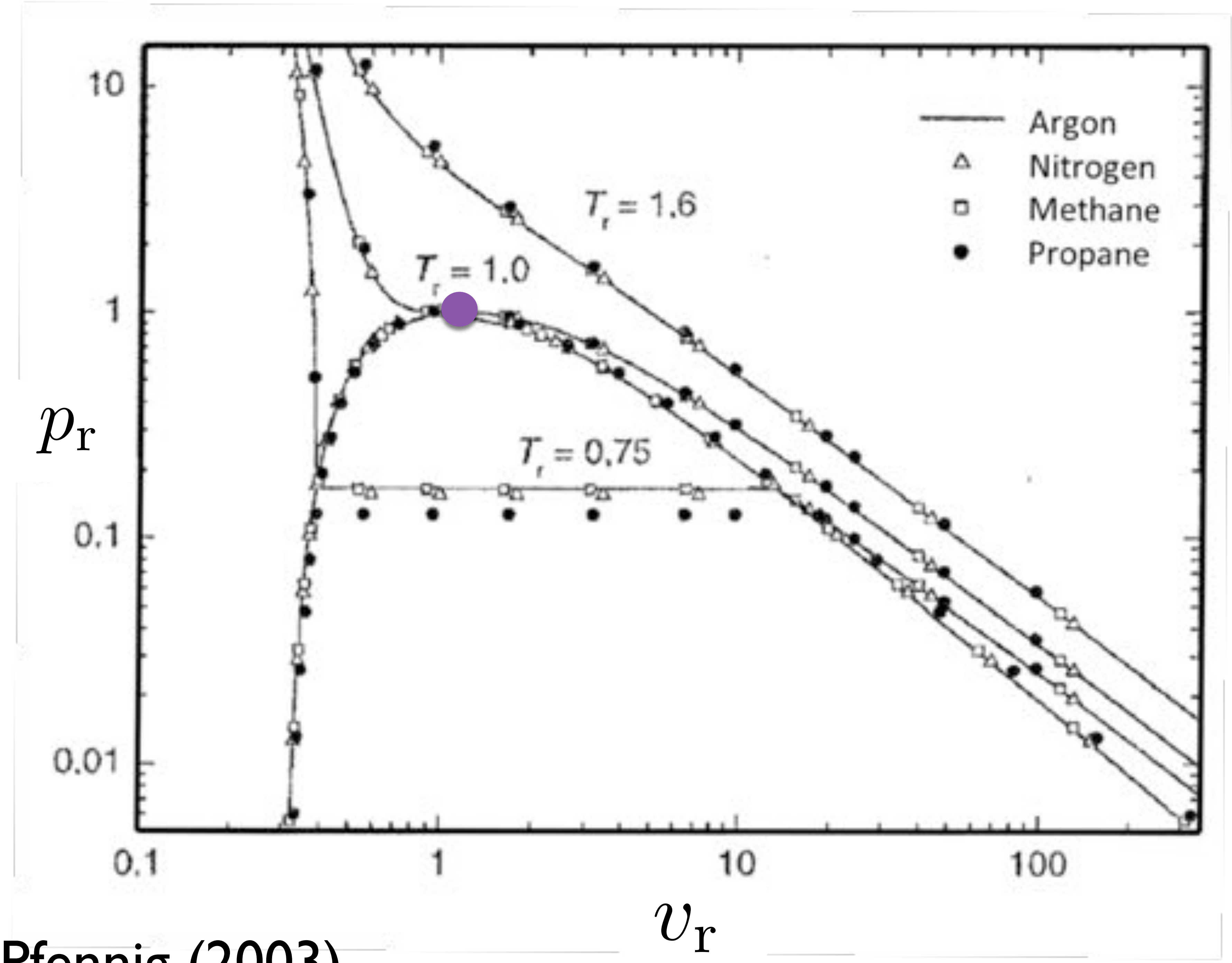
$$p = \frac{RT}{v-b} - \frac{a}{v^2}$$ van der Waals

$$p = \frac{RT}{v-b} - \frac{\alpha(T)}{v^2 + 2vb - b^2}$$ Peng-Robinson

$$p = \frac{RT}{v}\left(1 + \frac{B_1}{v} + \frac{B_2}{v^2} + \ldots\right)$$ virial

Reid / Prausnitz / Poling

$$p_{\mathrm{r}} = \frac{p}{p_{\mathrm{cr}}} \qquad v_{\mathrm{r}} = \frac{v}{v_{\mathrm{cr}}} \qquad T_{\mathrm{r}} = \frac{T}{T_{\mathrm{cr}}}$$



Pfennig (2003)

- Critical point:

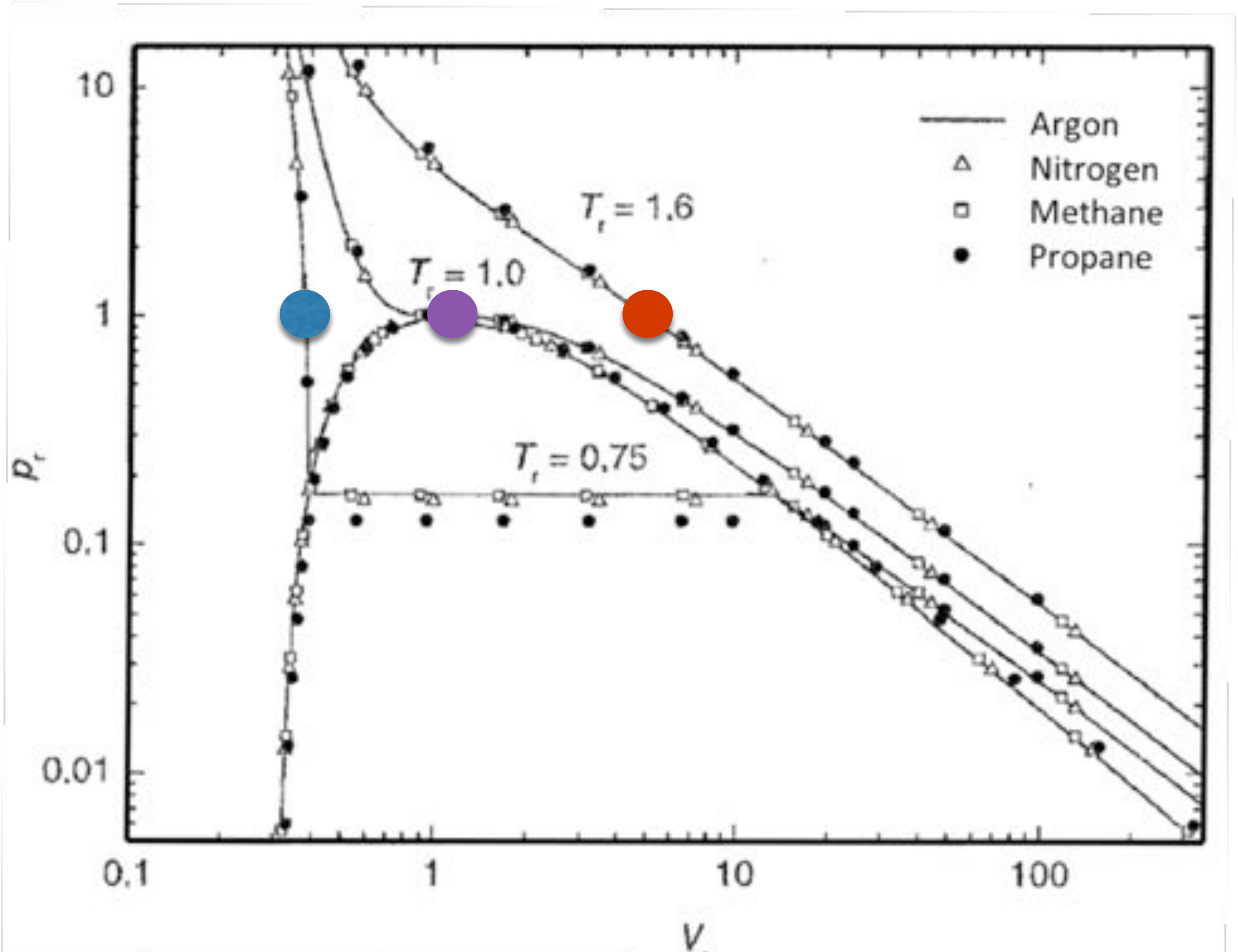
$$\left(\frac{\partial p}{\partial v}\right)_{T,\mathrm{cr}} = 0$$

$$\left(\frac{\partial^2 p}{\partial v^2}\right)_{T,\mathrm{cr}} = 0$$

Corresponding States Principle: Fluid pvT behavior collapses when nondimensionalized with the critical values

Isothermal compression

http://www.china-ec21.com



liquid:

$$\left(\frac{\partial p}{\partial v}\right)_T \text{ large}$$

critical:

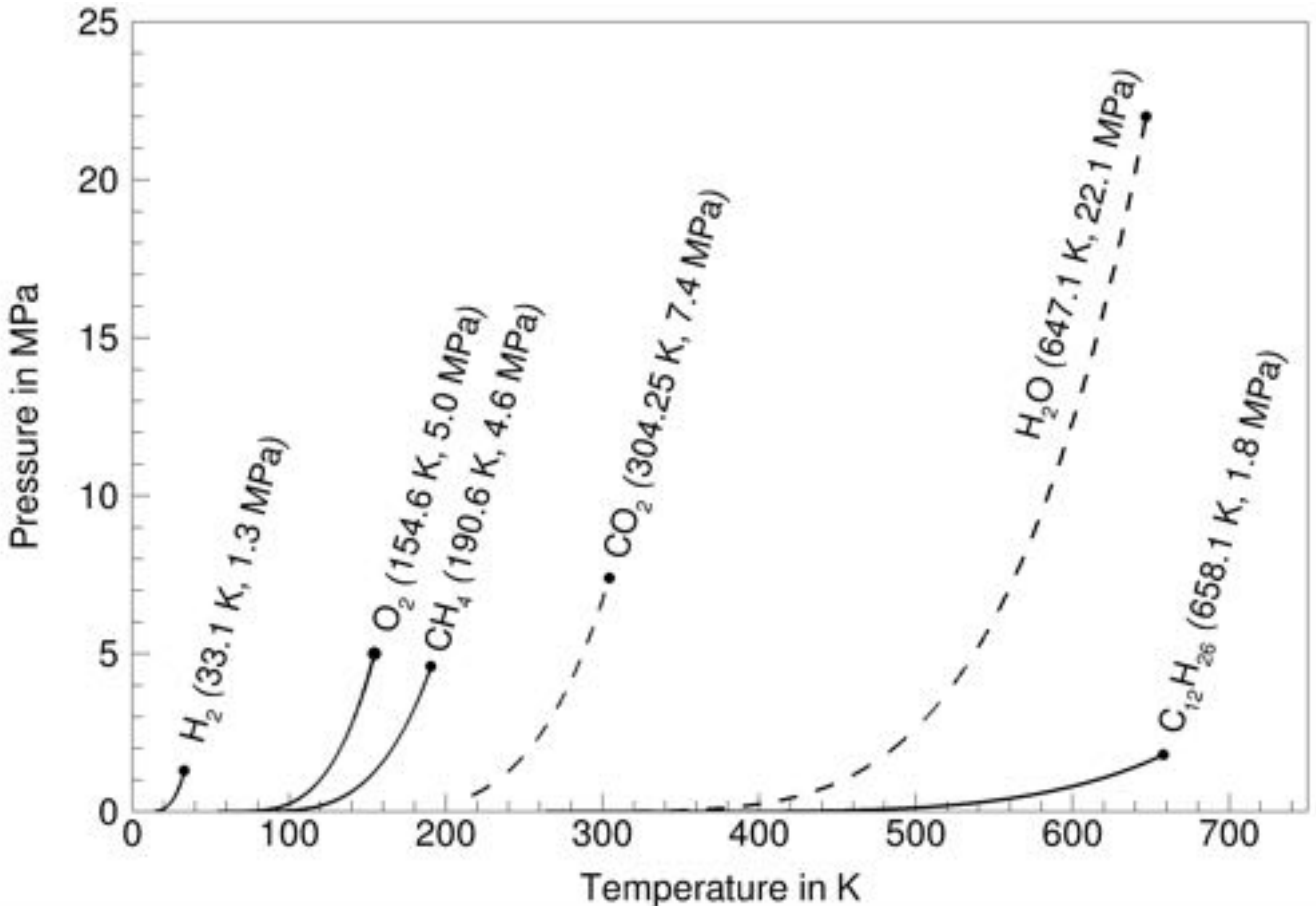
$$\left(\frac{\partial p}{\partial v}\right)_T \approx 0$$

ideal gas:

$$\left(\frac{\partial p}{\partial v}\right)_T = -\frac{p}{v}$$

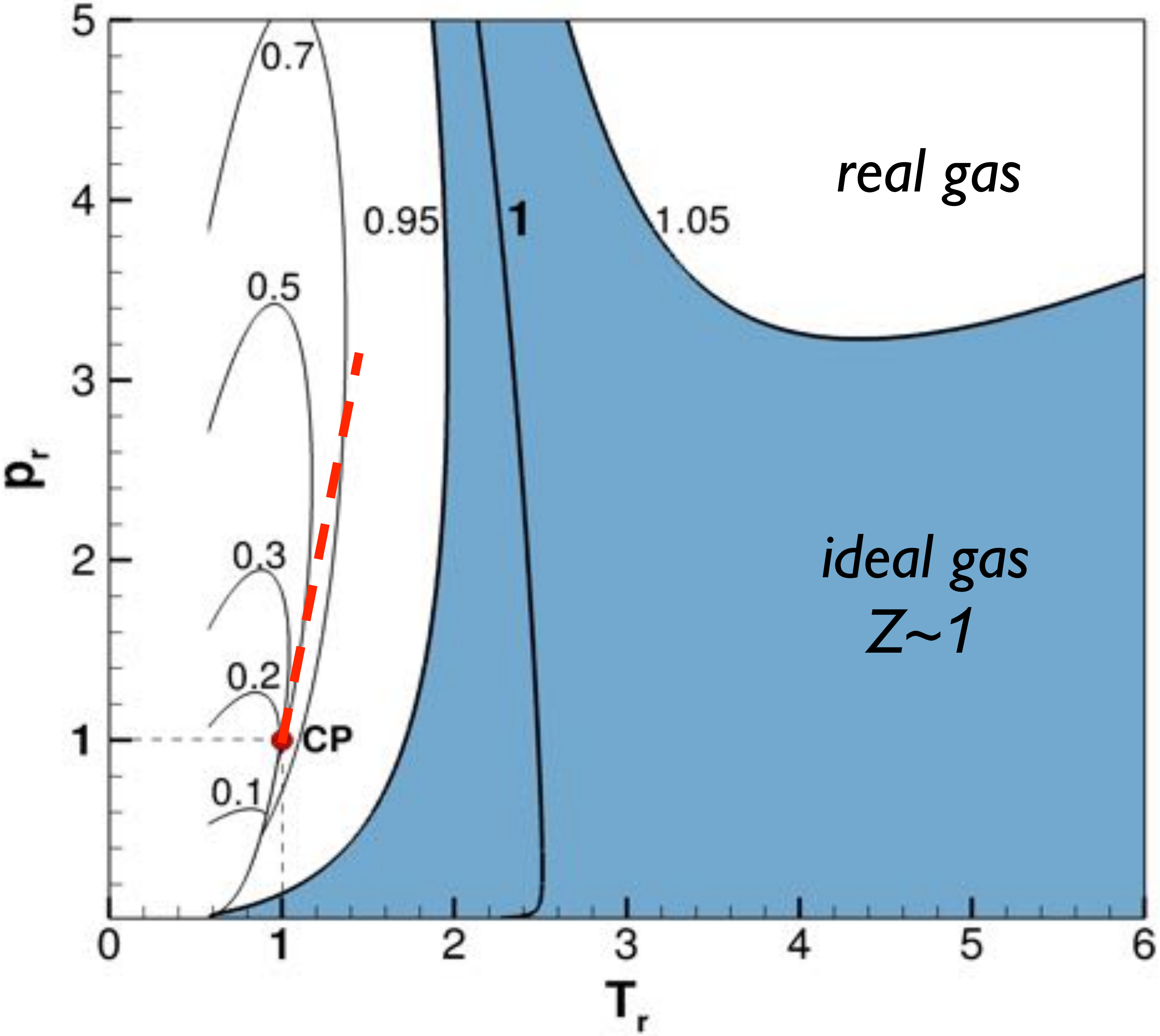
A fluid at near critical conditions does not build up pressure when compressed isothermally!

Species critical points



Real gas behavior in the phase plane

Compressibility factor $Z = \frac{p}{\rho R T} = \frac{p_{\mathrm{real}}}{p_{\mathrm{ideal}}}$

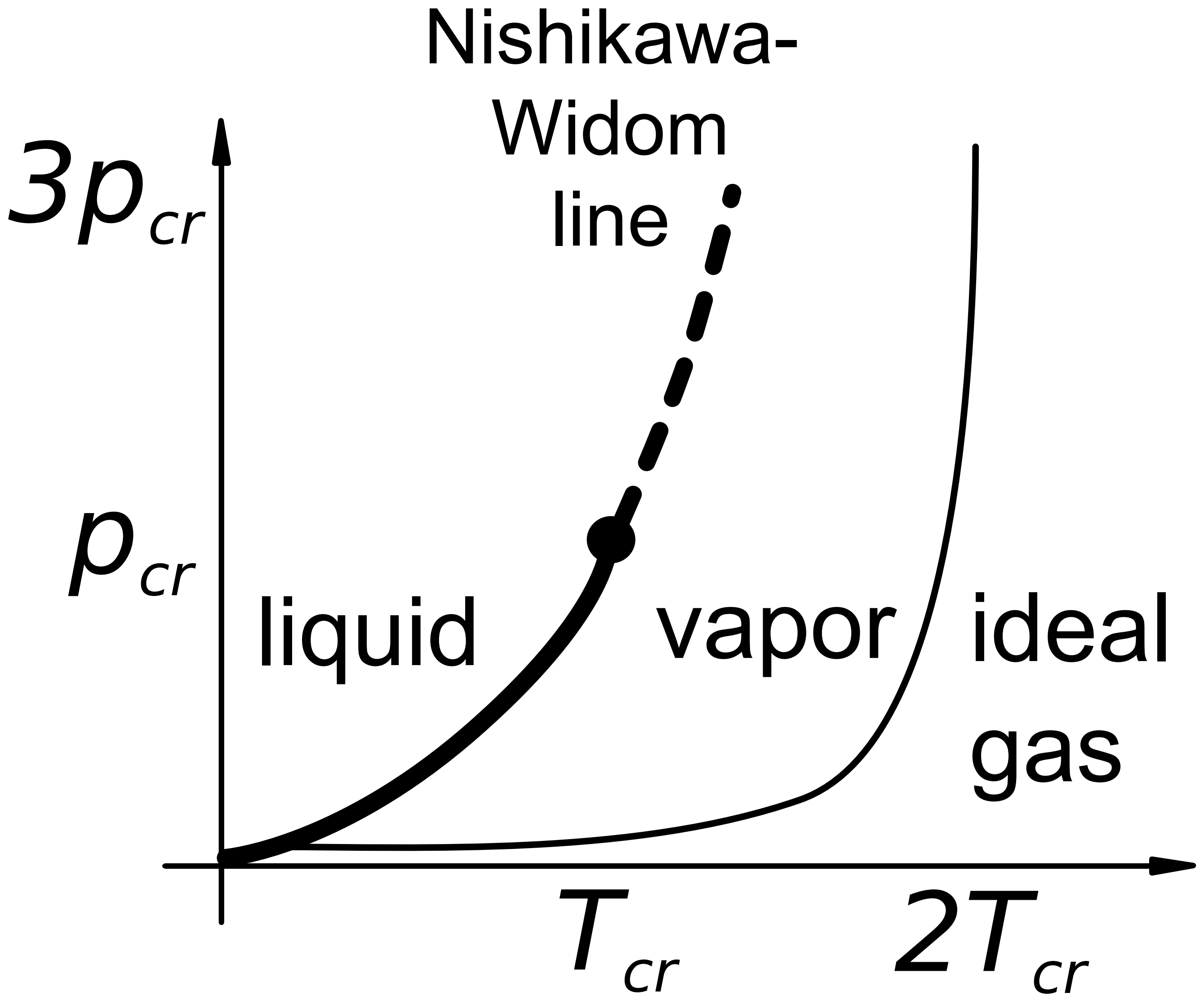


Banuti et al. (CnF 2016)

- Ideal gas at supercritical p
- Ideal gas only at higher T
- Vapor is not an ideal gas (except at very low p_r)
- E.g. 30% p error at p_r=0.5 (e.g. 10 bar dodecane)

Data from NIST

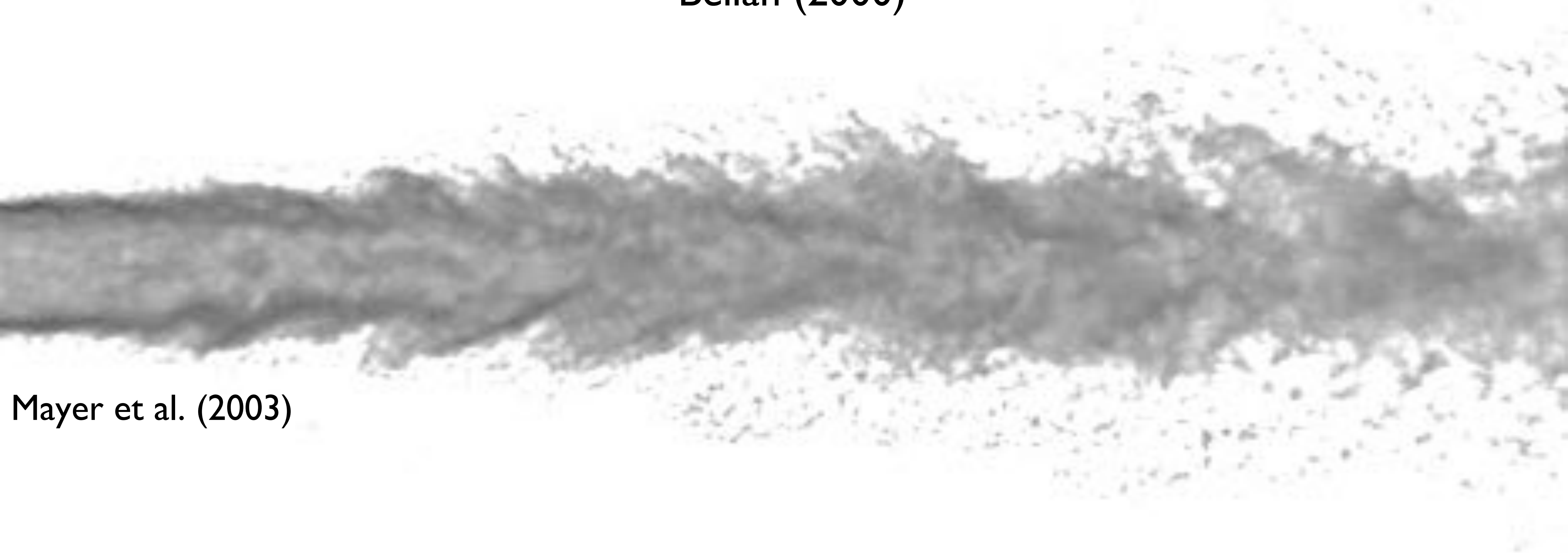
The real fluid phase plane



- Phase plane can be divided into liquids and gases
- Ideal gases for
  - $T>2T_{cr}$
  - $p<3p_{cr}$
- Pseudoboiling is supercritical phase transition from liquid to gas, with distributed latent heat
- Smooth transitions at $p>3p_{cr}$

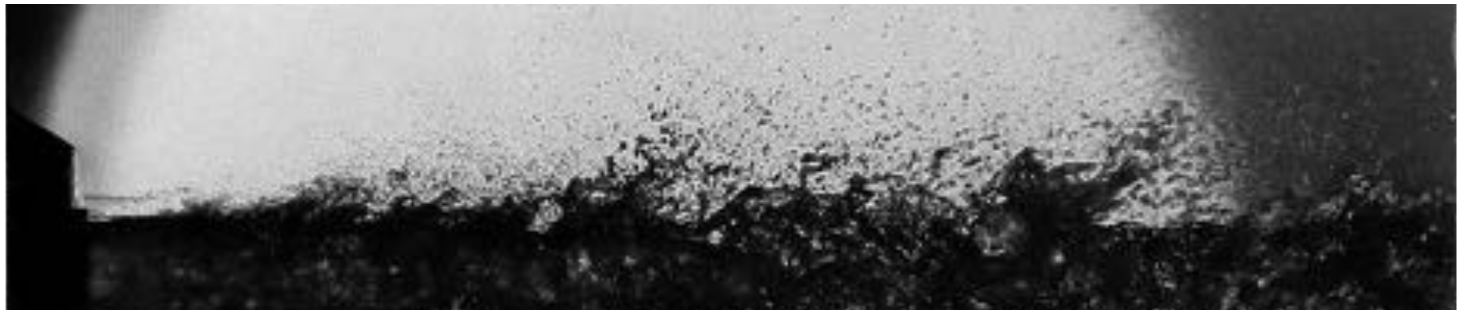
“Does a supercritical spray exist, and if so, what is it?”

