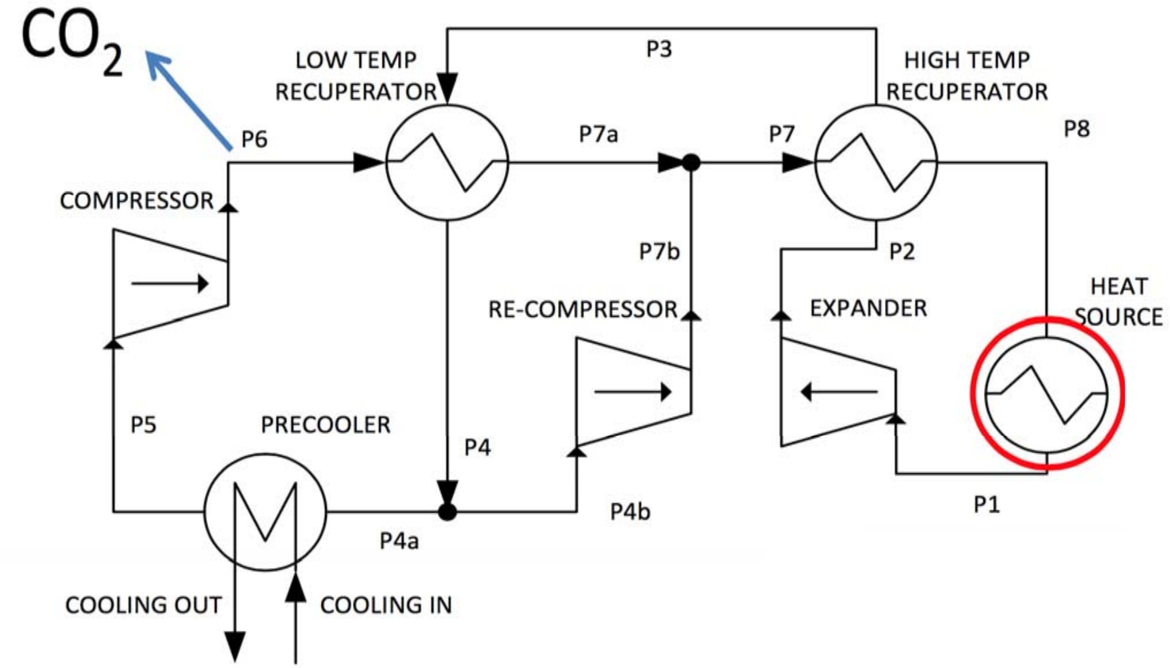
Large eddy simulations of oxy-fuel combustors for direct- fired supercritical CO2 power cycles

Daniel T. Banuti, Lee Shunn, Sanjeeb Bose, Dokyun Kim

CASCADE
TECHNOLOGIES

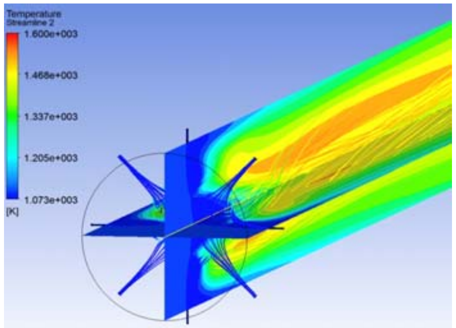
Direct-fired sCO2 cycle - Allam cycle



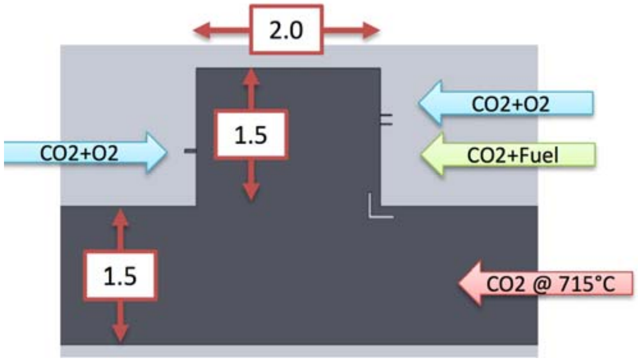
Delimont 2017

- Closed sCO2 loop
- Increased efficiency
- Small footprint
- Heat added by direct combustion (e.g. CH4+O2)
- Ideally, products in stoichiometric combustion (H2O, CO2) can be easily removed

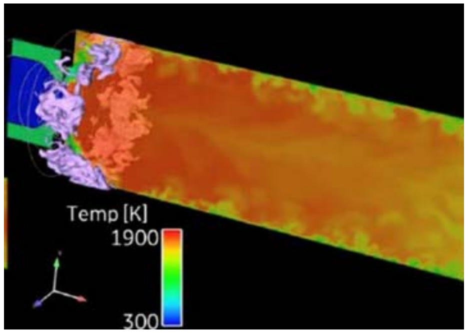
Problem: how *exactly* do we add heat?



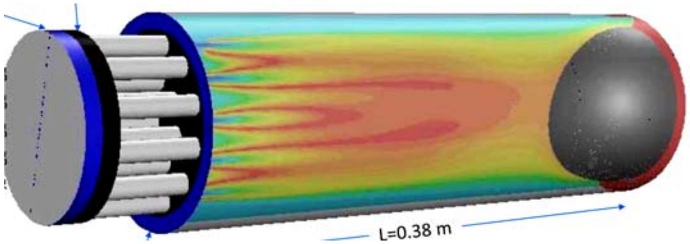
Radial jets in crossflow
(Delimont et al. UTSR 2016)



Trapped vortex chamber
(Delimont et al. UTSR 2017)