Bellan (2000)



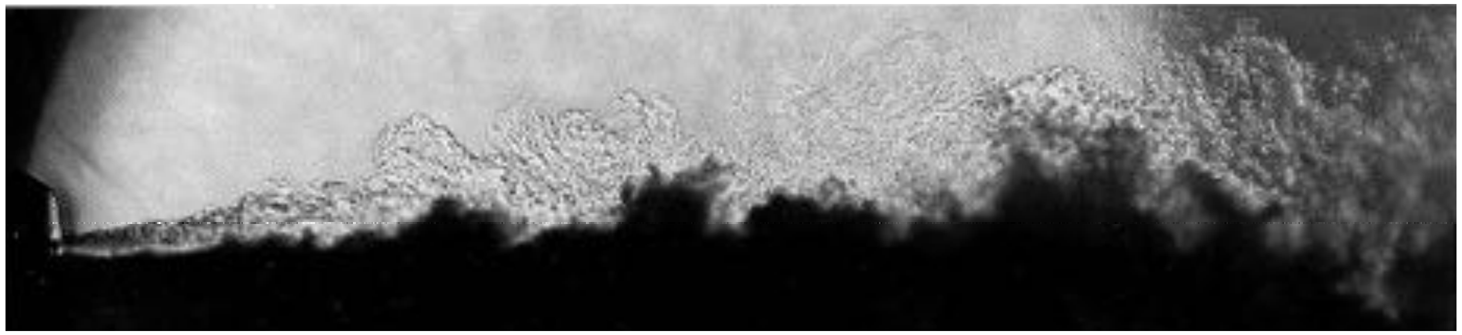
Mayer et al. (2003)

Key differences of high pressure break–up



Subcritical pressure

- Classical atomization
- Instabilities grow, ligaments and droplets detach

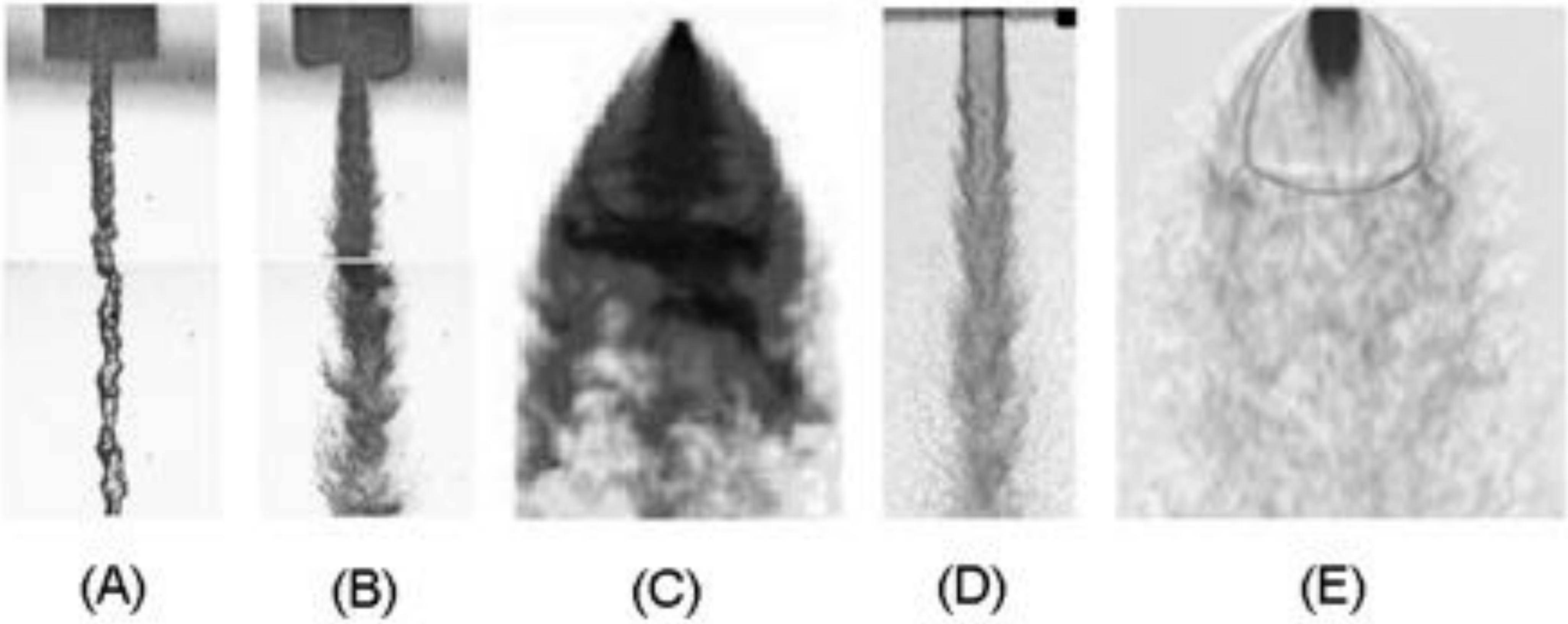


Supercritical pressure

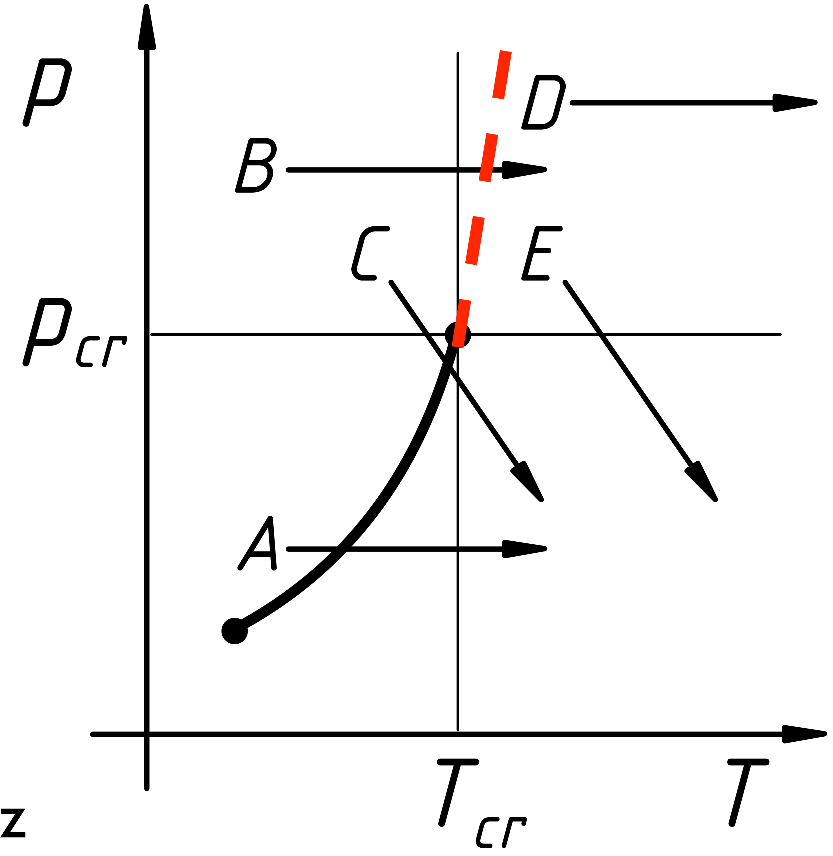
- Vanishing surface tension
- Mixing-like disintegration

Mayer et al. (1998)

Injection processes

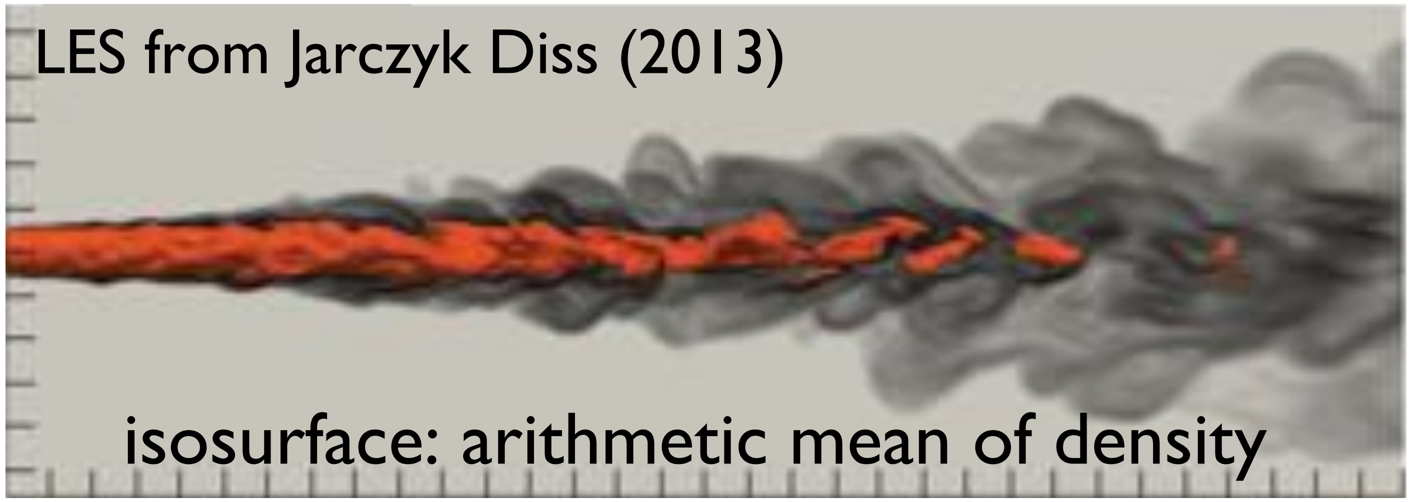


(A) Subcritical injection
(B) Transcritical injection
(C) Near critical flashing
(D) Supercritical injection
(E) High pressure ratio expansion



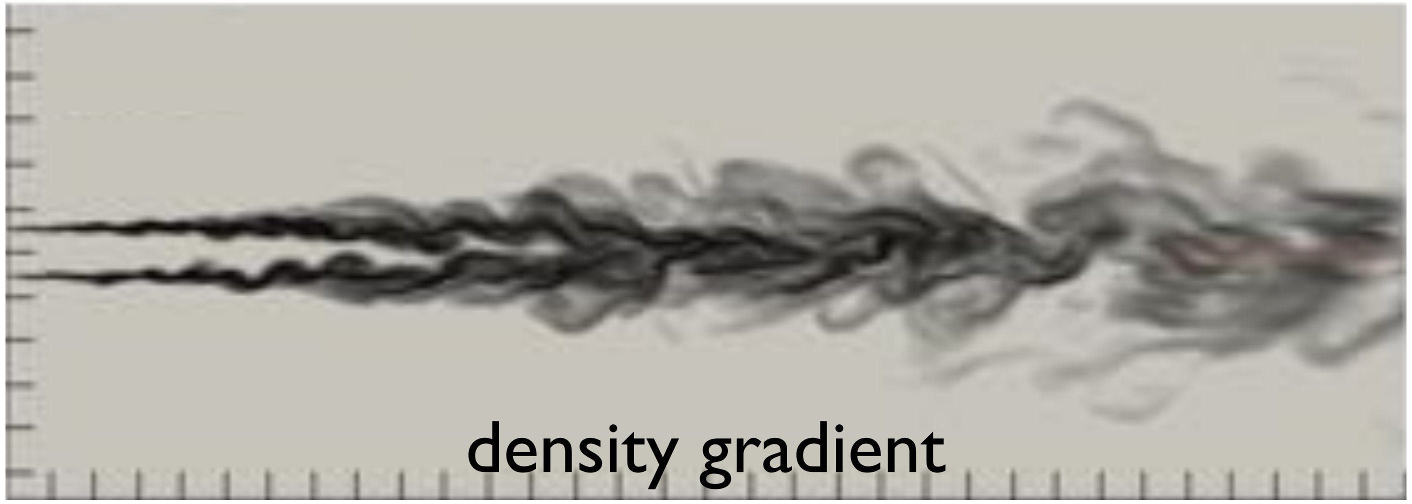
Banuti, Dissertation, 2015
(A), (B): Chehroudi; (C) Lamanna; (D) Branam; (E) Stotz

Boundary of a transcritical jet

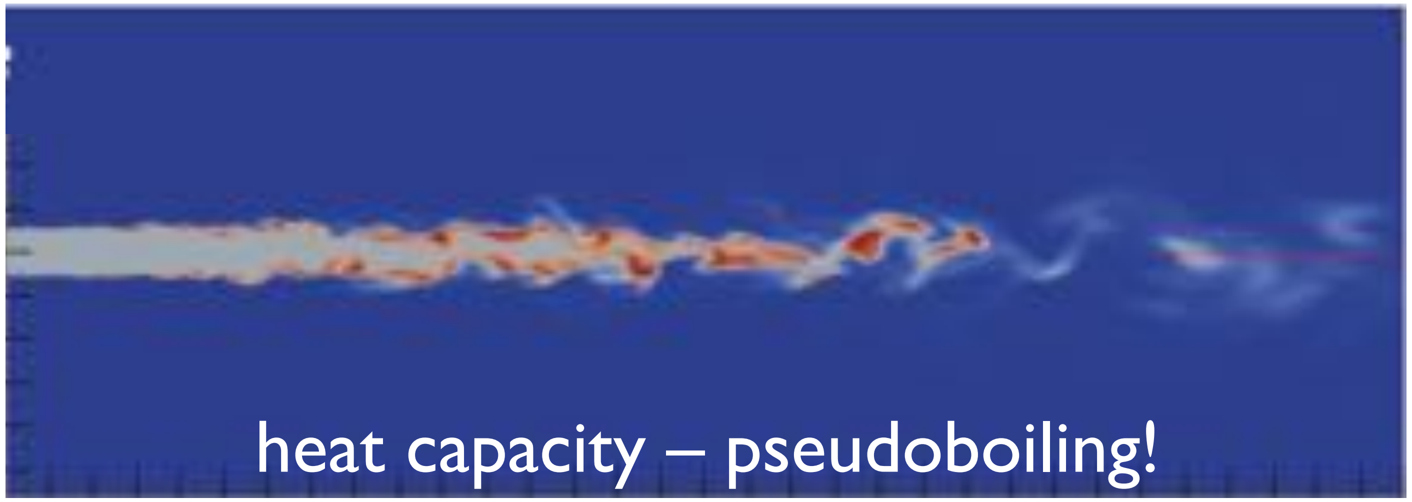


LES from Jarczyk Diss (2013)

isosurface: arithmetic mean of density



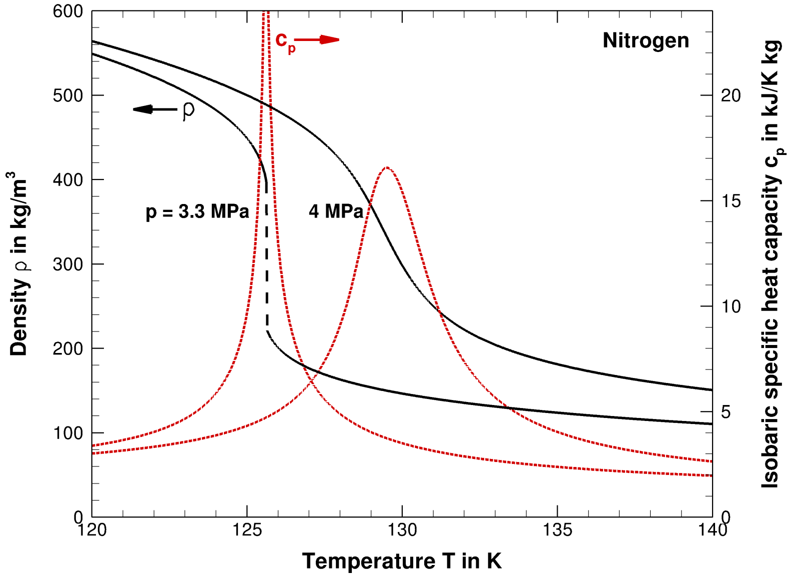
density gradient



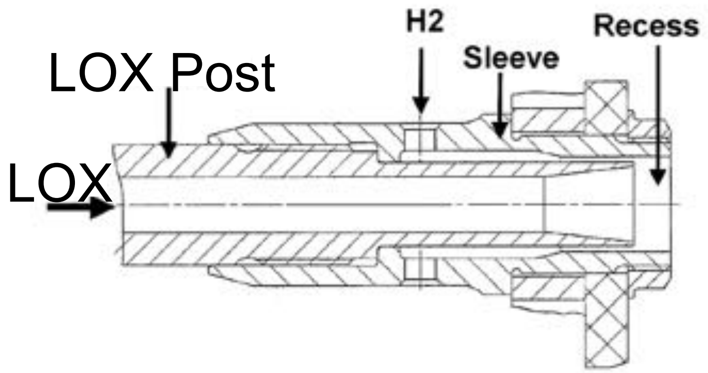
heat capacity – pseudoboiling!

Pseudoboiling provides a physical jet boundary criterion

- Highest density gradient
- Local identification via temperature!



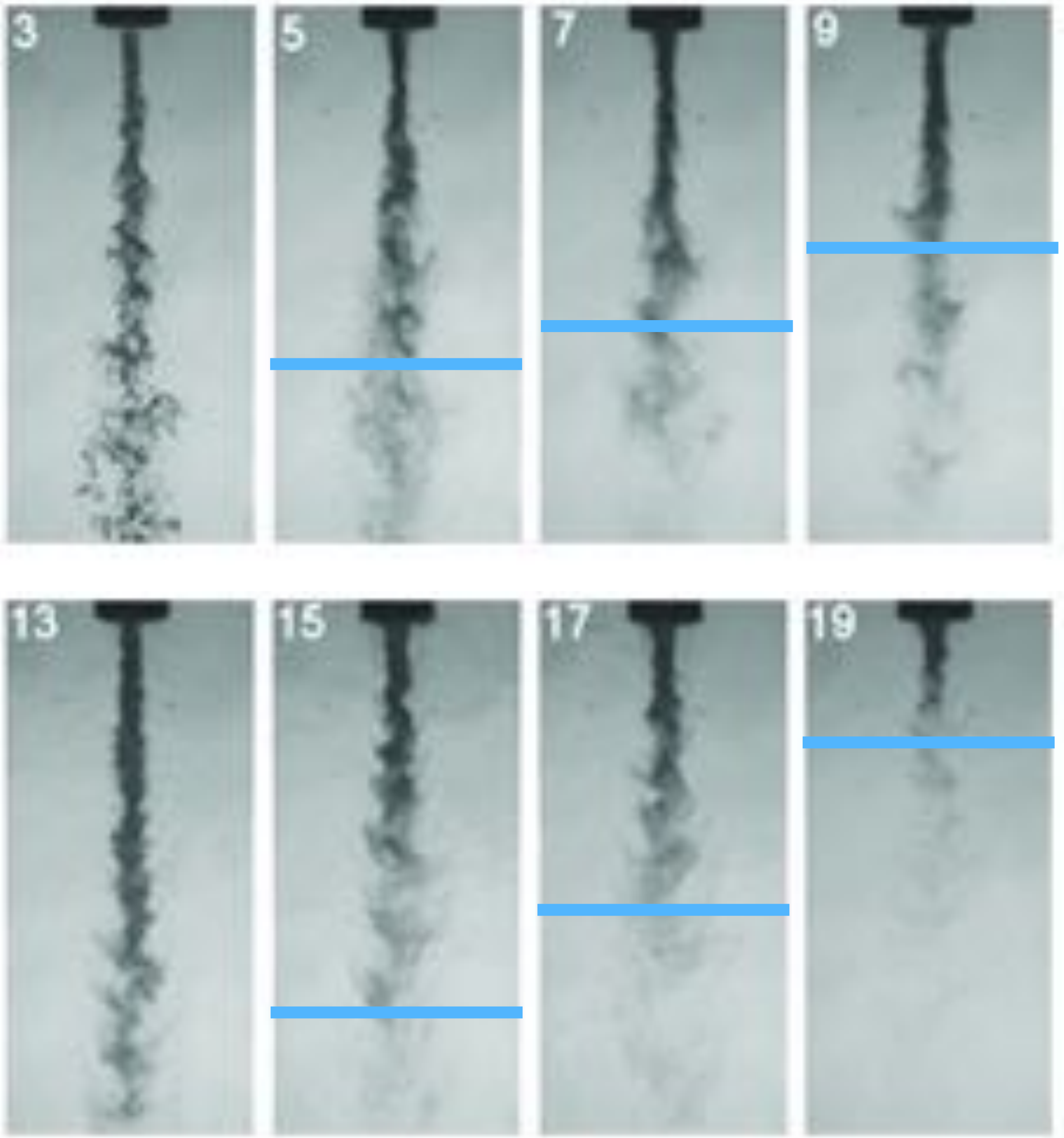
Coaxial injection LN2/GN2



Gaseous co-flow velocity

$p_r = 0.4$

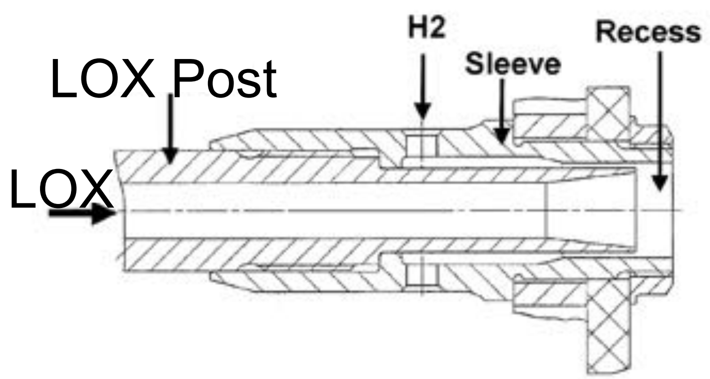
$p_r = 1.03$



- Increase in co-flow velocity shortens dense core (Davis and Chehroudi 2004)

Davis & Chehroudi (2004)

Coaxial injection LN2/GN2

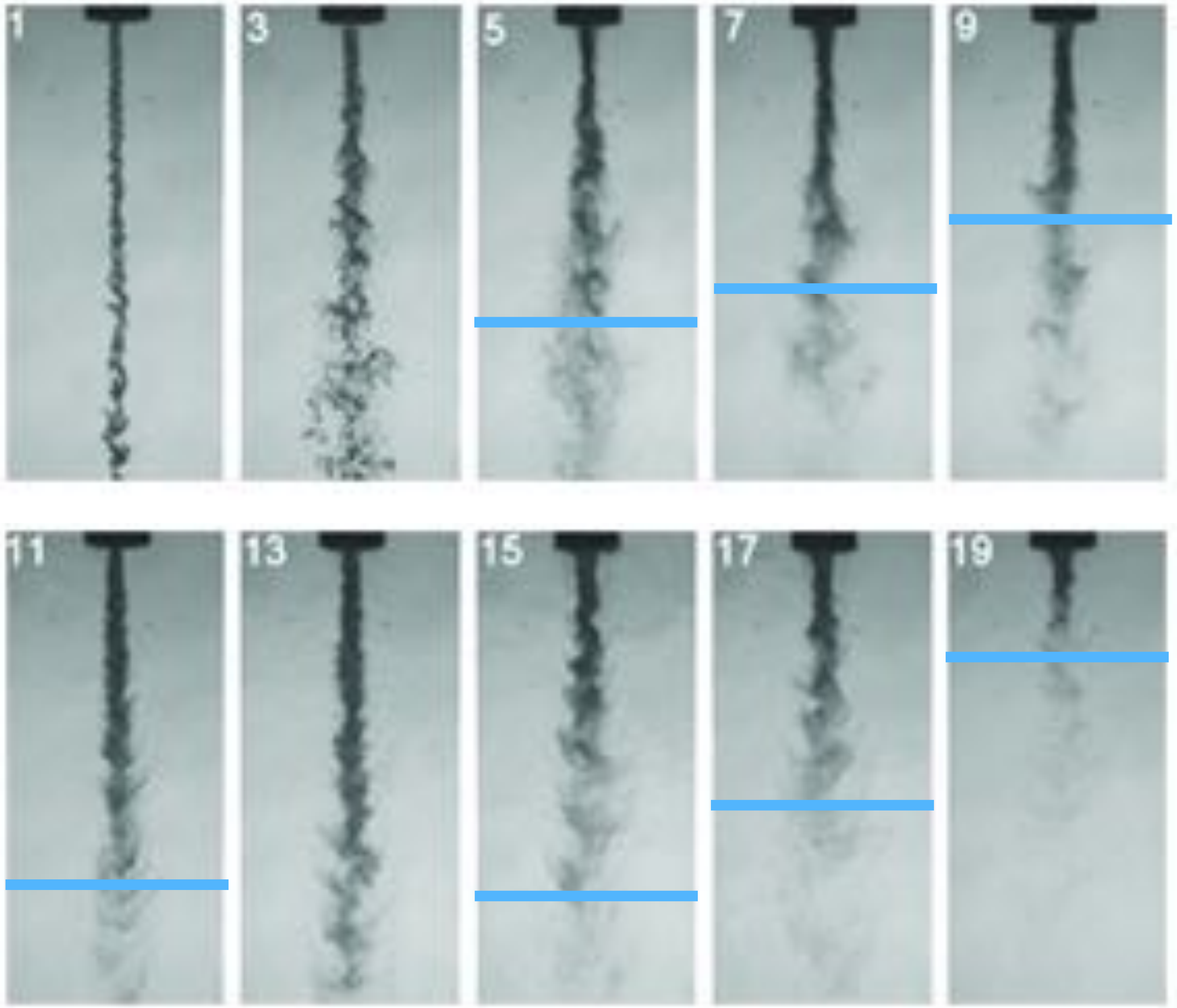


Gaseous co-flow velocity

Heat transfer

$p_r = 0.4$

$p_r = 1.03$

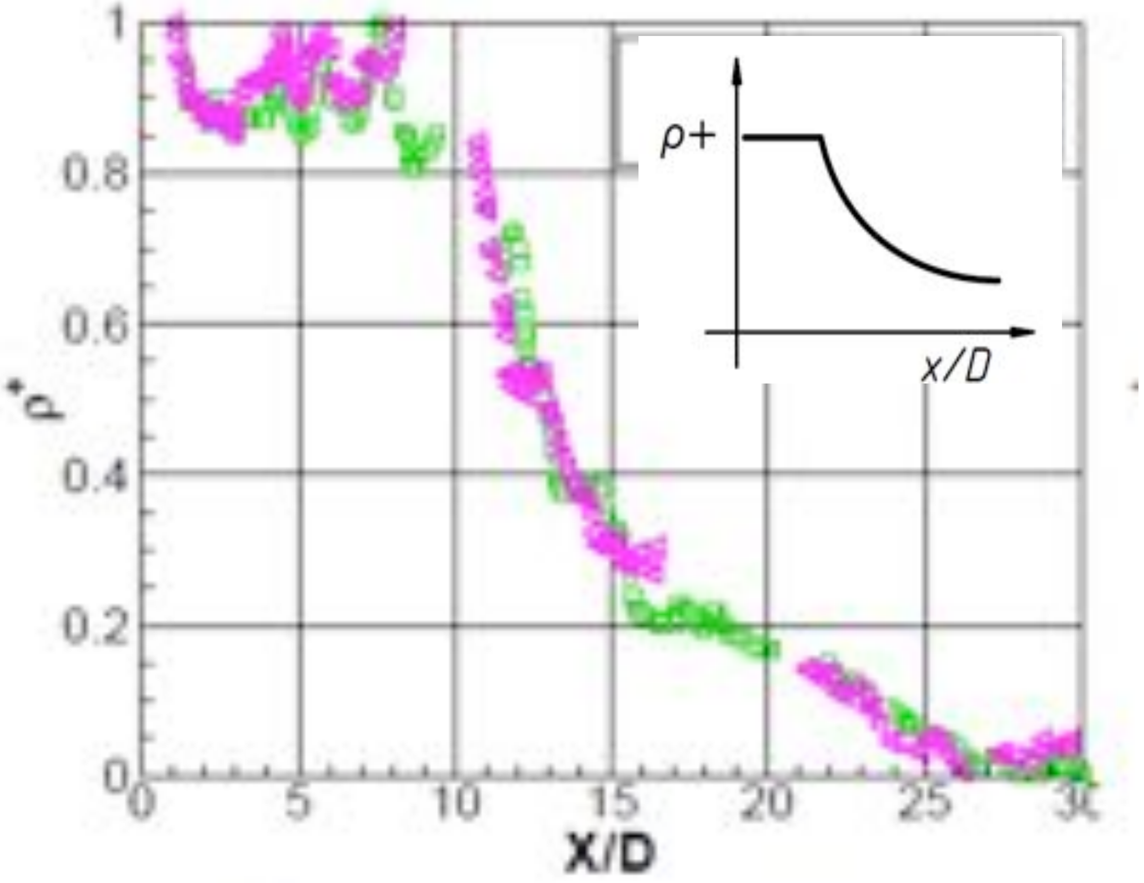


- Transcritical jet is uniquely sensitive to injector heat transfer
- Enhances break-up
- Acts like momentum flux ratio (Banuti and Hannemann AIAA 2014-3571)

Davis & Chehroudi (2004)

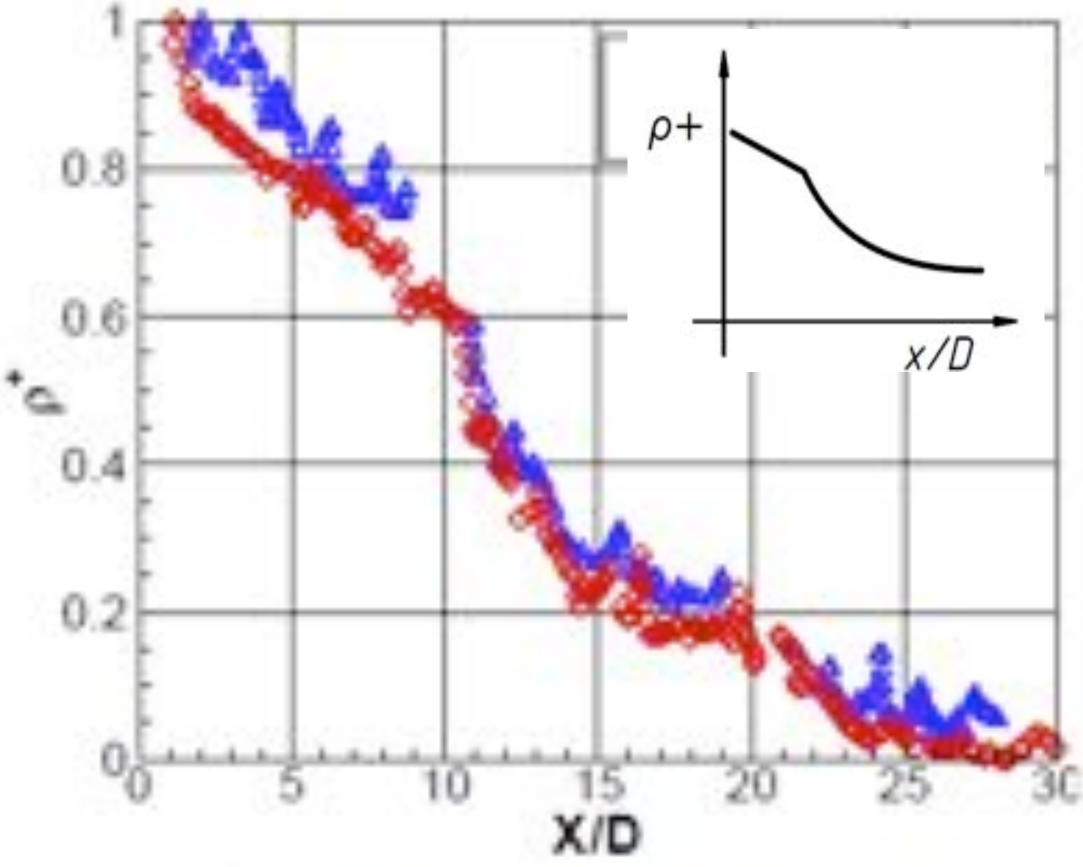
Thermally induced jet disintegration

mechanical

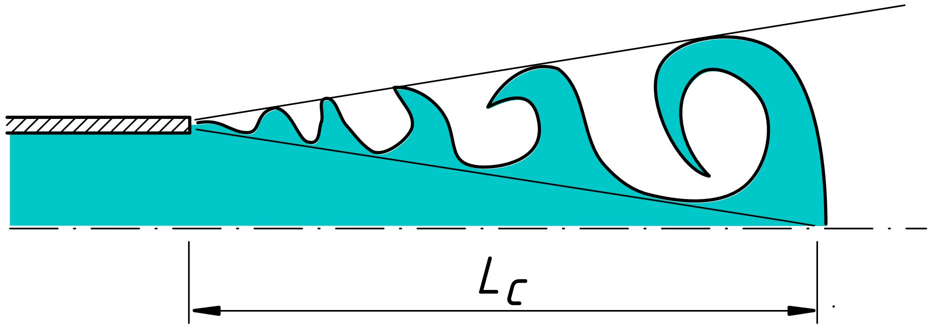


(a) $u = 5$ m/s $T = 120$ K

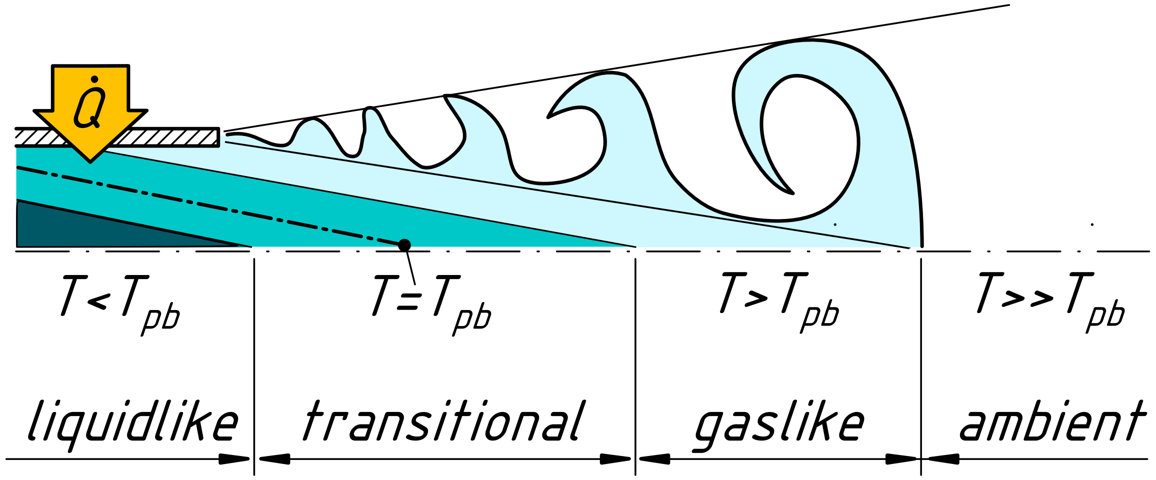
thermal



(b) $u = 5$ m/s $T = 130$ K



Experiments: Branam & Mayer (2003),
Transcritical injection of LN2 into GN2

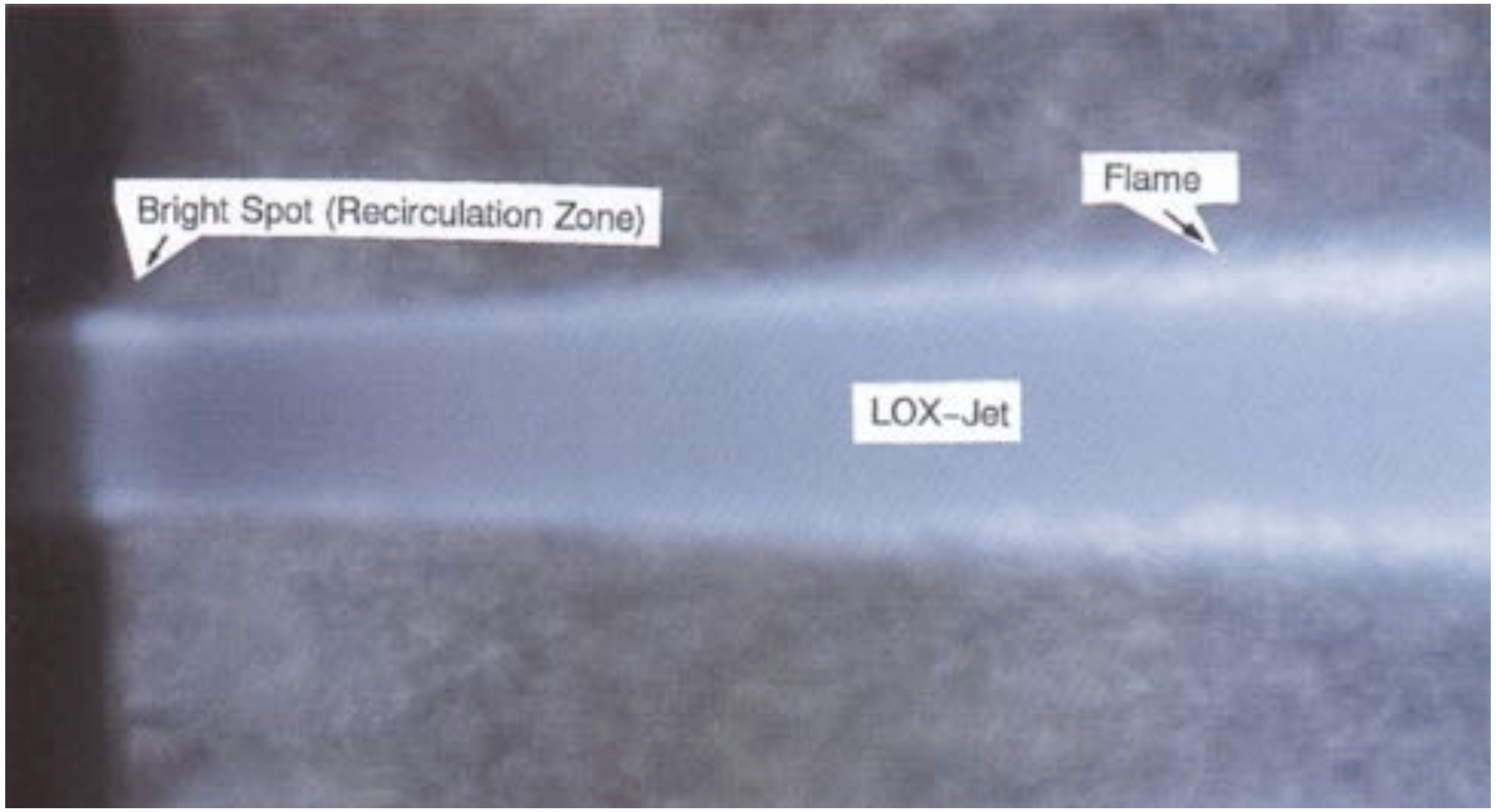


Banuti & Hannemann, PoF (2016)

Combustion

www.dlr.de

Experimental results LOX/GH2 combustion



- Mayer & Tamura (1996), Candel,
- Flame is anchored at LOX post
- Flame separates LOX and GH2 streams
- Practically impossible to quench at rocket conditions (Juniper et al. 2003)

One fluid mixing model

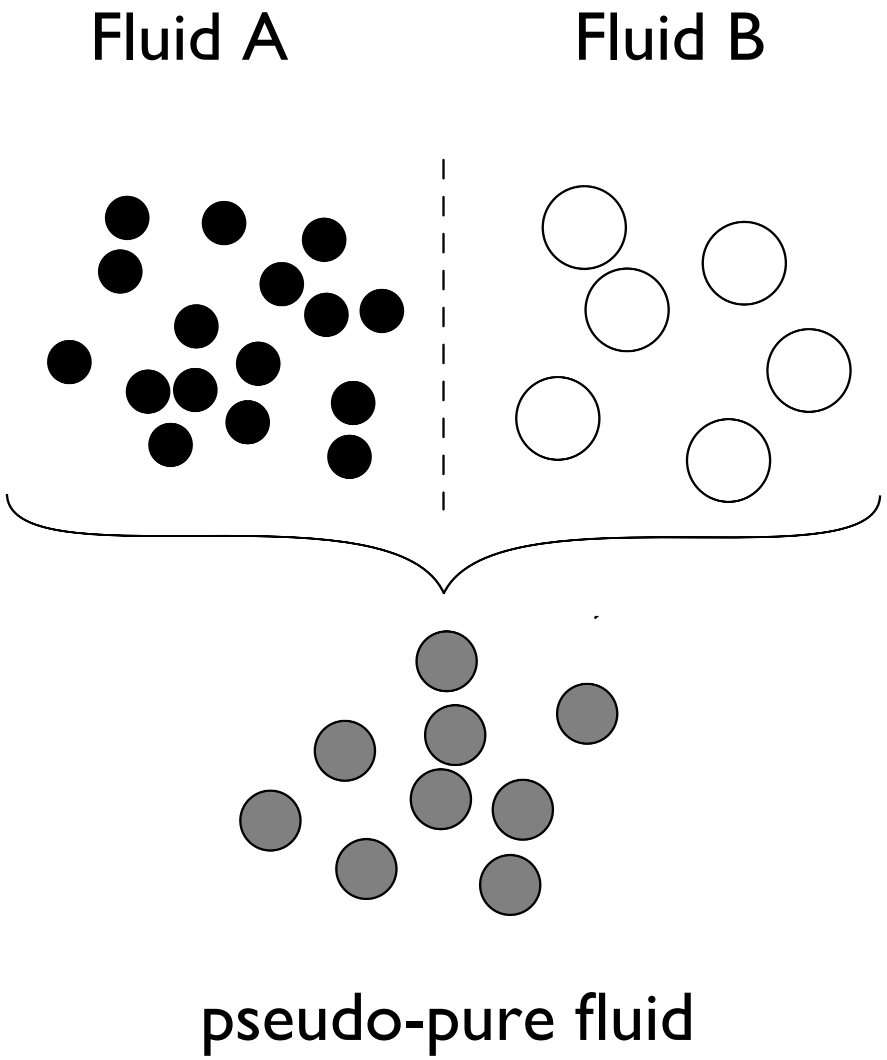
Peng-Robinson equation of state:

$$p = \frac{RT}{v-b} - \frac{a}{v^2+2bv-b^2}$$

$$a = 0.457236\frac{(RT_{\mathrm{cr}})^2}{p_{\mathrm{cr}}}\left[1+m(1-\sqrt{T_{\mathrm{r}}})\right]^2$$

$$m = 0.3746 + 1.54226\omega - 0.26992\omega^2$$

$$b = 0.077796\frac{RT_{\mathrm{cr}}}{p_{\mathrm{cr}}}.$$



Oefelein and Yang (1998)

One fluid mixing model – two approaches

Peng-Robinson equation of state:

$$p = \frac{RT}{v-b} - \frac{a}{v^2 + 2bv - b^2}$$

$$a = 0.457236\frac{(RT_{\mathrm{cr}})^2}{p_{\mathrm{cr}}}\left[1 + m(1-\sqrt{T_{\mathrm{r}}})\right]^2$$

$$m = 0.3746 + 1.54226\omega - 0.26992\omega^2$$

$$b = 0.077796\frac{RT_{\mathrm{cr}}}{p_{\mathrm{cr}}}.$$

Oefelein and Yang (1998)

Mixing rules

van der Waals

$$a = \sum_{i=1}^{N}\sum_{j=1}^{N} y_i y_j \sqrt{a_i a_j}(1-k_{i,j})$$

$$b = \sum_{i=1}^{N} y_i b_i$$

$$\omega = \sum_{i=1}^{N} y_i \omega_i$$

pseudocritical point

$$T_{\mathrm{cr},i,j} = \left(T_{\mathrm{cr},i}\cdot T_{\mathrm{cr},j}\right)^{1/2},$$

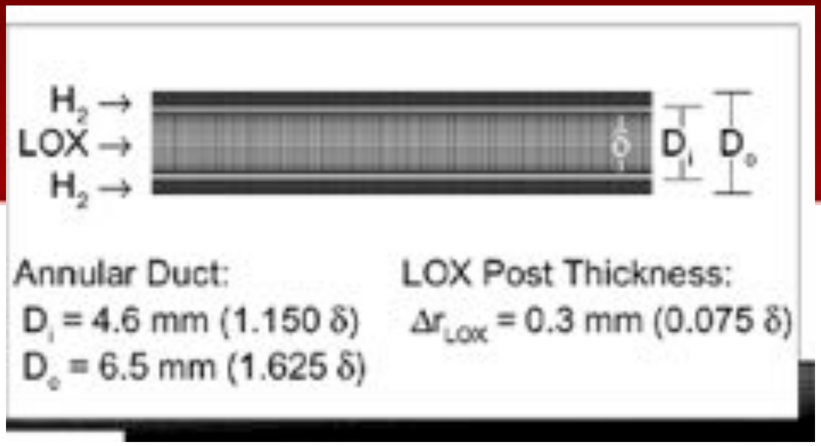
$$v_{\mathrm{cr},i,j} = \left(\frac{1}{2}\left(v_{\mathrm{cr},i}^{1/3} + v_{\mathrm{cr},j}^{1/3}\right)\right)^3,$$

$$Z_{\mathrm{cr},i,j} = \frac{1}{2}\left(Z_{\mathrm{cr},i} + Z_{\mathrm{cr},j}\right),$$

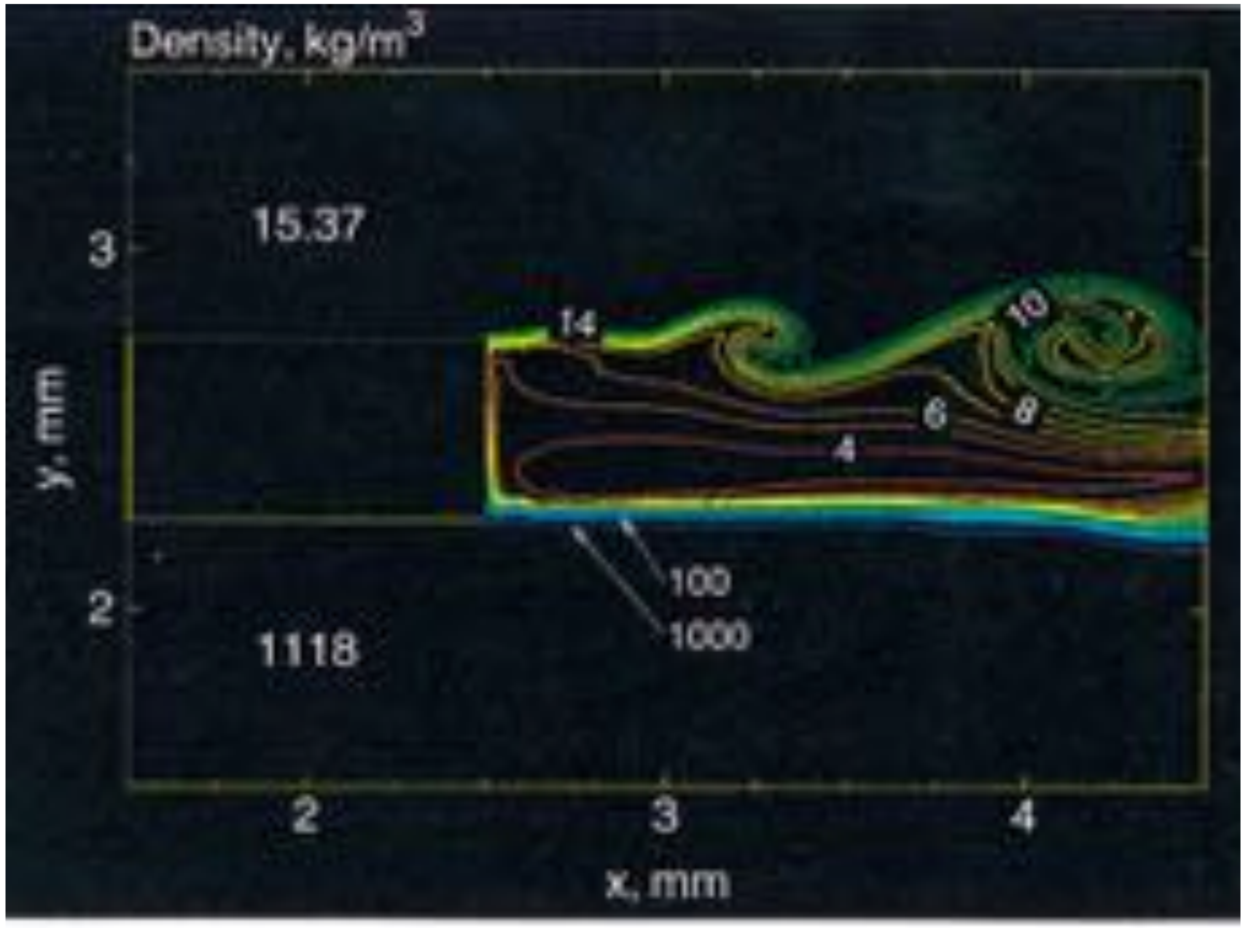
$$p_{\mathrm{cr},i,j} = \frac{Z_{\mathrm{cr},i,j}RT_{\mathrm{cr},i,j}}{v_{\mathrm{cr},i,j}},$$

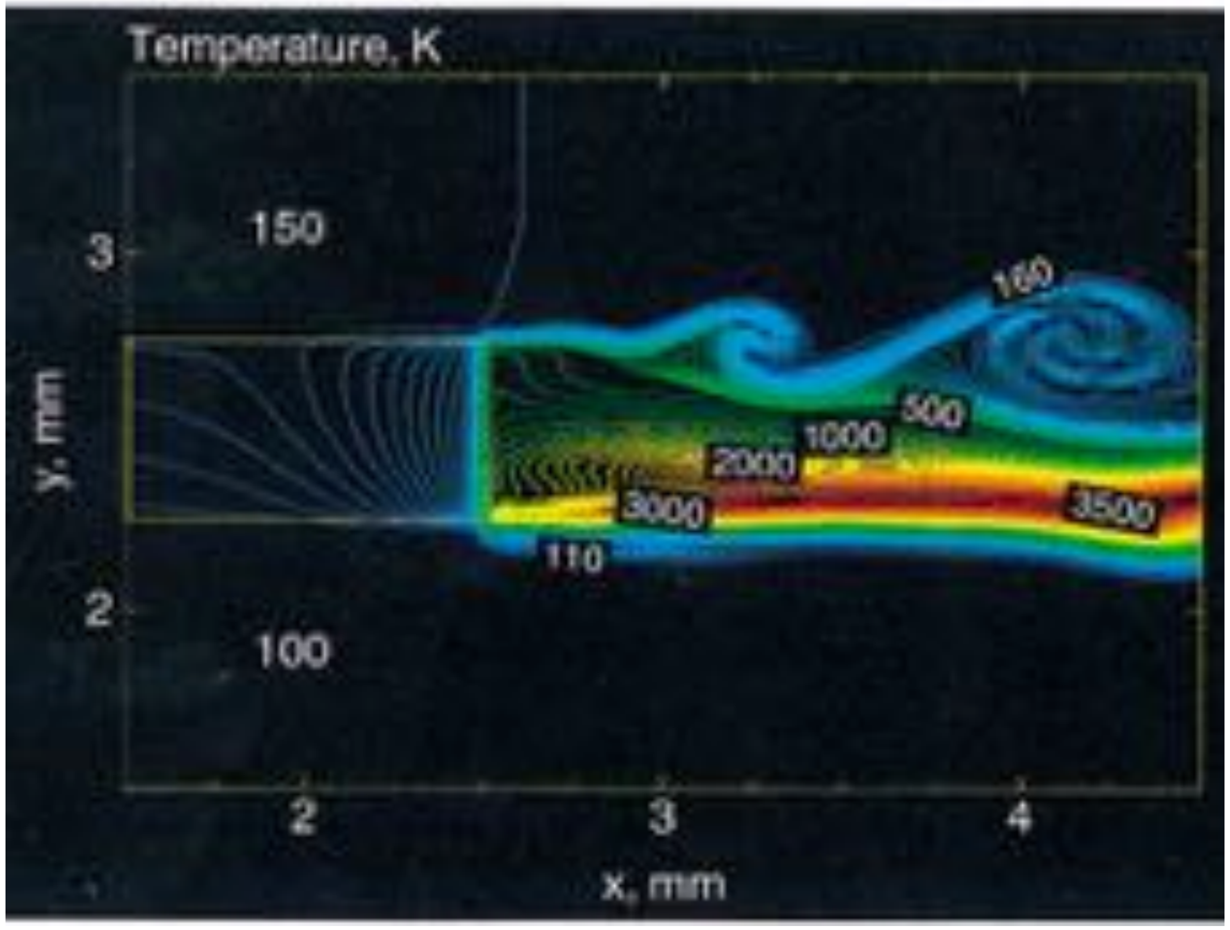
$$\omega_{i,j} = \frac{1}{2}\left(\omega_i + \omega_j\right).$$

Large eddy simulation



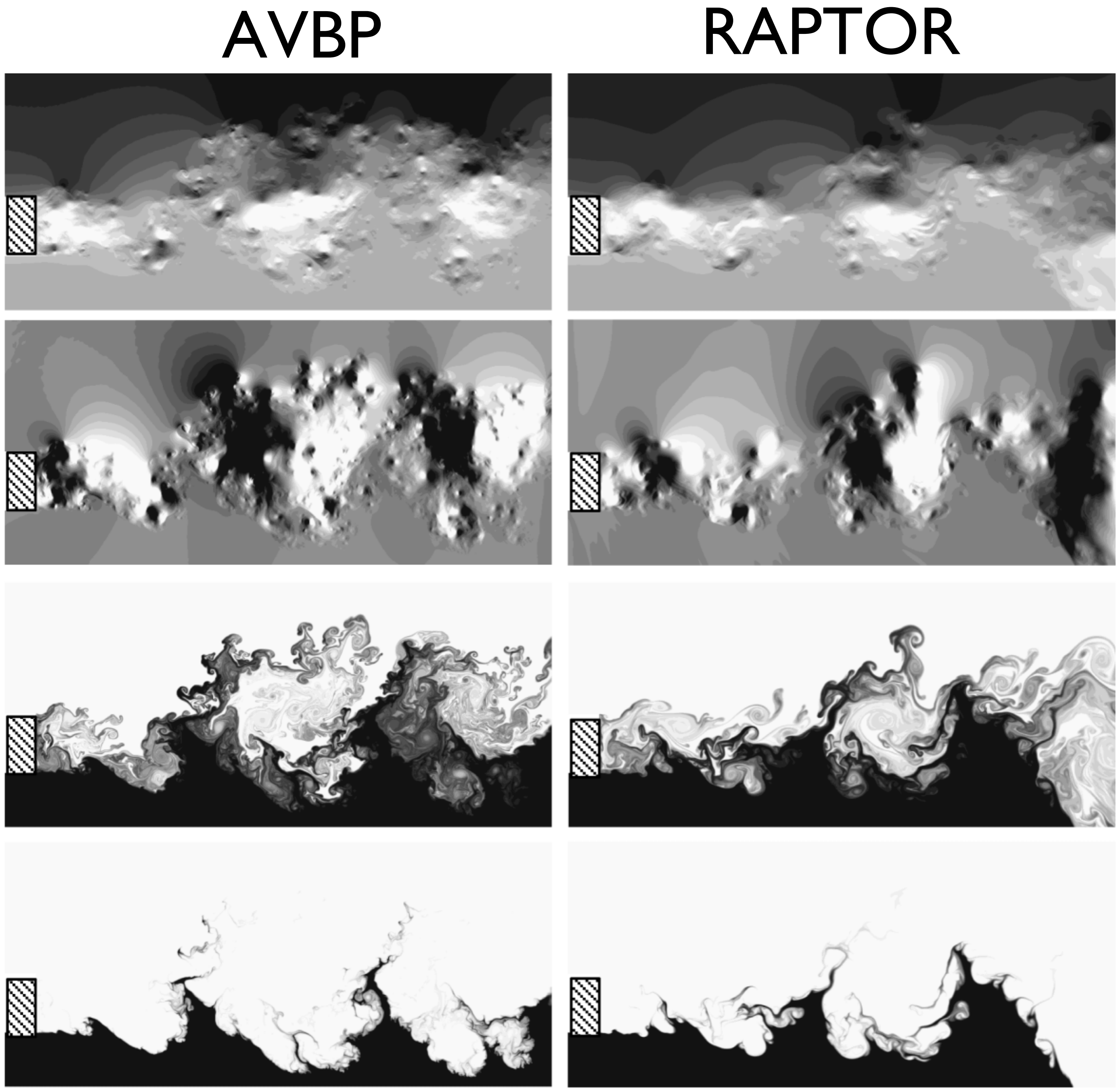
- Transcritical injection (Oefelein & Yang 1998)
- $p = 100$ bar, $T_{LOX} = 100$ K, $T_{H2} = 150$ K



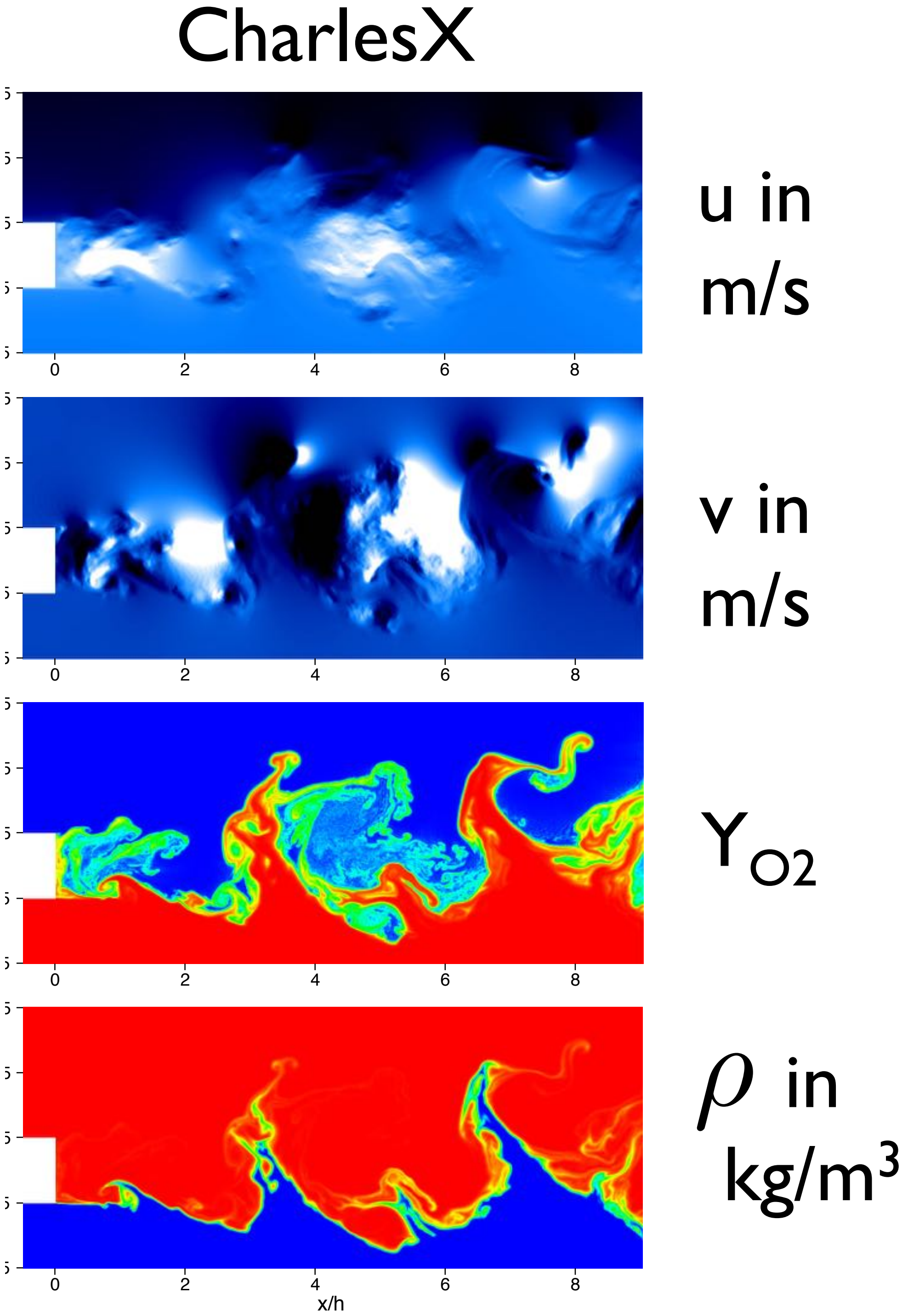


- Flame is anchored at LOX post; wall heat transfer taken into account
- Steep transition with density ratio >250 across few cells

LOX/GH2 as numerical benchmark case



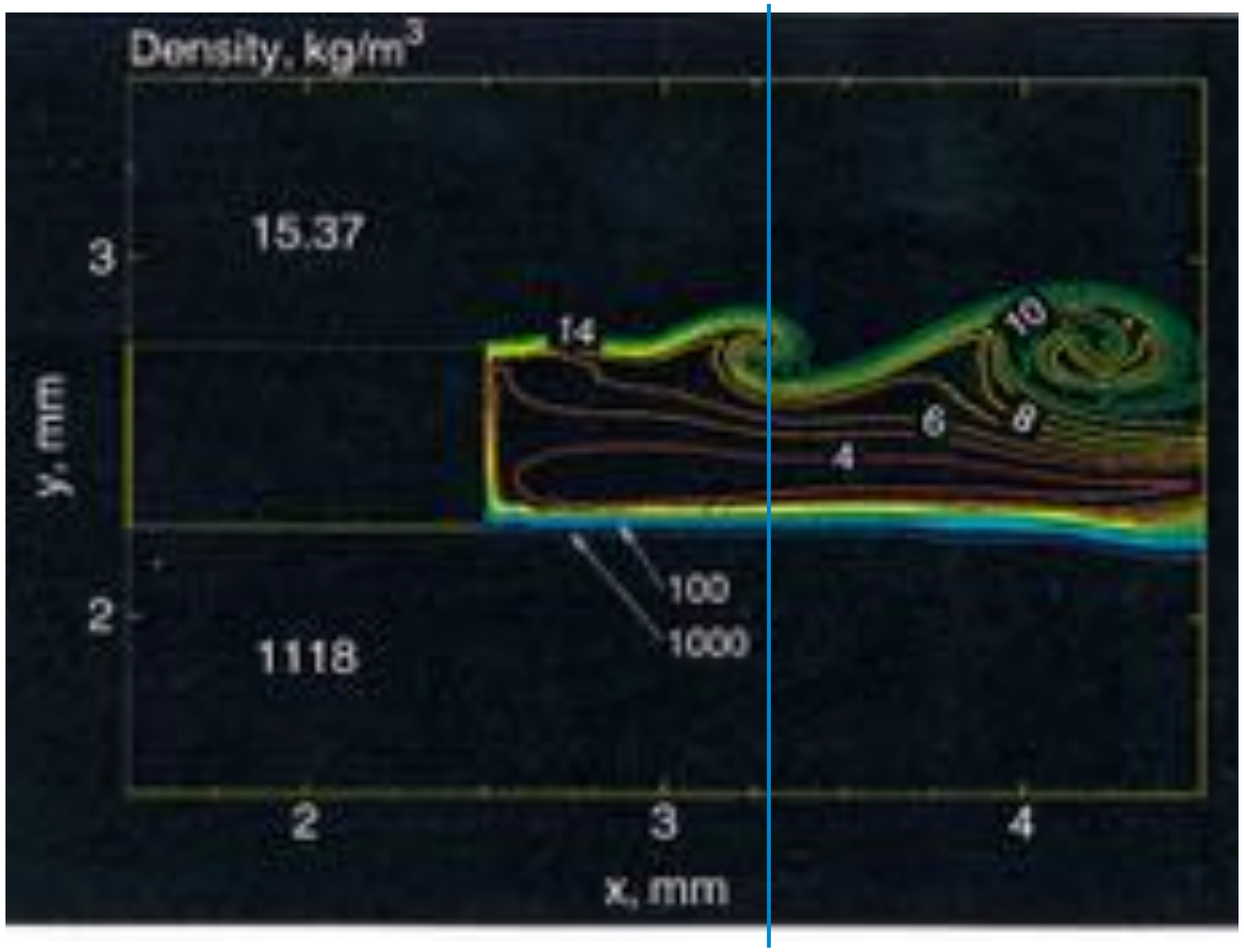
Ruiz et al. (2016)

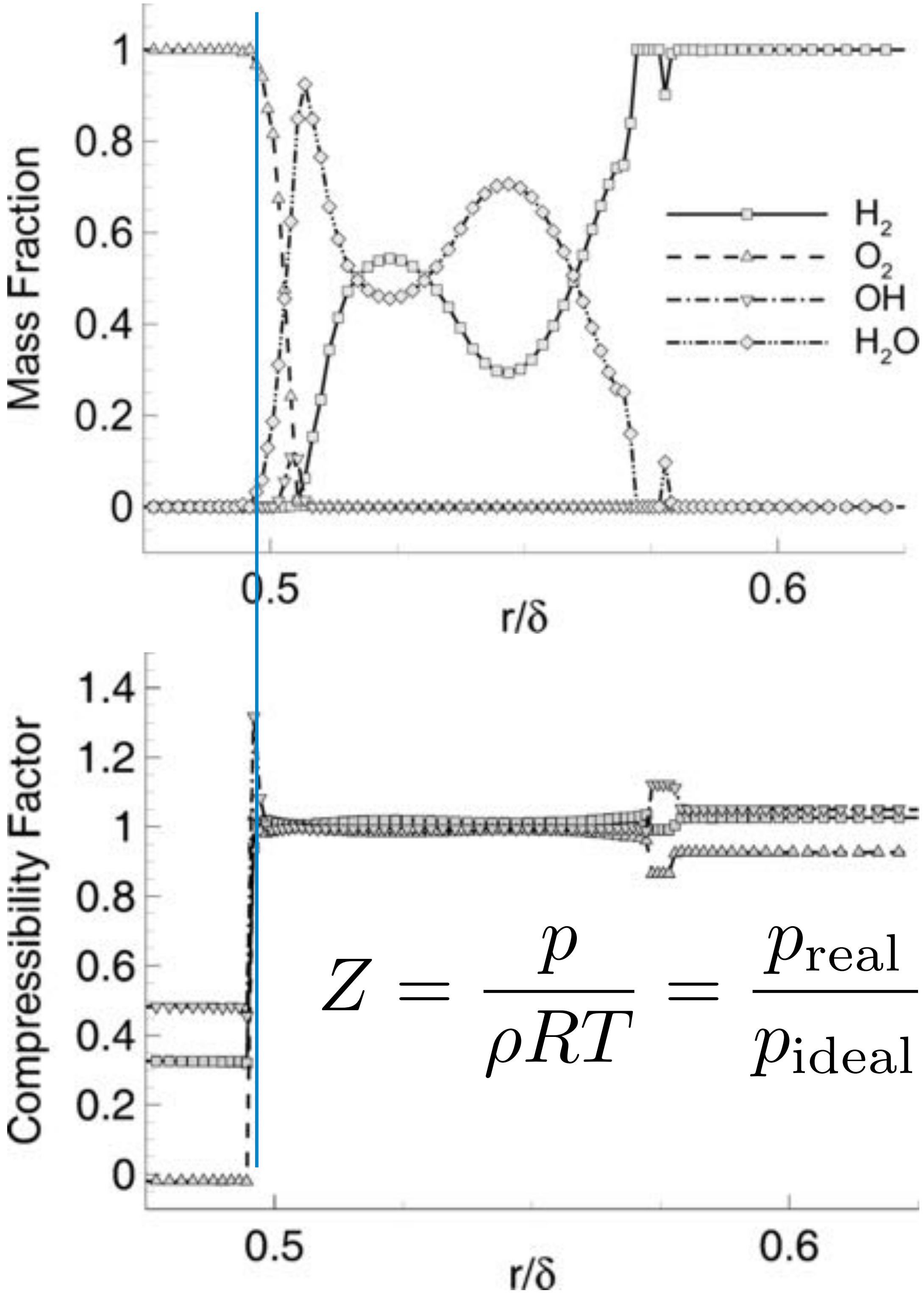


Courtesy of Peter C. Ma

Large eddy simulation

- Transcritical injection (Oefelein & Yang 1998, Oefelein 2006)
- p = 100 bar, T_{LOX} = 100 K, T_{H2} = 150 K

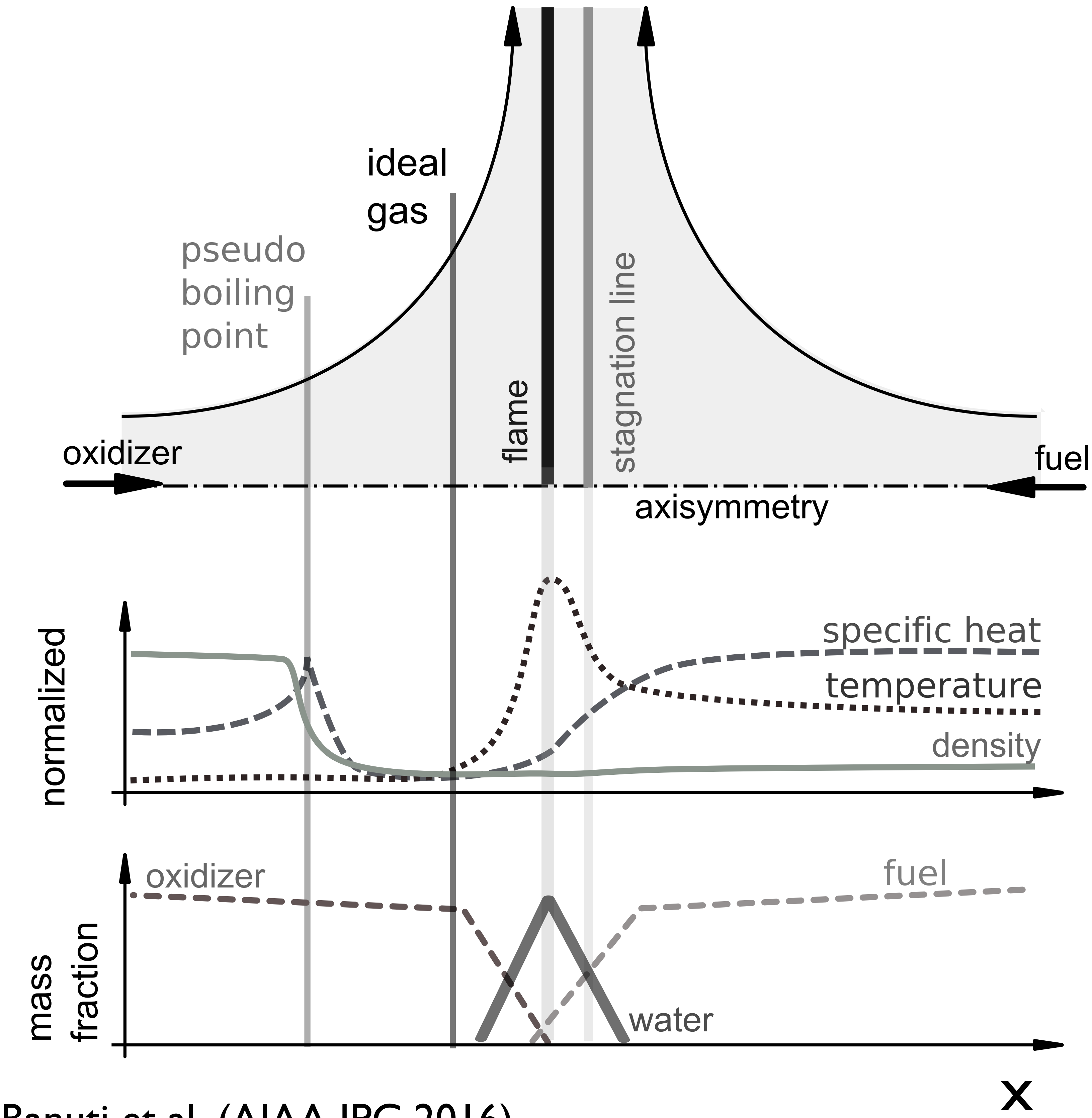




$$Z = \frac{p}{\rho R T} = \frac{p_{\text{real}}}{p_{\text{ideal}}}$$

- Transition to ideal gas occurs before mixing
- Mixing process is ideal
- Real fluid phenomena found in O2 only

Structure of transcritical diffusion flames



Banuti et al. (AIAA JPC 2016)

- Two thermodynamic transitions
  - Pseudoboiling
  - Ideal gas
- Mixing occurs in ideal gas only
- Real fluid behavior is essentially confined to pure oxygen
- **Understanding of pure fluid behavior needed!**

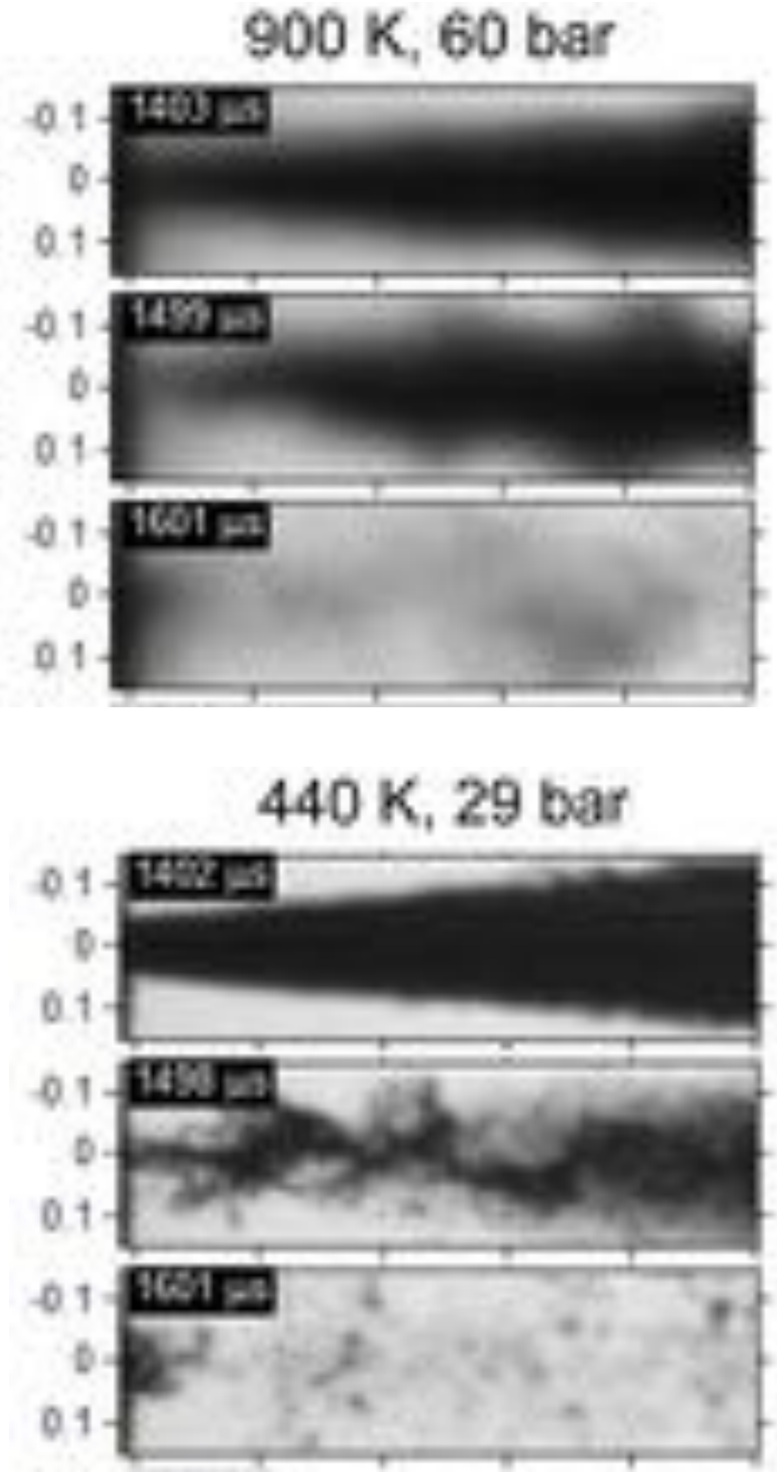
Assumptions and limits

State-of-the-art mixing rules adhere to single fluid formalism

- Assumptions (Ely & Hanley 1981/83)
  - Mixing rules are valid
  - Single phase
  - Similar fluids
  - No polar substances

- Works very well for intended purpose (LOX/GH2 combustion)

- What about
  - Mixing?
  - Lifted off flames (hydrocarbons)?
  - Residual surface tension?



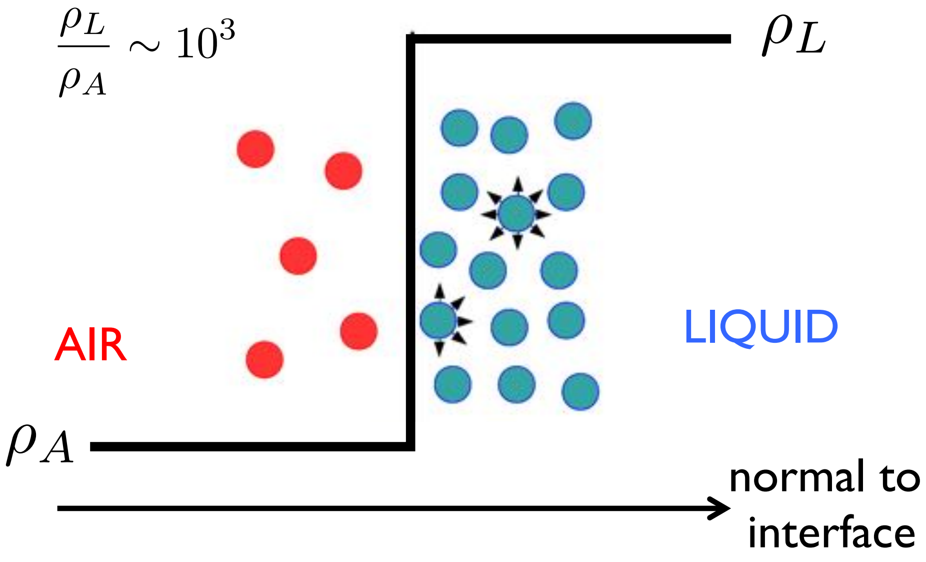
Dahms et al. 2013, Manin et al. 2014

IV. Transcritical Atomization

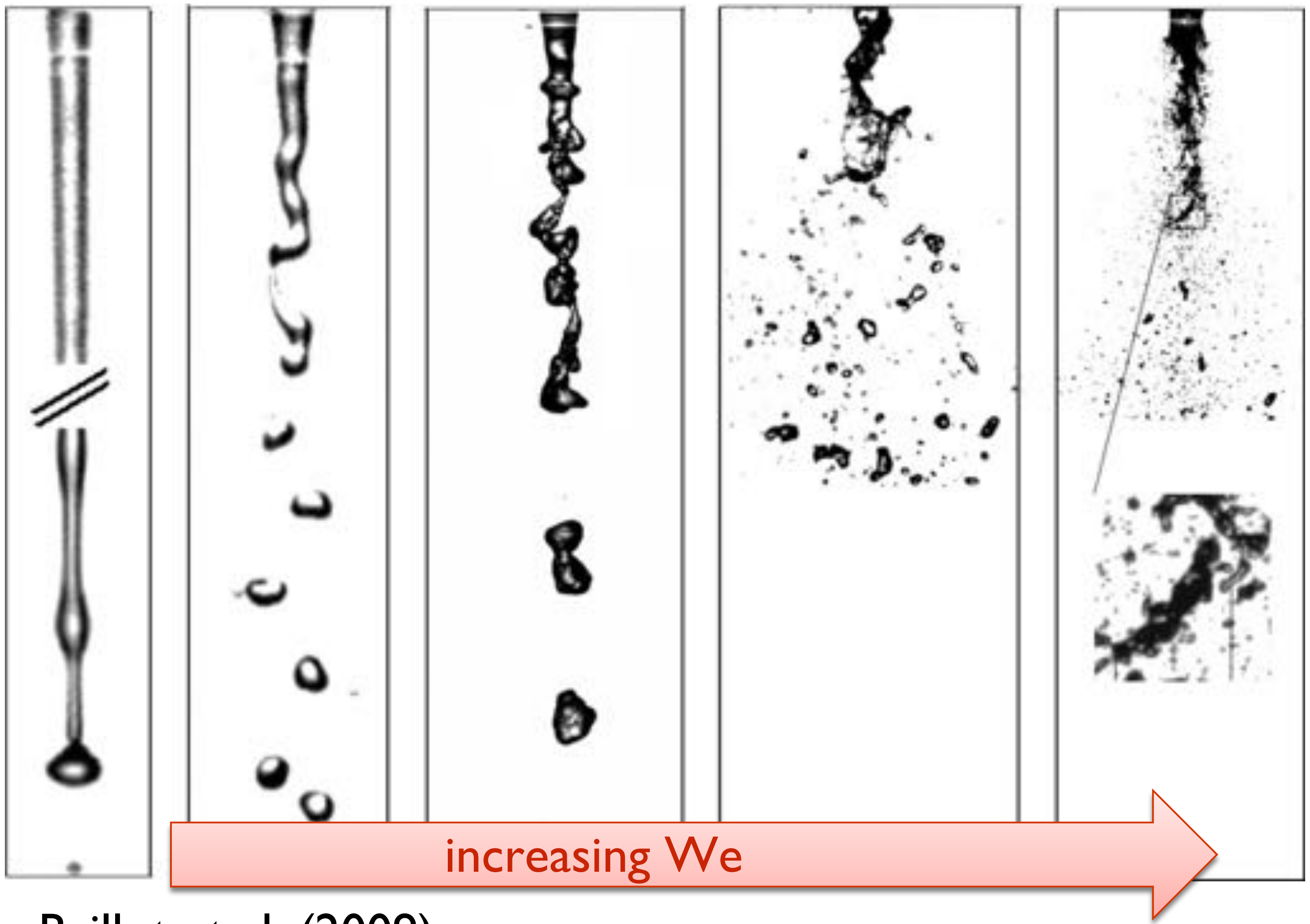
Classic atomization description at low pressures

Weber no. $\mathrm{We} = \dfrac{\rho U^2 D}{\sigma}$

ratio of aerodynamic stress
to surface tension stress



→ Sharp interface
(~single-molecule thick)



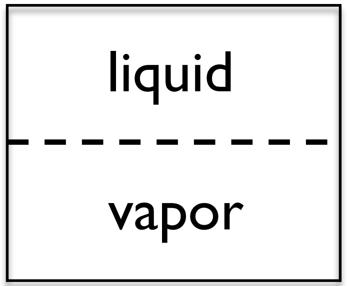
Baillot et al. (2009)

Computational techniques:

1. VoF: Hirt & Nichols (1981), Jofre et al. (2014), Ivey & Moin (2015)
2. Level-Set: Osher & Sethian (1988), Desjardins et al. (2008), Herrmann et al. (2008)
3. Front-Tracking: Unverdi, Tryggvason et al. (1992, 2001)

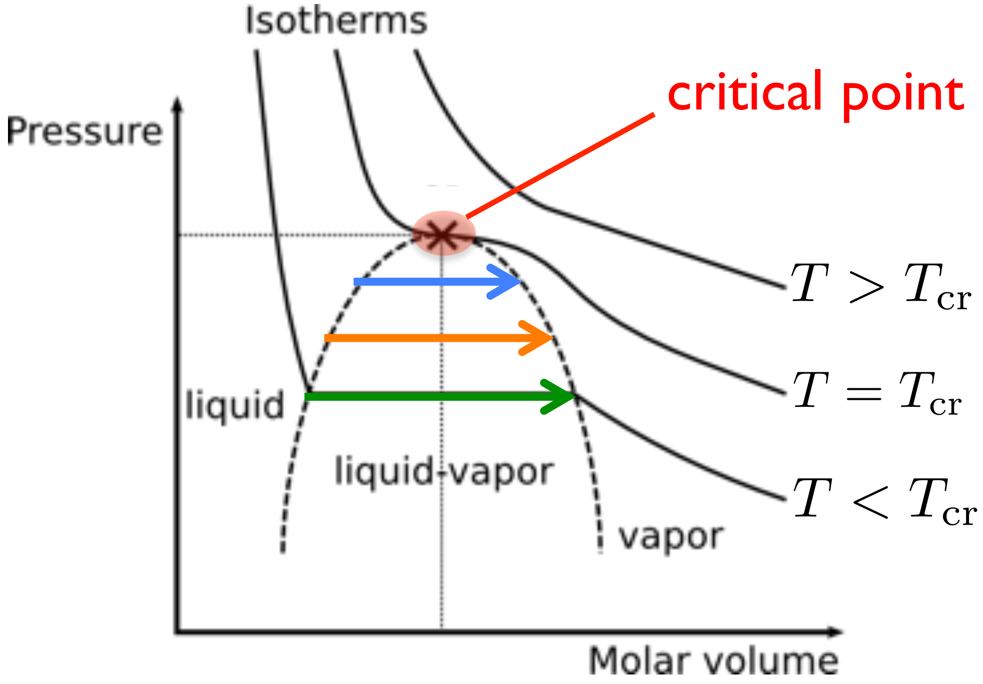
Interface broadening at high pressures

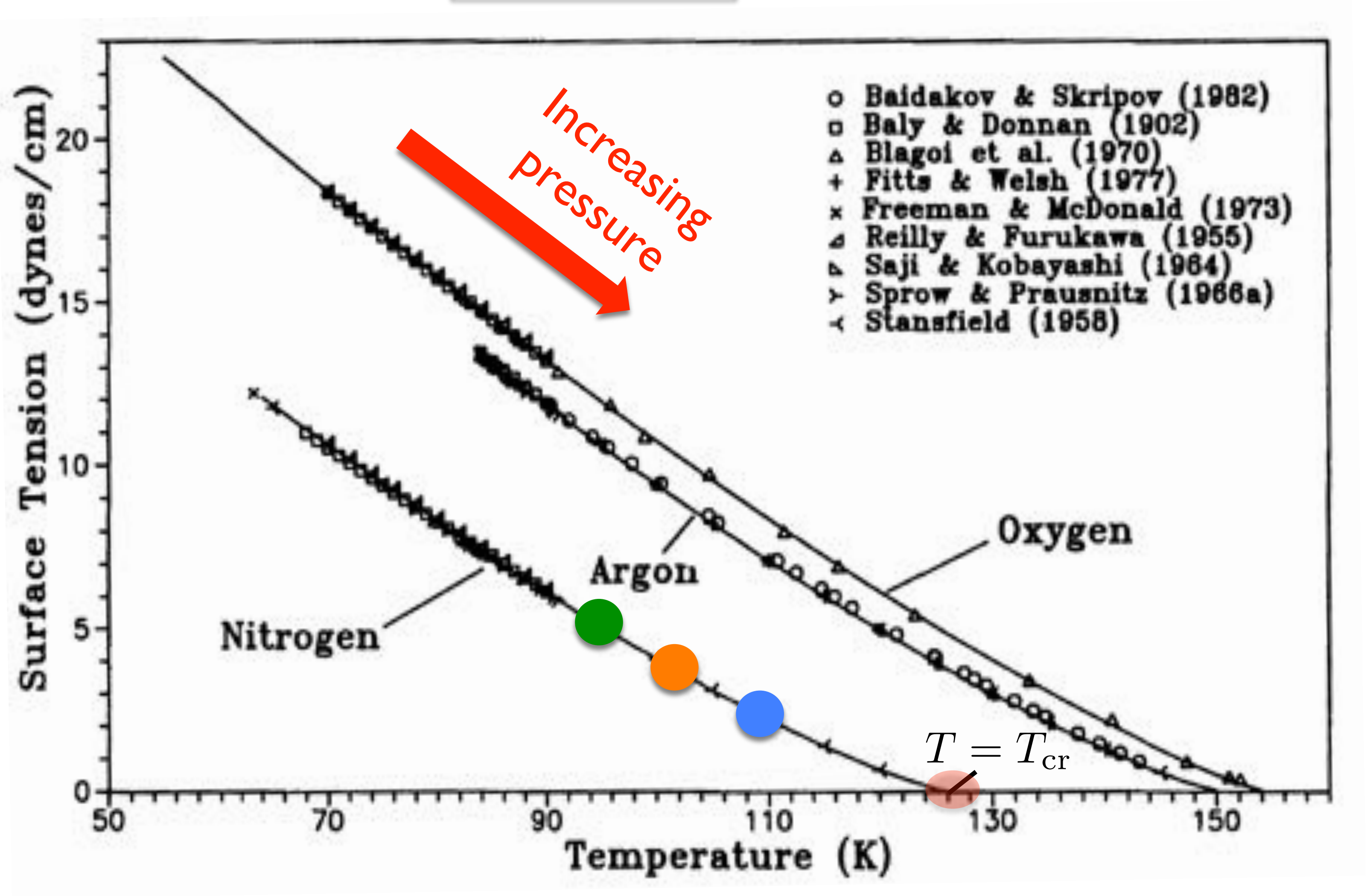
Single-component equilibrium systems



closed chamber

$P = P(T)$
in phase equilibrium



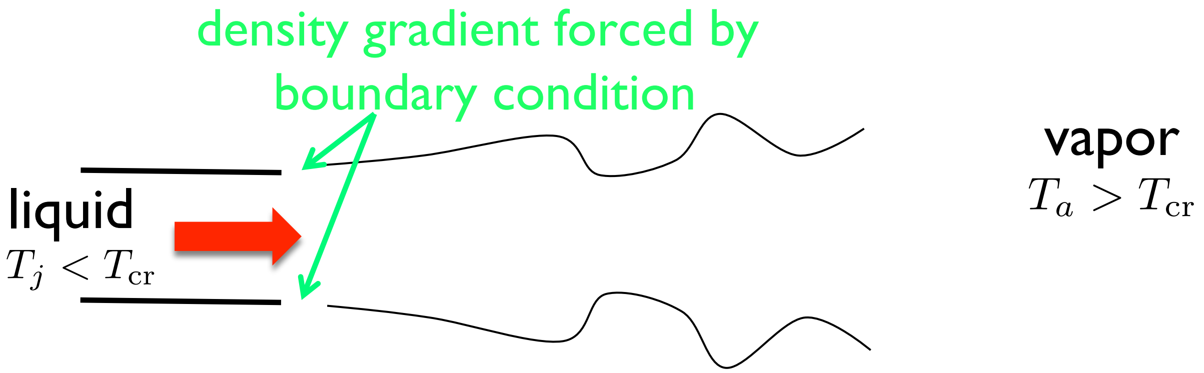


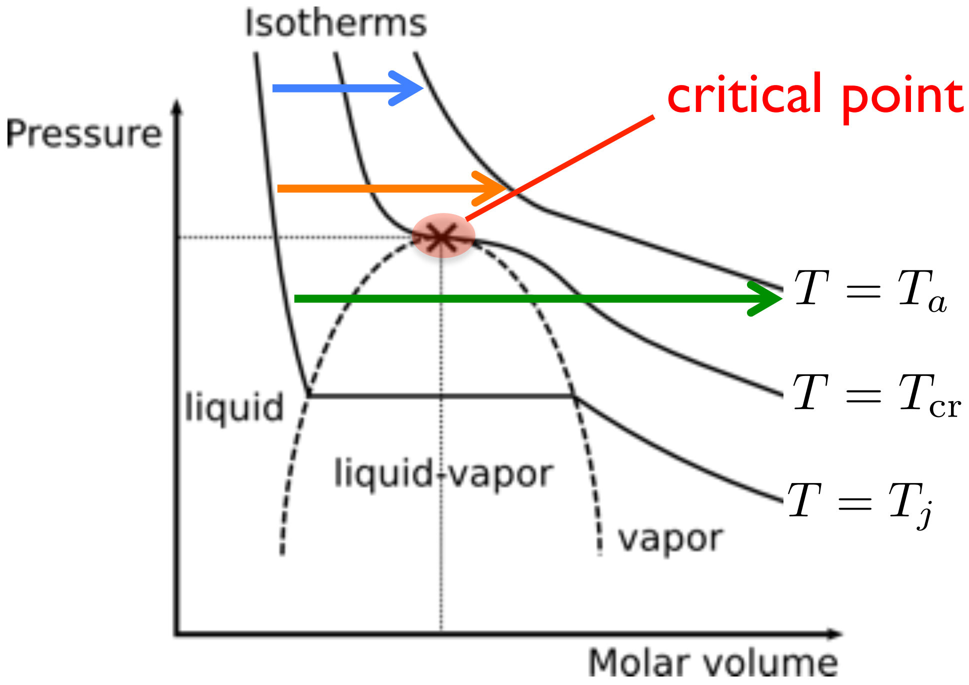
Lemmon & Penoncello (1994)

Surface tension vanishes and interface disappears above the critical point

Interface broadening at high pressures

Single-component evolution systems



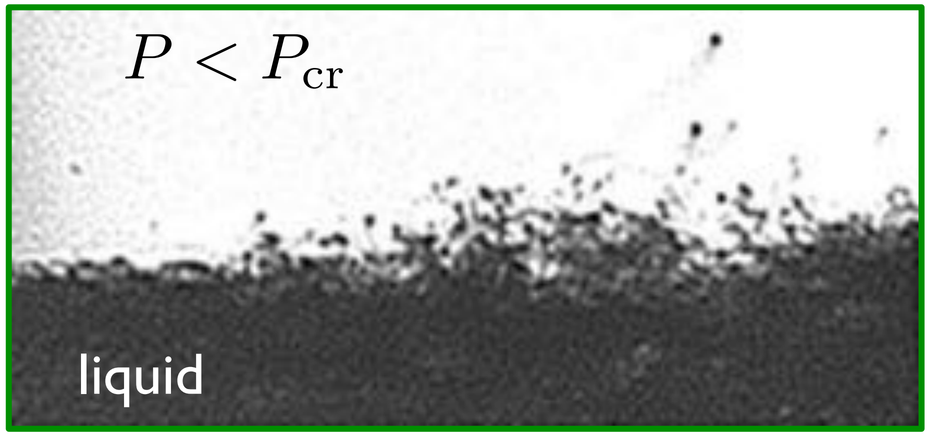


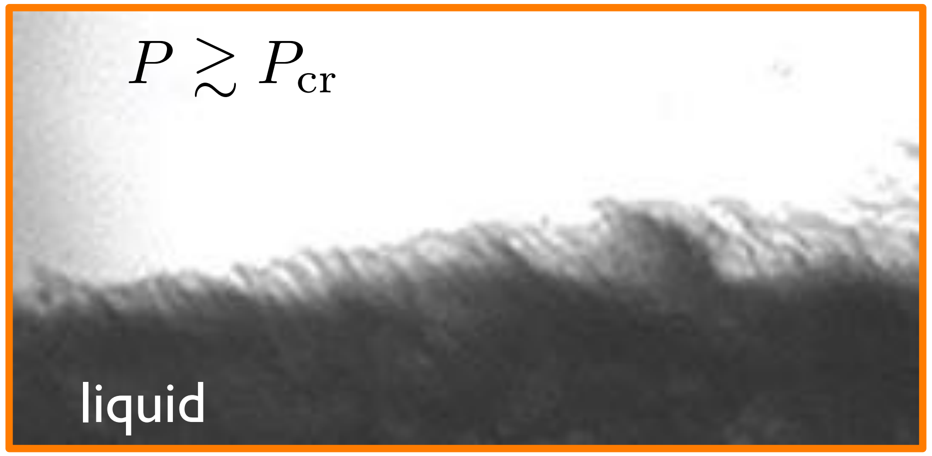
There is a transition from jet breakup to diffusive mixing as pressure increases above the critical value

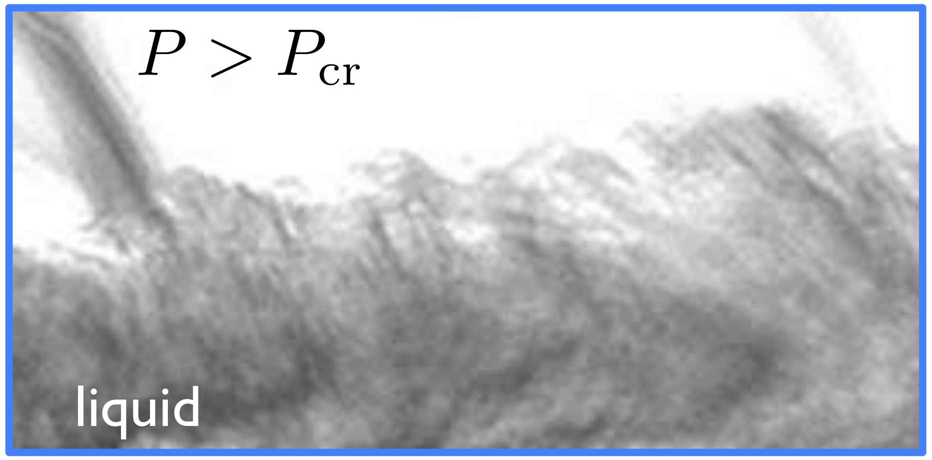
In general, surface tension does not necessarily vanish instantaneously → transient surface tension

LN$_2$ jet into GN$_2$ ambient:

$P_{\mathrm{cr}} = 34\mathrm{bar}$
$T_{\mathrm{cr}} = 126\mathrm{K}$







Cheroudi (2012)

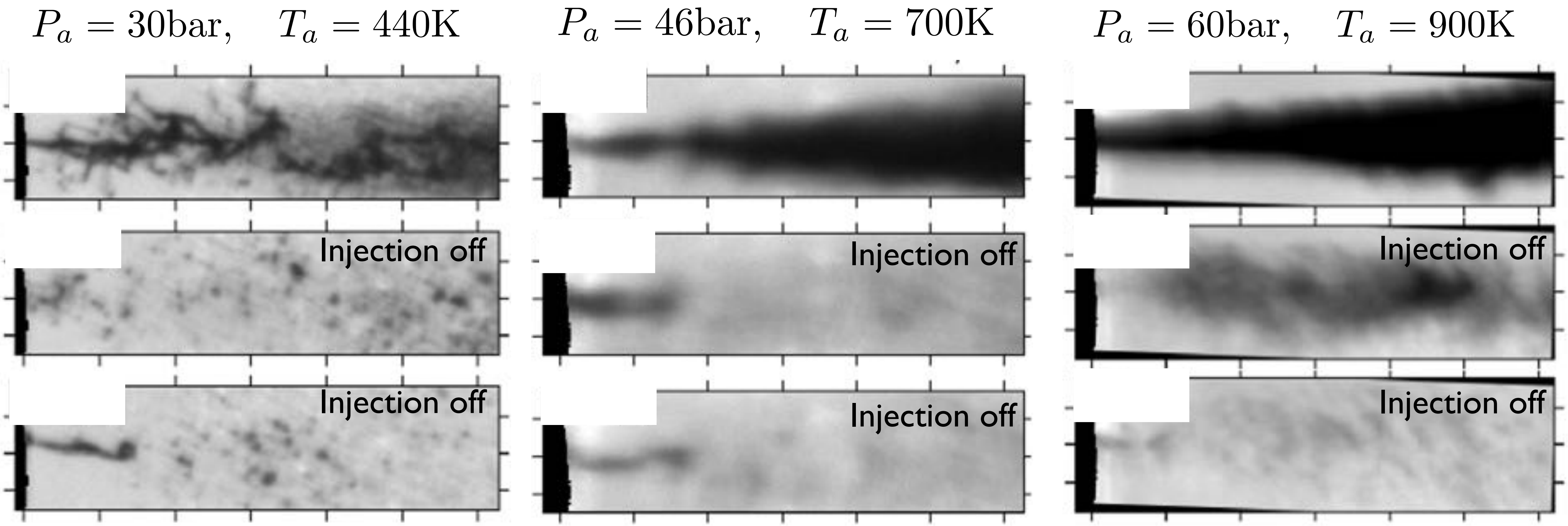
High-pressure injection of hydrocarbon fuels

n-Dodecane spray into GN_2 ambient

Manin et al. (2014)

n-Dodecane: $P_{\rm cr} = 18\rm bar \quad T_{\rm cr} = 658K$

GN_2: $P_{\rm cr} = 34\rm bar \quad T_{\rm cr} = 126K$



$\downarrow P_a \quad \downarrow T_a$

Ligaments and droplets: surface tension

$\uparrow P_a \quad \uparrow T_a$

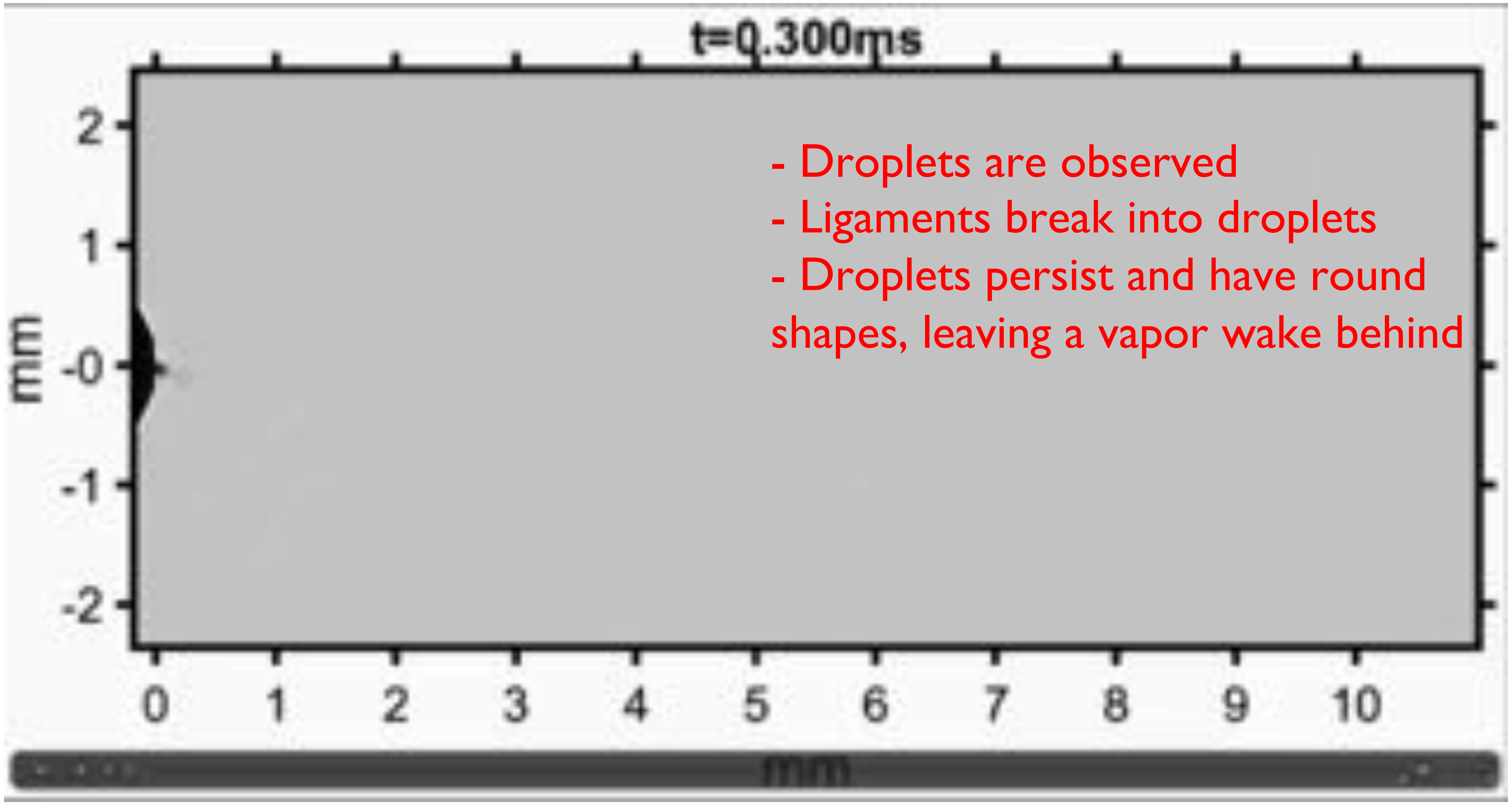
Blurred interfaces: diffusive mixing

High–pressure injection of hydrocarbon fuels

Atomization and classical evaporation:

n-Hexadecane: P_{cr} = 14 bar, T_{cr} = 722 K

n-Hexadecane into O_2 at 900 K, 79 bar



- Droplets are observed
- Ligaments break into droplets
- Droplets persist and have round shapes, leaving a vapor wake behind

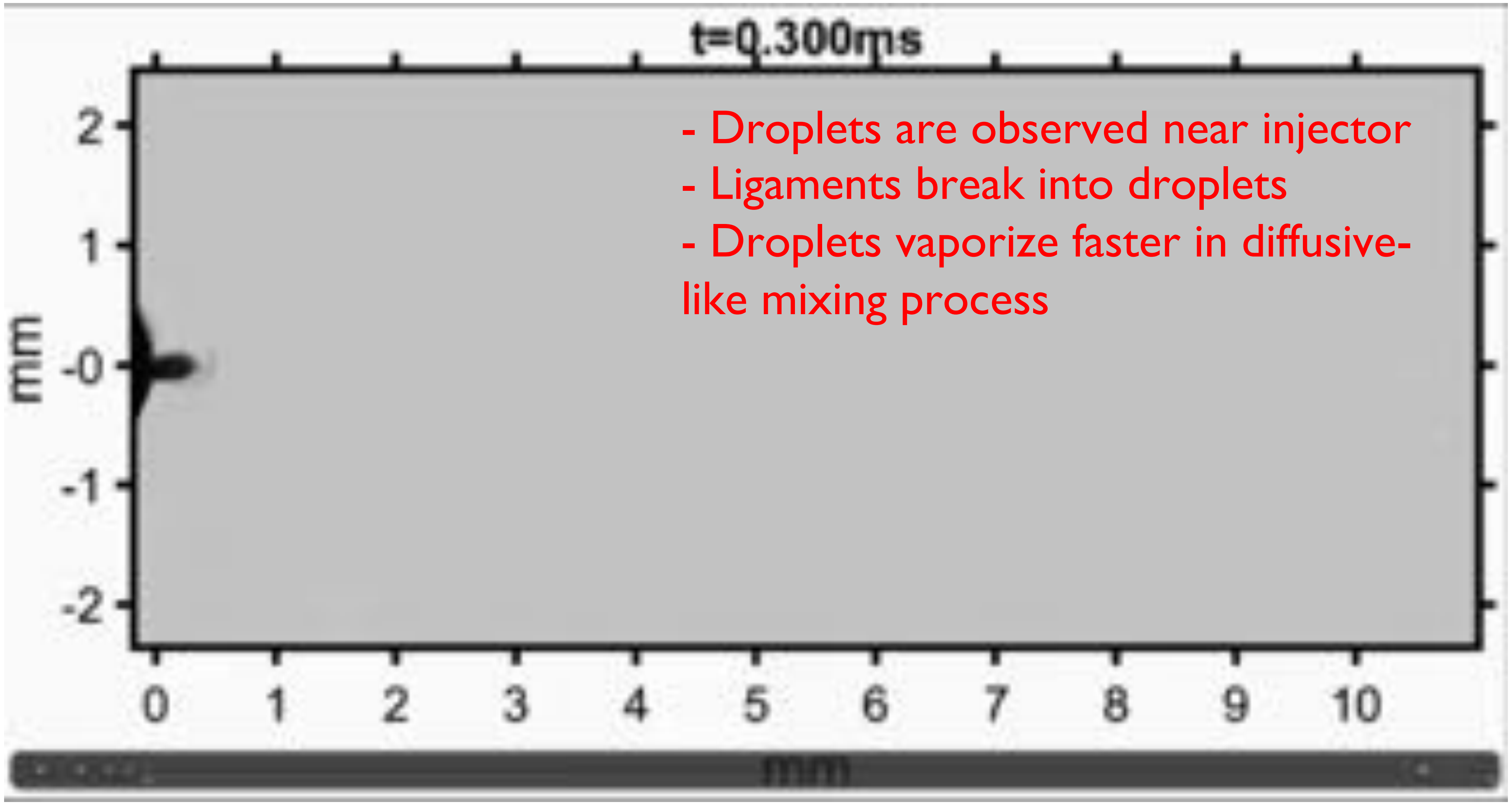
Crua et al. (2015)

High–pressure injection of hydrocarbon fuels

Atomization and miscible mixing:

n-Hexadecane: P_{cr} = 14 bar, T_{cr} = 722 K

n-Hexadecane into O_2 at 1200 K, 107 bar



- Droplets are observed near injector
- Ligaments break into droplets
- Droplets vaporize faster in diffusive-like mixing process

Crua et al. (2015)

The critical locus of a binary mixture

Vapor-liquid equilibrium:

Mechanical: $P_V = P_L$

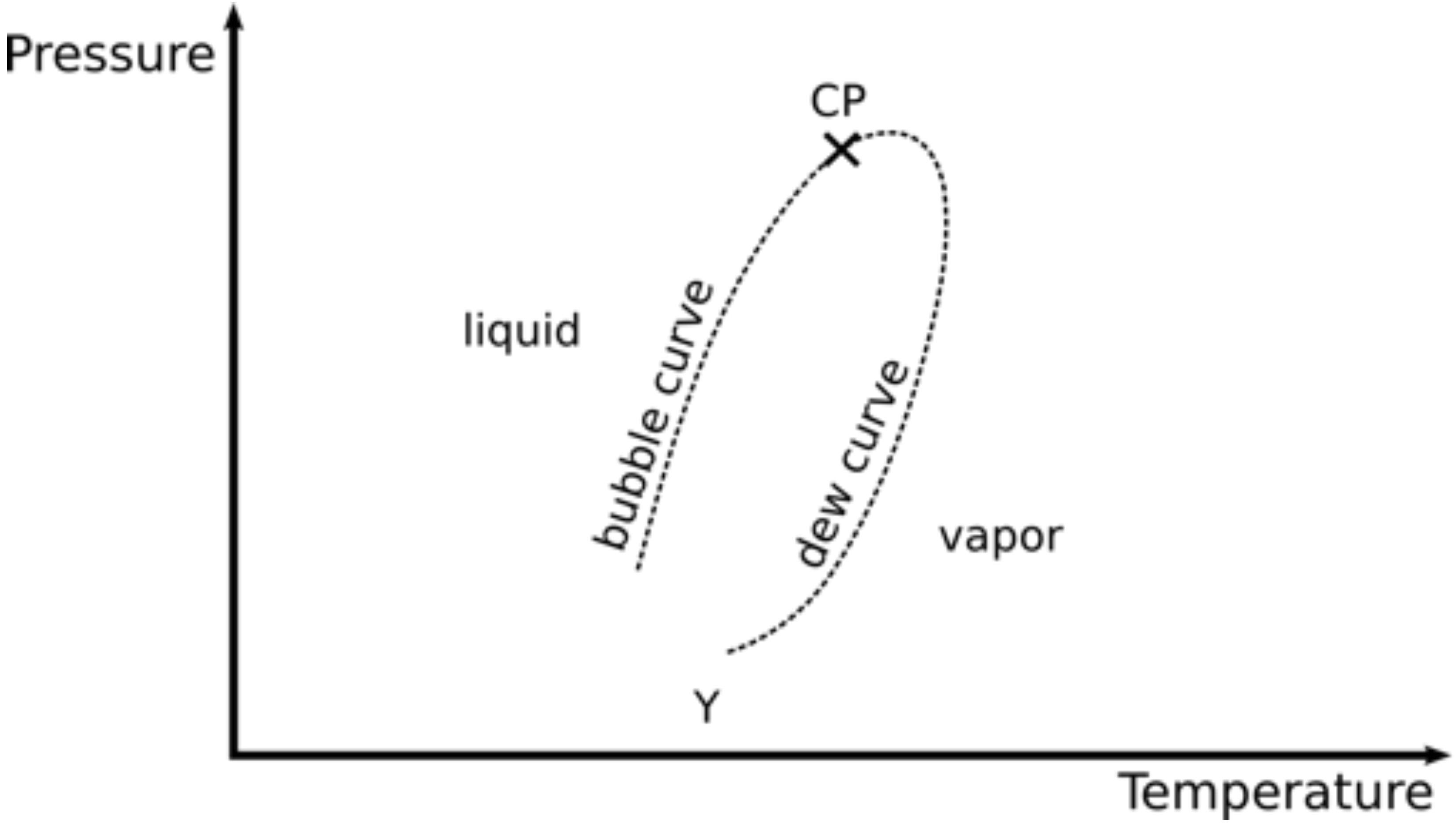
Thermal: $T_V = T_L$

Chemical: $\mu_{V\,i} = \mu_{L\,i}$

Critical point: $\rho_V = \rho_L$

$$\left(\frac{\partial \mu}{\partial Y}\right)_{P_{cr},T_{cr}} = \left(\frac{\partial^2 \mu}{\partial Y^2}\right)_{P_{cr},T_{cr}} = 0$$

PT diagram: one mixture composition



The critical locus of a binary mixture

Vapor-liquid equilibrium:

Mechanical: $P_V = P_L$

Thermal: $T_V = T_L$

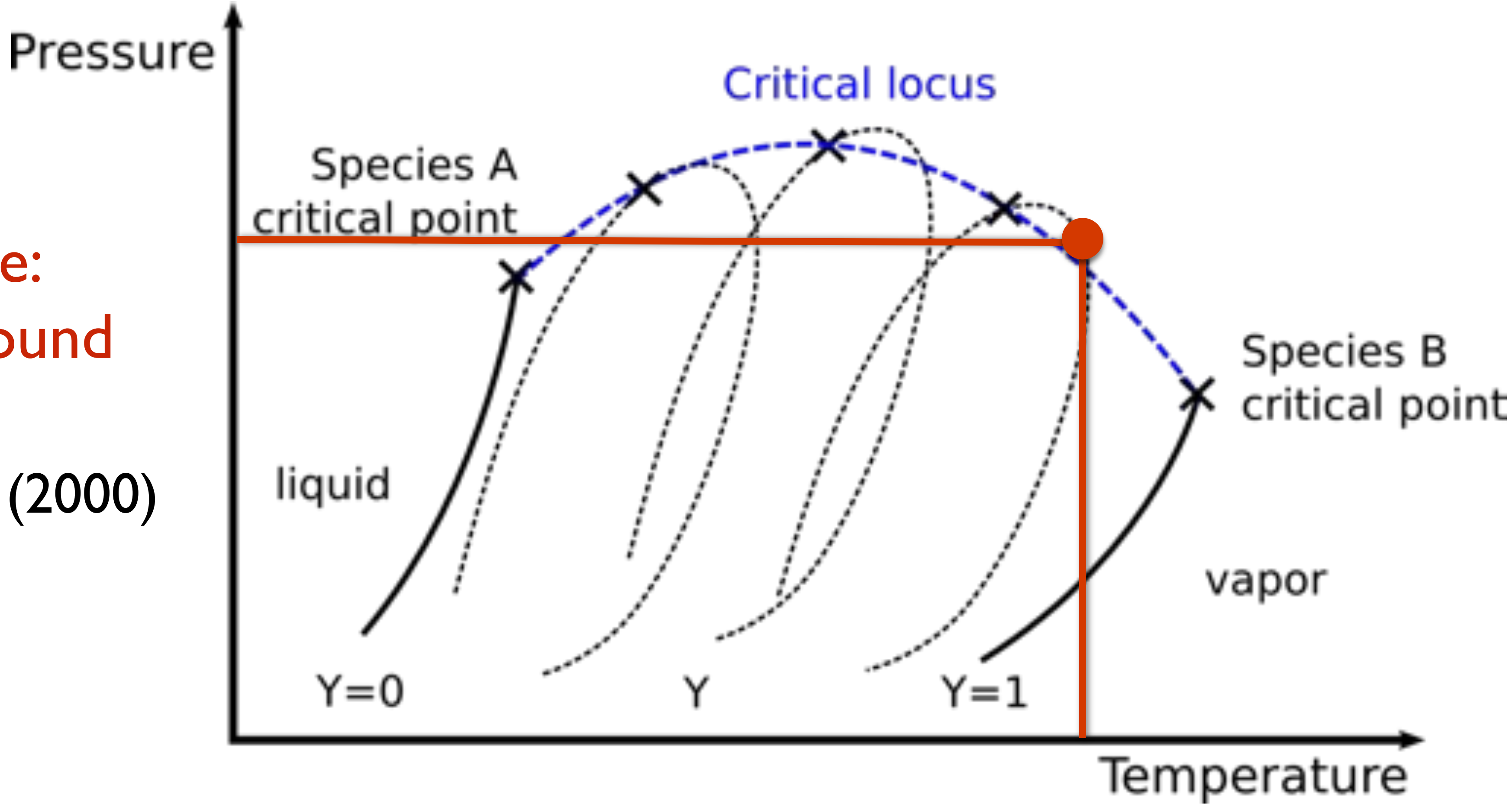
Chemical: ${\mu_V}_i = {\mu_L}_i$

Critical locus: $\rho_V = \rho_L$ for $Y \in [0,1]$

$$\left(\frac{\partial \mu}{\partial Y}\right)_{P_{cr},T_{cr}} = \left(\frac{\partial^2 \mu}{\partial Y^2}\right)_{P_{cr},T_{cr}} = 0$$

PT diagram: all mixture compositions

Critical mixing temperature: two-phase region upper bound for a given pressure

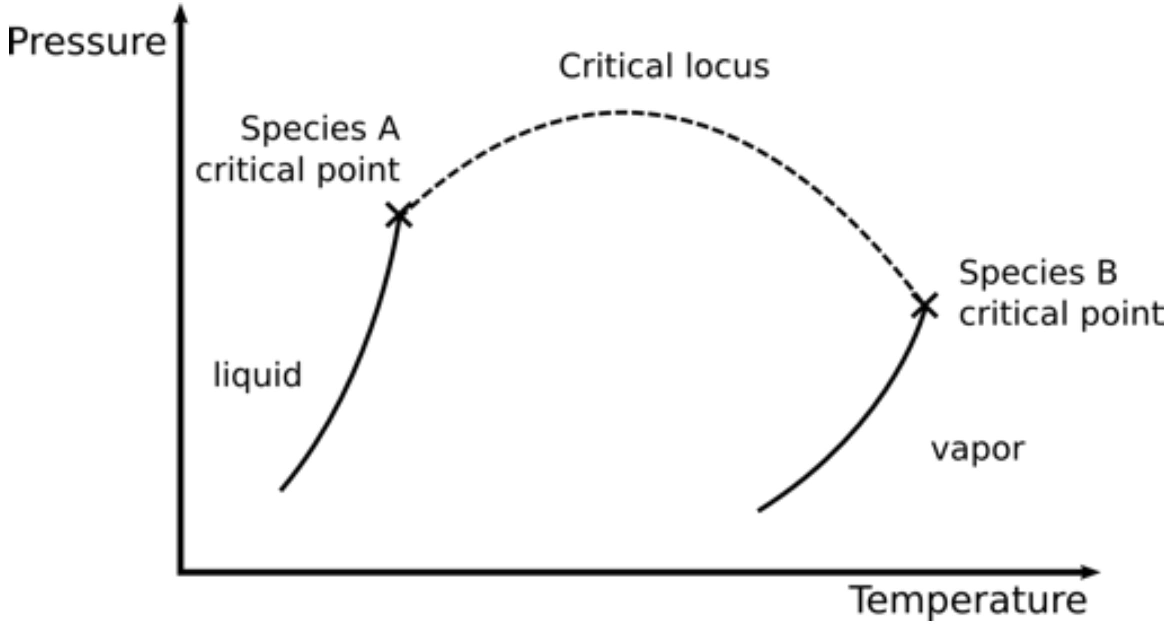


Yang (2000)

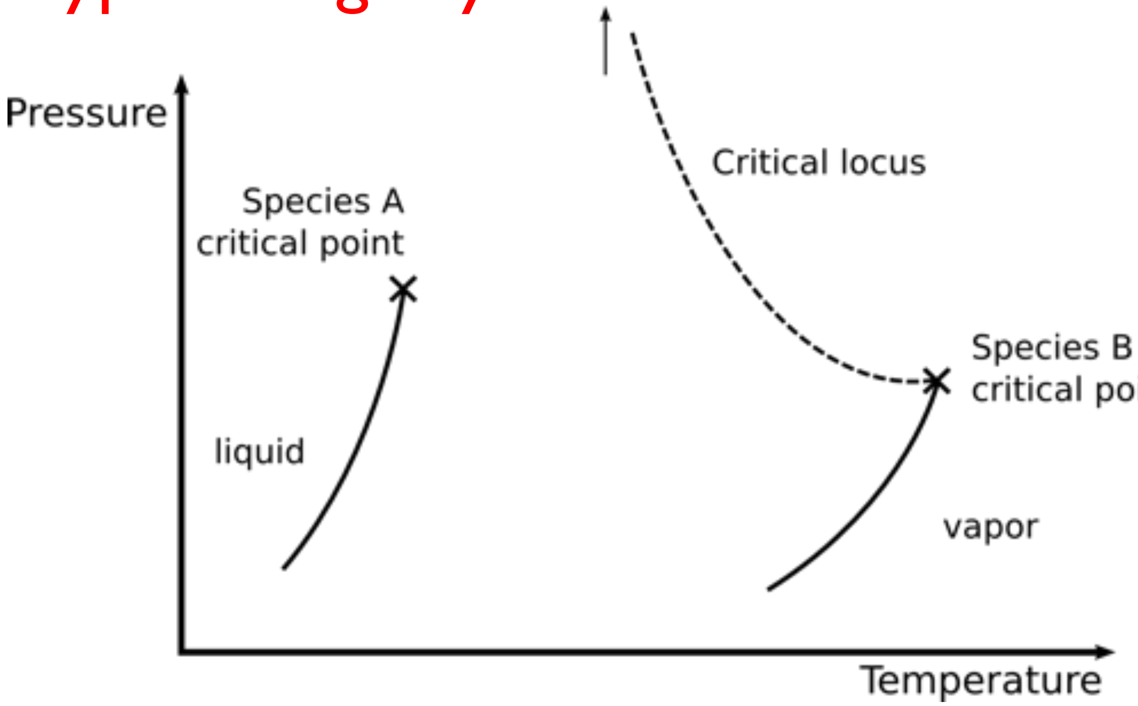
The critical point of a binary mixture

Mixture types: van Konynenburg & Scott (1980)

Type I: e.g. Mixtures of Hydrocarbons

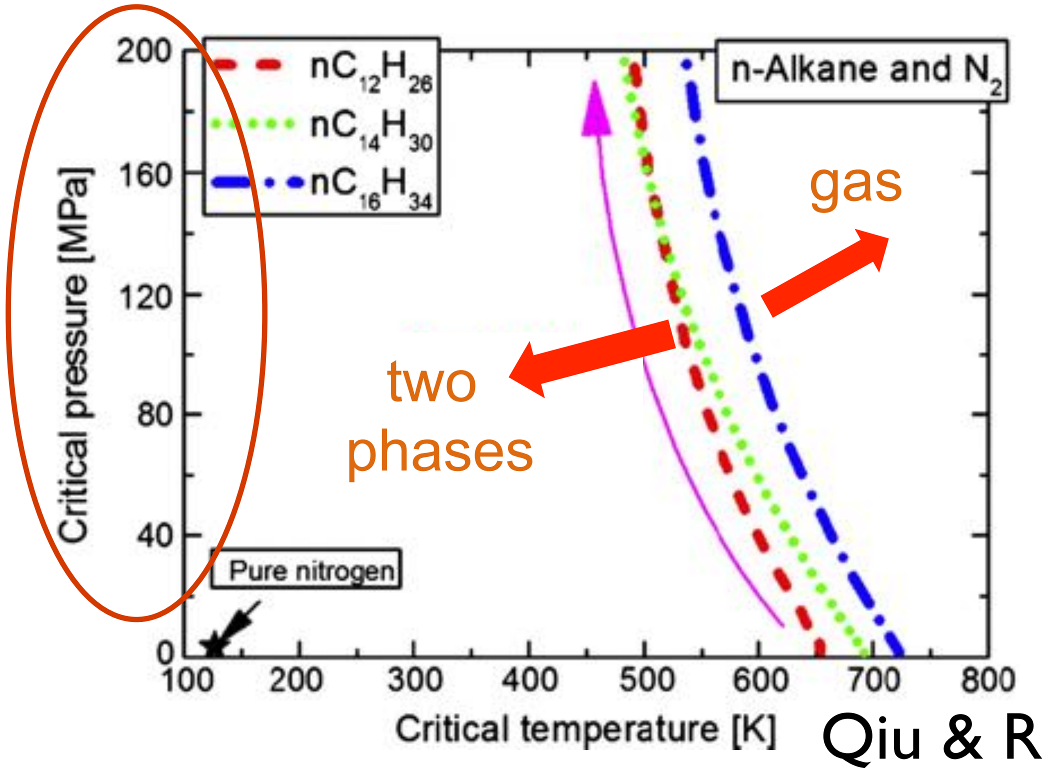


Type III: e.g. Hydrocarbons and Nitrogen



There is a "telescopic effect" on the mixture critical pressure in hydrocarbon-air systems

→ System appears to be shifted into the two-phase region upon mixing



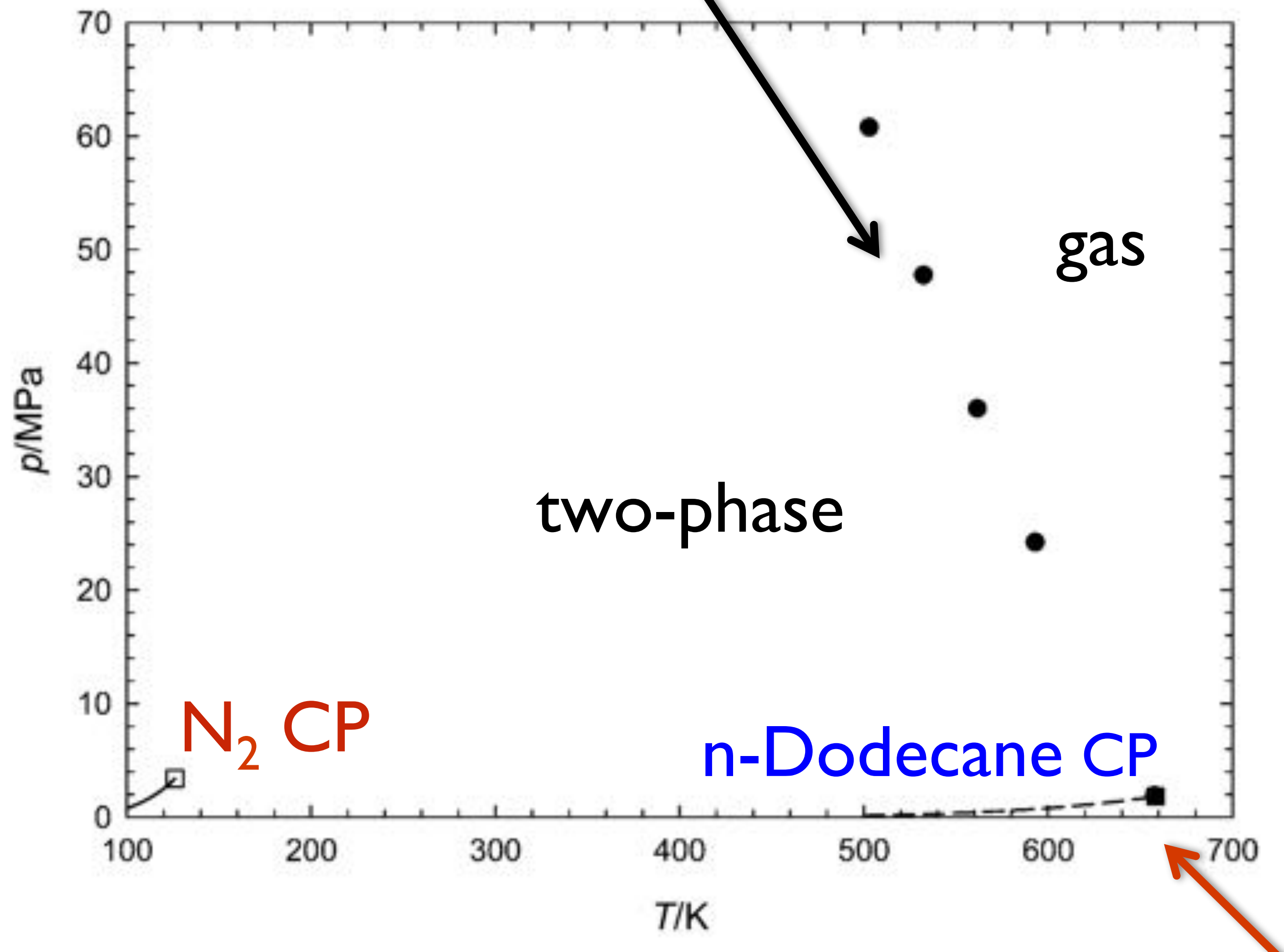
Qiu & Reitz (2015)

Surface–tension effects in hydrocarbon fueled sprays

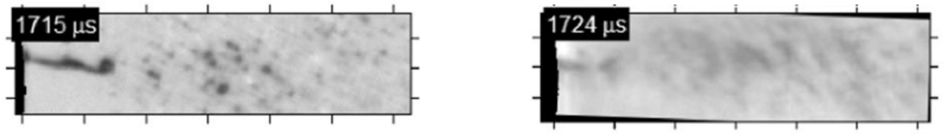
n-Dodecane / GN_2 equilibrium system

n-Dodecane spray into GN_2

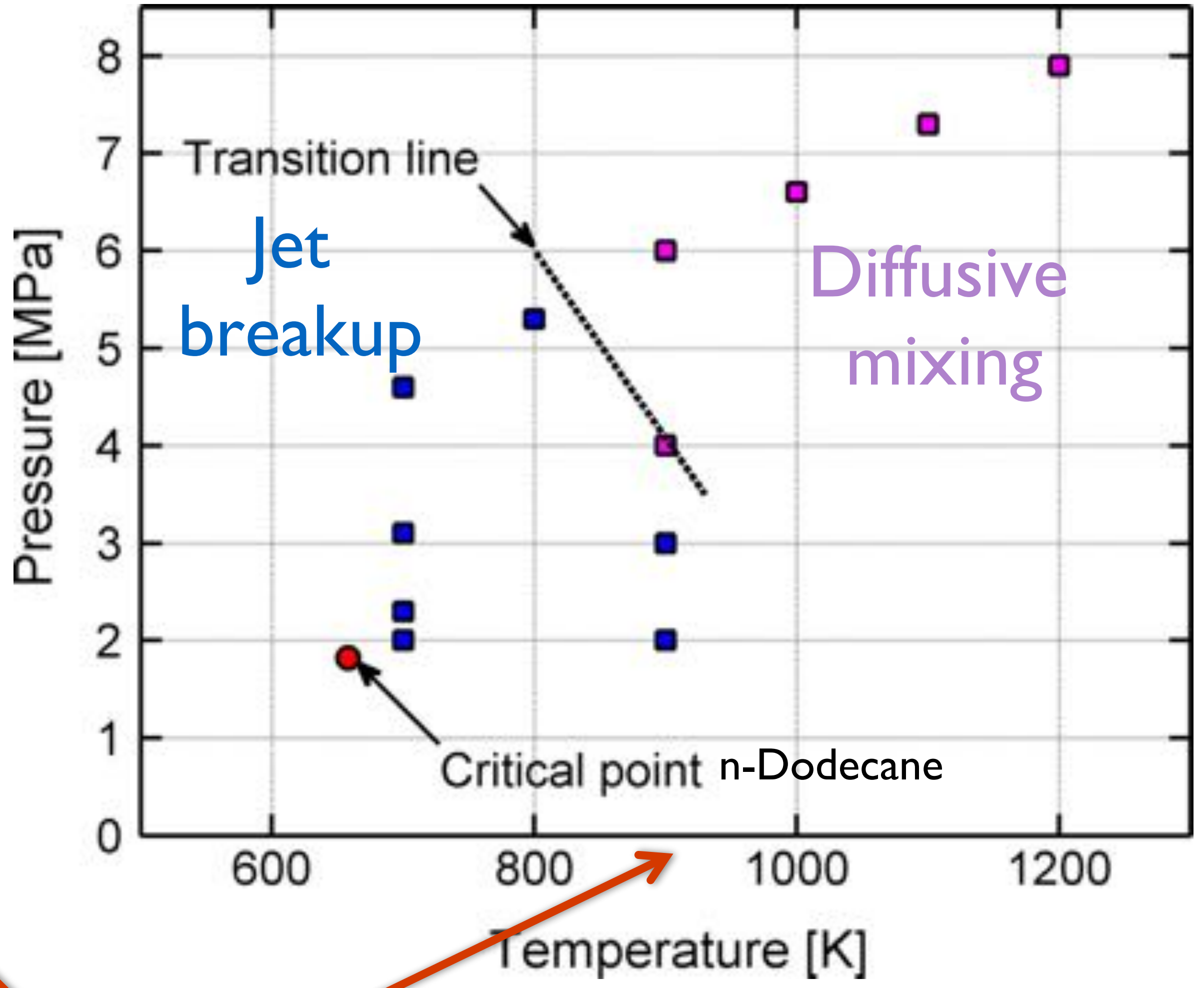
VLE: critical locus



Experiments by Garcia et al. (2011)



Jet-breakup / Diffusive mixing



Manin et al. (2014)

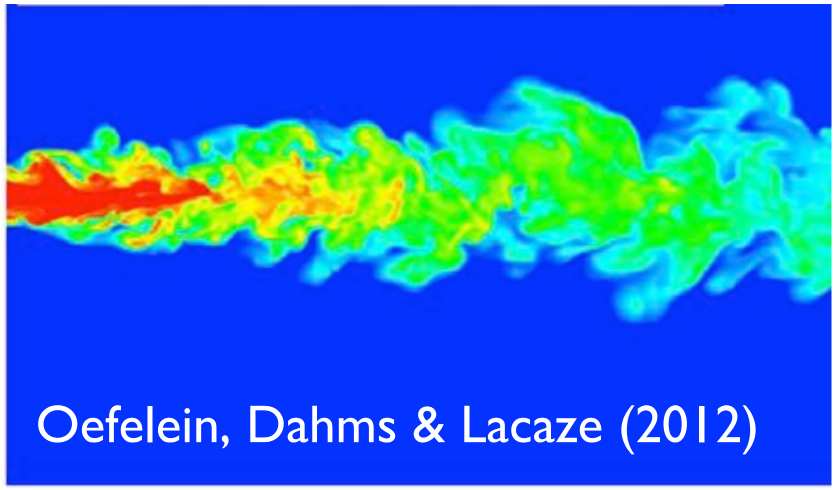
Surface tension may exist above critical locus

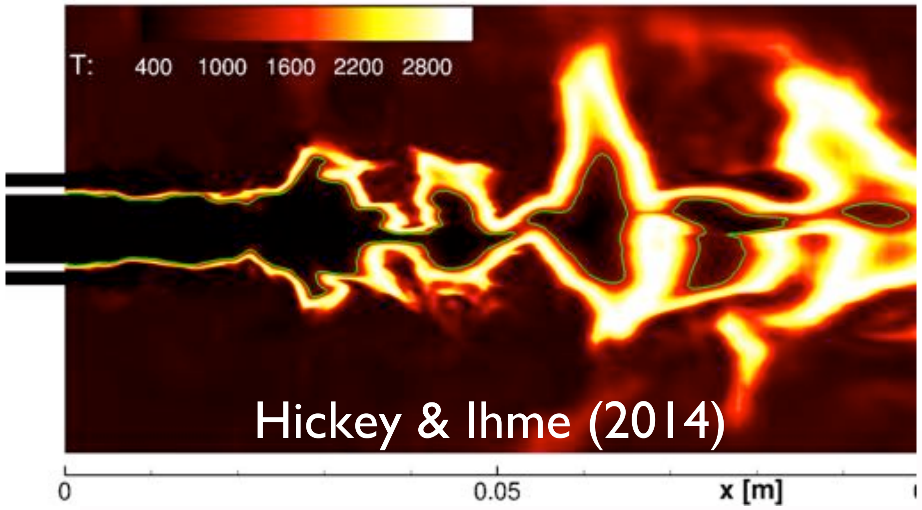
Computational modeling of high-pressure flows

State-of-the-art: single-phase formulations

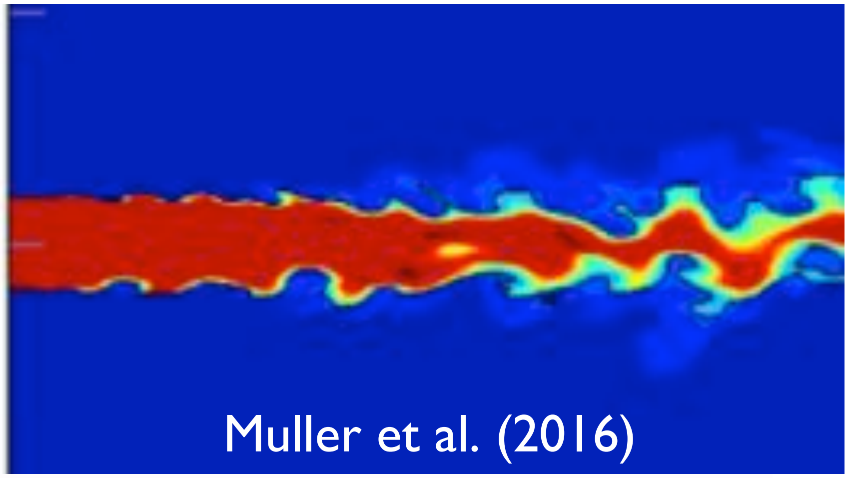
- Conservation equations for compressible miscible fluids without interfacial phenomena
- Real-gas equation of state + mixing rules
- Experimental correlations for transport properties at high pressures
- Conditions typically chosen when transcritical range does not play a significant role

LES of jet flows

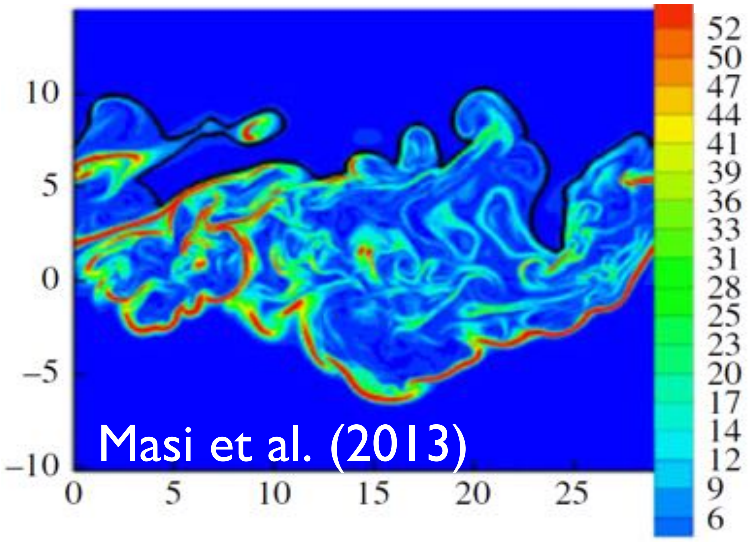

Oefelein, Dahms & Lacaze (2012)



Hickey & Ihme (2014)

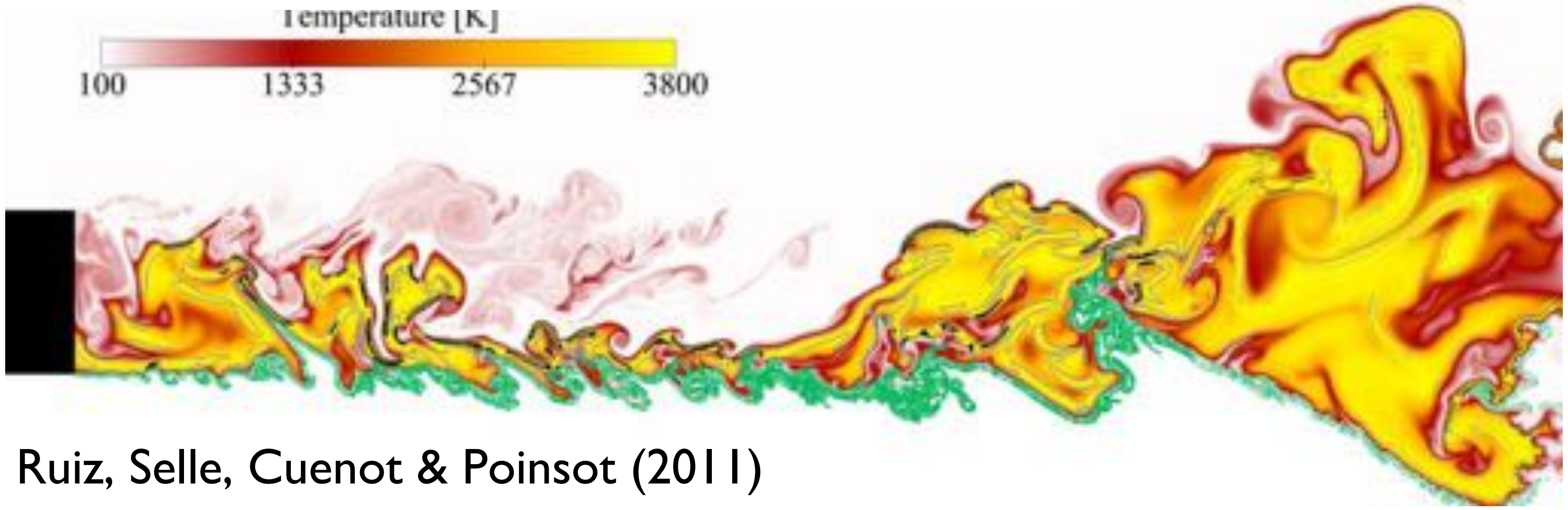

Muller et al. (2016)

DNS of mixing layers



Masi et al. (2013)

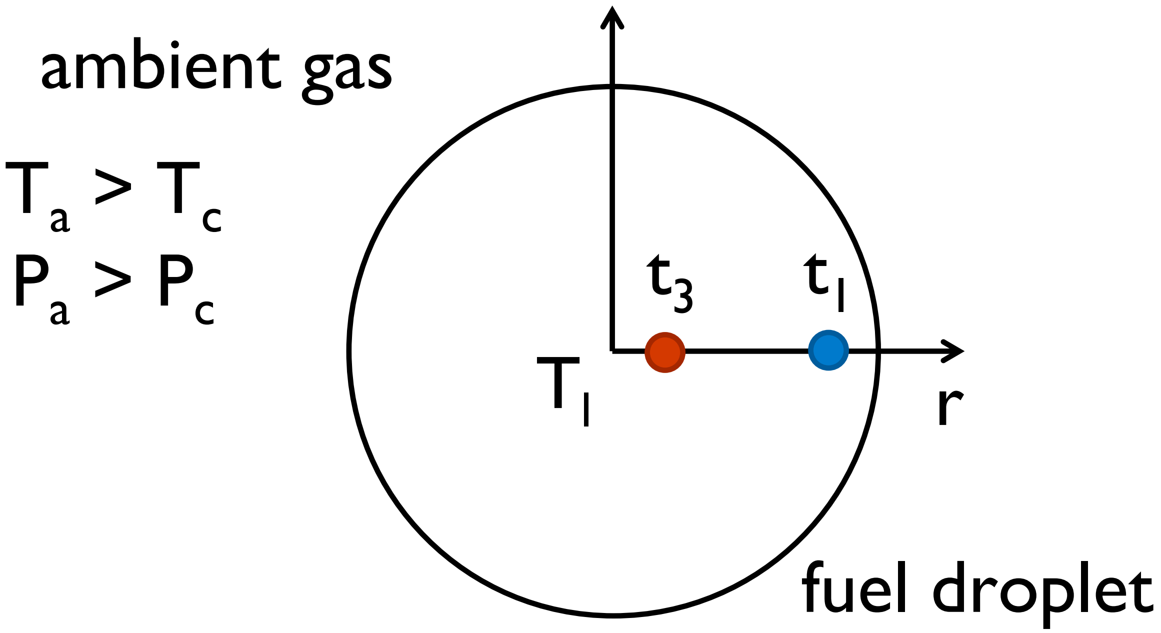
Simulations of flame stabilization

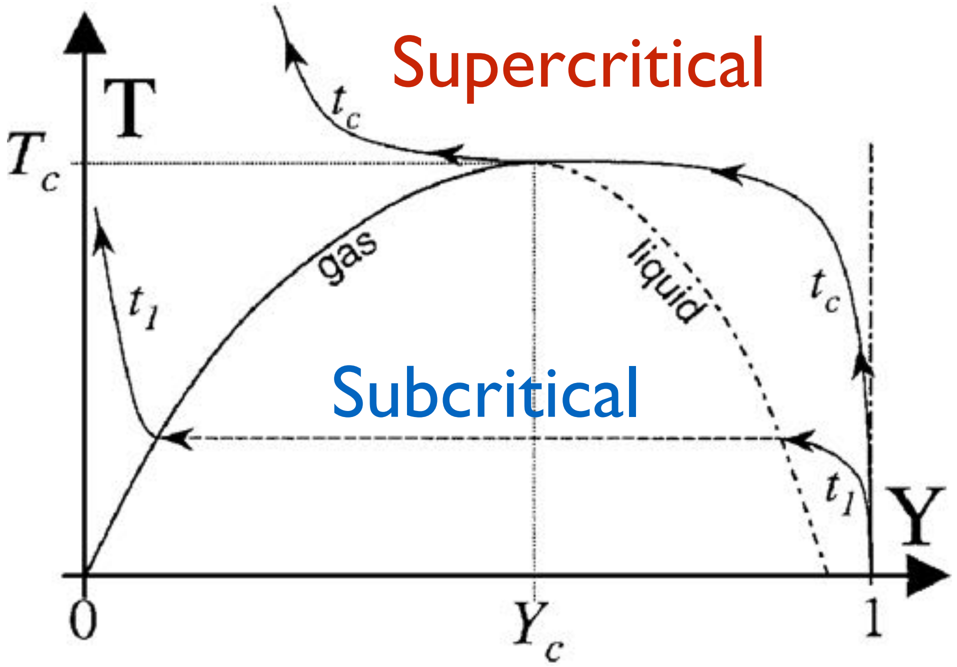


Ruiz, Selle, Cuenot & Poinsot (2011)

Reduced-order analysis of transcritical flows

Transcritical vaporization of liquid fuels Sirignano & Delplanque (1999)

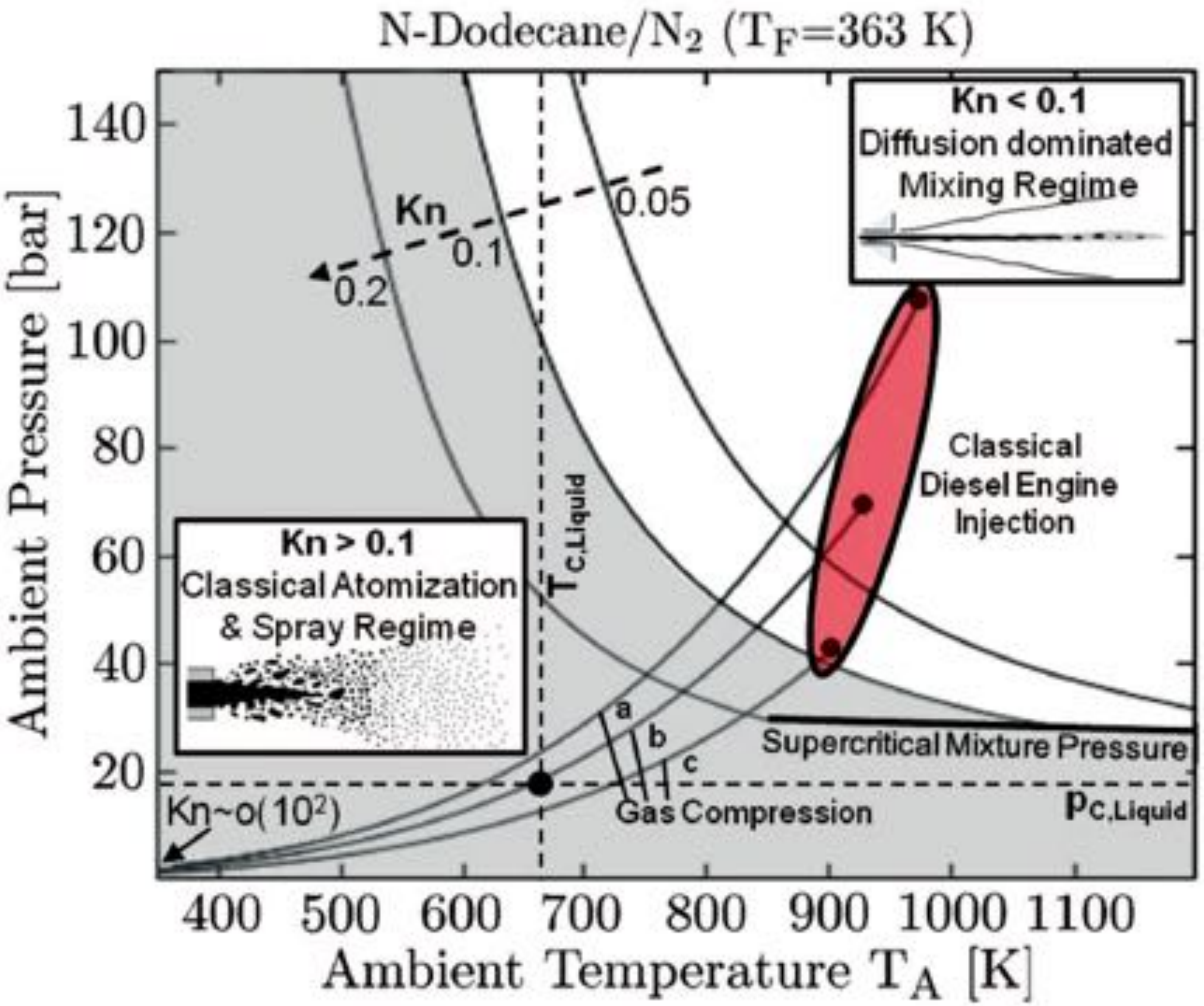




Subcritical and supercritical trajectories may exist simultaneously

Reduced-order modeling of transcritical flows

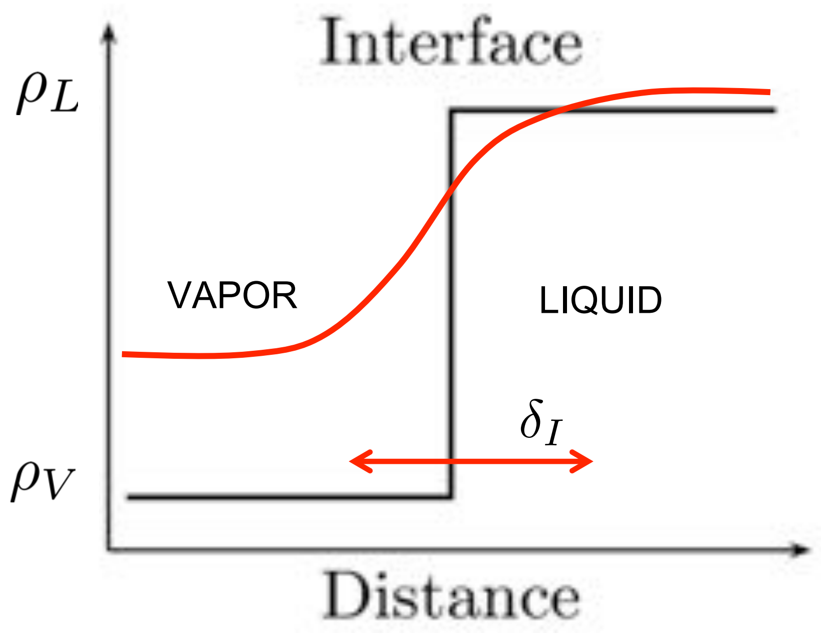
Global thermodynamic (i.e. static) analysis of transcritical flows



Dahms & Oefelein (2013)

The diffuse–interface approach

Hydrodynamic modeling of transcritical flows



Example: LN_2 into GN_2

$\delta_I = 0.5\times$ mean free path at $P = 0.2P_{\mathrm{cr}}$

$\delta_I = 15\times$ mean free path at $P = 0.9P_{\mathrm{cr}}$

At high pressures, the interface is still thin in hydrodynamic scales (~O(10nm)) but enters the continuum range

Dahms & Oefelein (2013)

Theoretical foundations:

The thermodynamic potentials are non-local → dependence on composition gradients.

Poisson (1831), Van Der Waals (1892), Landau (1937), Cahn & Hilliard (1958)

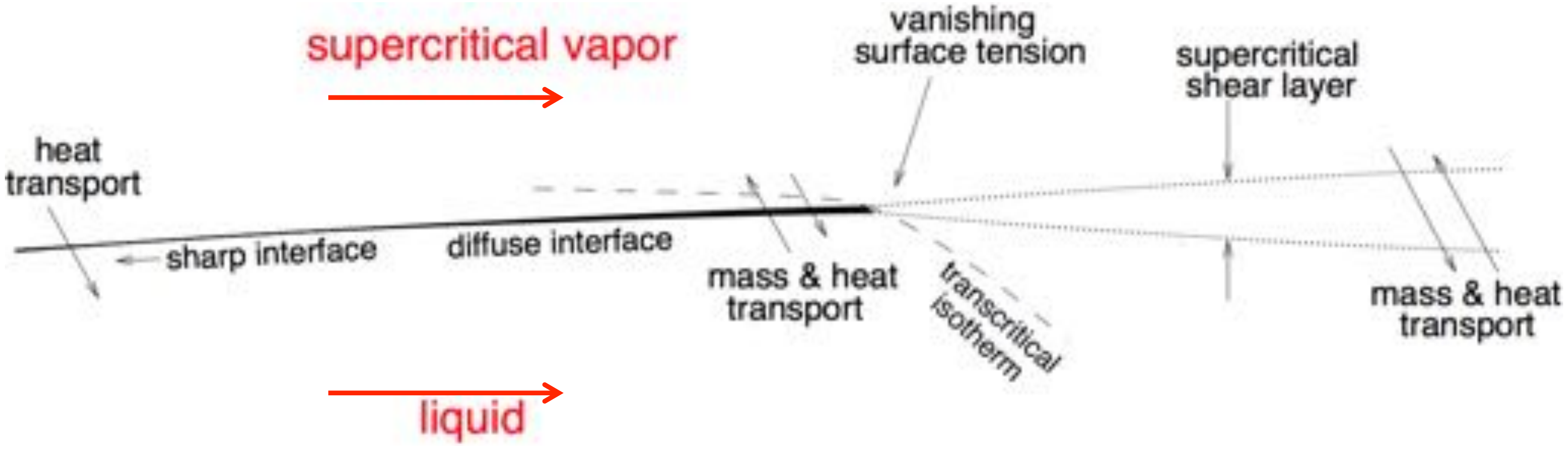
Some recent works on diffuse interface:

- Anderson (1998): Utilization of diffuse interface method in equations of fluid motion
- Dahms & Oefelein (2013): One of the first applications to address high-pressure combustion
- Gaillard et al. (2016): Multi-component transcritical diffusion flame structure

The diffuse–interface approach

Wish list:

A continuum single set of conservation equations accounting for interfacial phenomena



Mixture continuity: $$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i) = 0$$

Mixture momentum conservation: $$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j}(\rho u_i u_j) = \frac{\partial \tau_{ij}}{\partial x_j} + \frac{\partial \mathcal{K}_{ij}}{\partial x_j}$$

Must include pressure and surface-tension stresses

Mixture energy conservation: $$\frac{\partial(\rho e_t)}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i e_t) = -\frac{\partial q_i}{\partial x_i} - \frac{\partial \mathcal{Q}_i}{\partial x_i} + \frac{\partial}{\partial x_j}\left[(\tau_{ij} + \mathcal{K}_{ij})u_i\right]$$

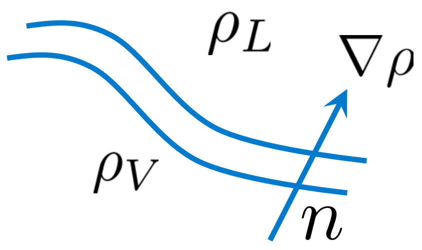
Must include work done by surface-tension stresses and modified heat conduction

Species mass conservation: $$\frac{\partial(\rho Y_k)}{\partial t} + \frac{\partial}{\partial x_i}(\rho u_i Y_k) = -\frac{\partial J_{i,k}}{\partial x_i} - \frac{\partial \mathcal{J}_{i,k}}{\partial x_i}$$

Must include modified molecular diffusion

\+ Real gas equation of state

The diffuse–interface approach



Single-component mechanical equilibrium: $\dfrac{\partial \mathcal{K}_{ij}}{\partial x_j} = 0$

Minimization of interface's Helmholtz free energy

$$F = \int_{\mathcal{V}} \left[\rho f + \frac{\kappa}{2} \left(\frac{\partial \rho}{\partial x_i} \frac{\partial \rho}{\partial x_i} \right) \right] d\mathcal{V}$$

Non local correction (first approx.)

$\kappa =$ Gradient coefficient
Pismen (2001)

Capillary stress tensor
Korteweg (1901)

$$\mathcal{K}_{ij} = -P\delta_{ij} + \rho\kappa \frac{\partial^2 \rho}{\partial x_k \partial x_k} + \frac{1}{2}\kappa \left(\frac{\partial \rho}{\partial x_m} \frac{\partial \rho}{\partial x_m} \right) \delta_{ij} - \kappa \frac{\partial \rho}{\partial x_i} \frac{\partial \rho}{\partial x_j}$$

Gradient theory (1D)
Lin et al. (2007)

$$\frac{1}{2}\kappa \left(\frac{d\rho}{dn} \right)^2 = \rho(f - \mu) + P_0 \quad \text{subject to} \quad \rho \to \rho_L \quad \text{at} \quad n \to \infty$$

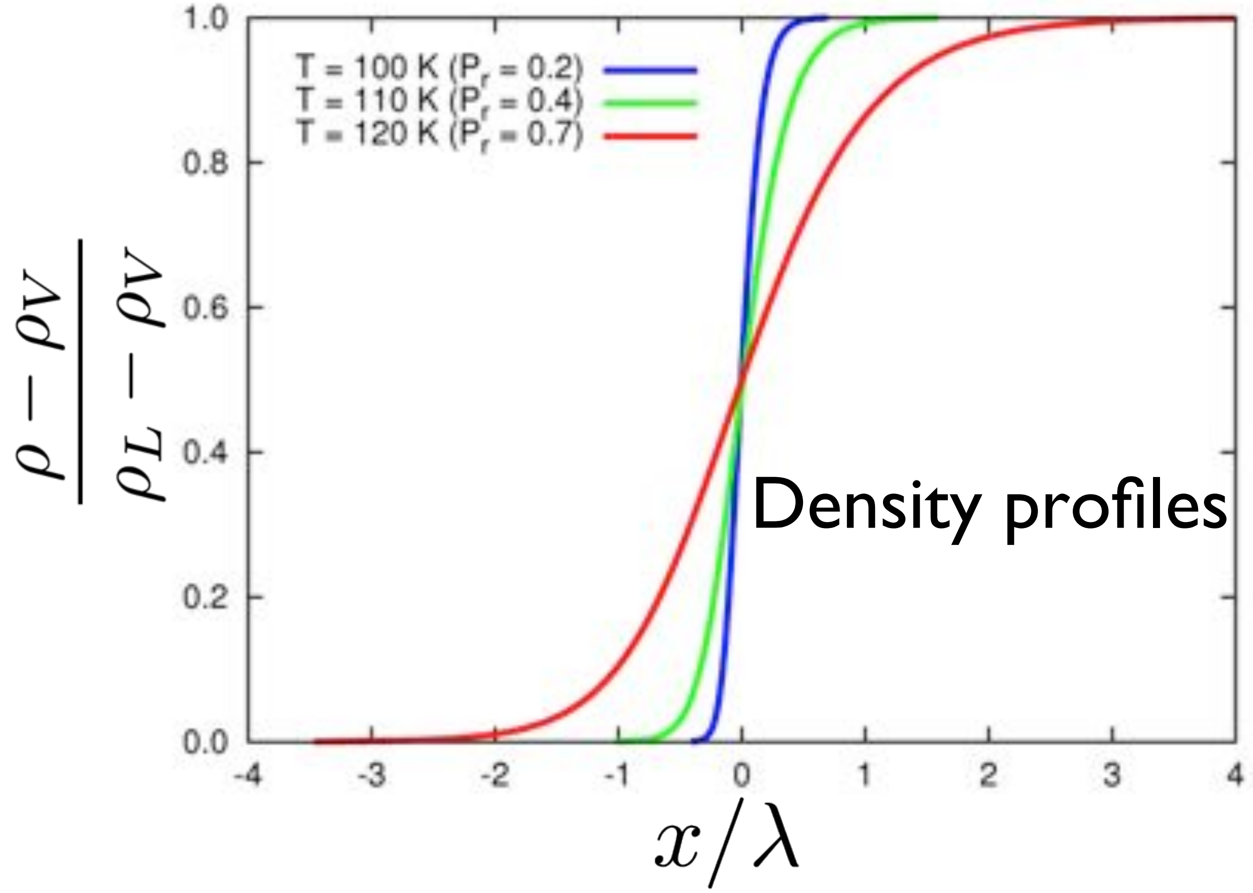
Local surface tension coefficient

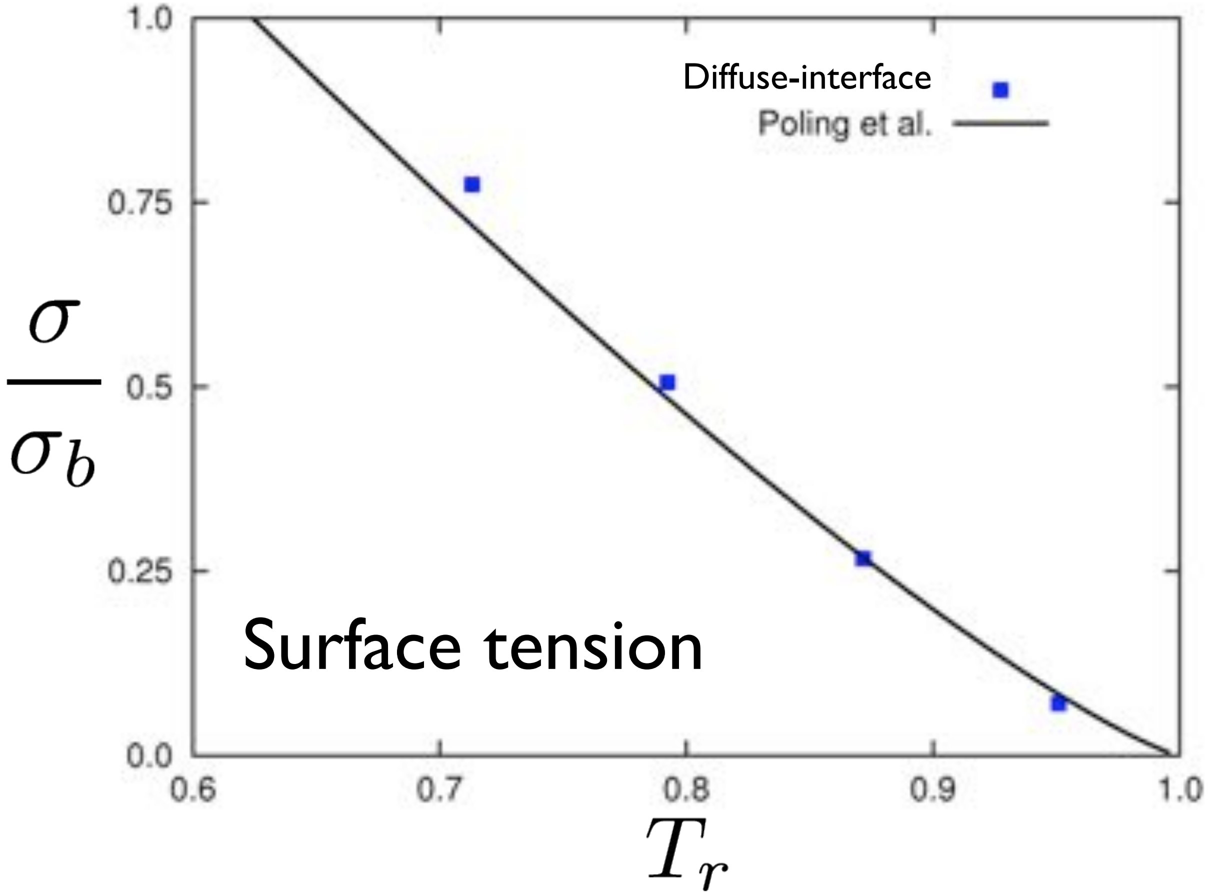
$$\sigma = \kappa \int_{-\infty}^{+\infty} \left(\frac{d\rho}{dn} \right)^2 dn$$

Note surface tension coefficient does not appear explicitly in the diffuse-interface-based conservation equations.

Diffuse–interface profiles

N_2 at vapor-liquid equilibrium:

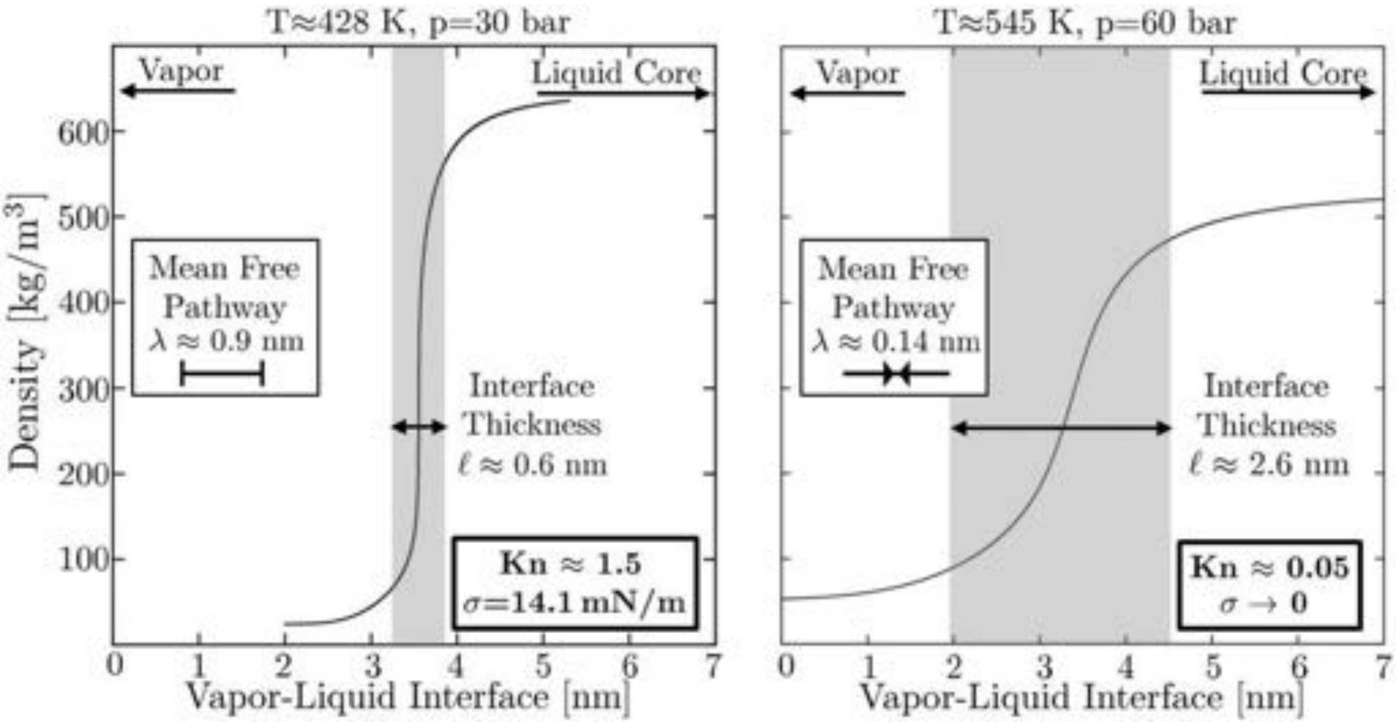




Extension to multi-species:

- Interface thickness increases with temperature
- Mean free path decreases with pressure

Dahms & Oefelein (2013)



Toward multi–component flows

Non local correction
(first approx.)

Interface's Helmholtz free energy:

$$F = \int_{\mathcal{V}} \left[f_0(\rho) + \sum_{i,j} \frac{1}{2} \kappa_{ij} \nabla \rho_i \nabla \rho_j \right] d\mathcal{V}$$

Species mass conservation (Cahn-Hilliard type):

$$\frac{\partial \left(\rho Y_k \right)}{\partial t} + \frac{\partial}{\partial x_i} \left(\rho u_i Y_k \right) = - \frac{\partial J_{i,k}}{\partial x_i} - \frac{\partial \mathcal{J}_{i,k}}{\partial x_i}$$

Must asymptotically collapse to zero (sharp interfaces, subcritical) and to Stefan-Maxwell-type diffusion (diffusive mixing, supercritical)

See more details in Gaillard et al., *Comb. Theor. Modelling* (2016)

"Another perspective of high scientific interest would be to perform DNS as well as LES of the transition between subcritical and supercritical flames using [this] compressible formulation, which is fully valid in several dimensions."

V. Conclusions & Open Challenges

Summary

- The **supercritical** p,T phase plane is divided into **liquid and gaseous** states.
- **Pseudoboiling** is the transition from supercritical liquid to gas. It occurs across the Widom line $p< 3p_{cr}$. A distributed **latent heat** is required to overcome **intermolecular forces**.
- Transcritical jets are sensitive to heating in the injector, causing **thermal break-up.**
- In LOX/GH2 non premixed combustion, **real-fluid effects are confined to O_2** .
- Liquid-gas interfaces become broader at high pressures and enter the continuum range.
- Surface tension persists in hydrocarbon-air systems above the critical pressure of the components, leading to simultaneous occurrence of classic-like jet breakup and diffusive mixing.
- Current trends of increasing combustor pressures will make the transcritical problem increasingly more relevant in internal combustion engines and gas turbines.

Open challenges

- Experimental diagnostics: Quantitative diagnostics and optical access are hindered by the high pressures & temperatures → lack of data for validation.

- Thermodynamics of transcritical fluids: Fundamental understanding is required to model thermodynamic coefficients, critical points, equations of state and mixing rules for real fluid mixtures in combustion systems.

- Aerodynamics of hydrocarbon-air jets in transcritical regimes: A predictive, thermodynamically consistent set of conservation equations is required to model transition from delayed classic atomization (sharp interfaces) to diffuse mixing (smeared interfaces) simultaneously in the same flow field → diffuse interface method (?)

- Subgrid-scale modeling for interfaces: High-pressure interfaces are thicker but still thin in hydrodynamic scales → thickened interface models (?)

- Combustion of transcritical hydrocarbon-air jets: Unexplored problem that becomes additionally complicated by the occurrence of high-pressure low-temperature complex hydrocarbon chemistry and transport.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1891

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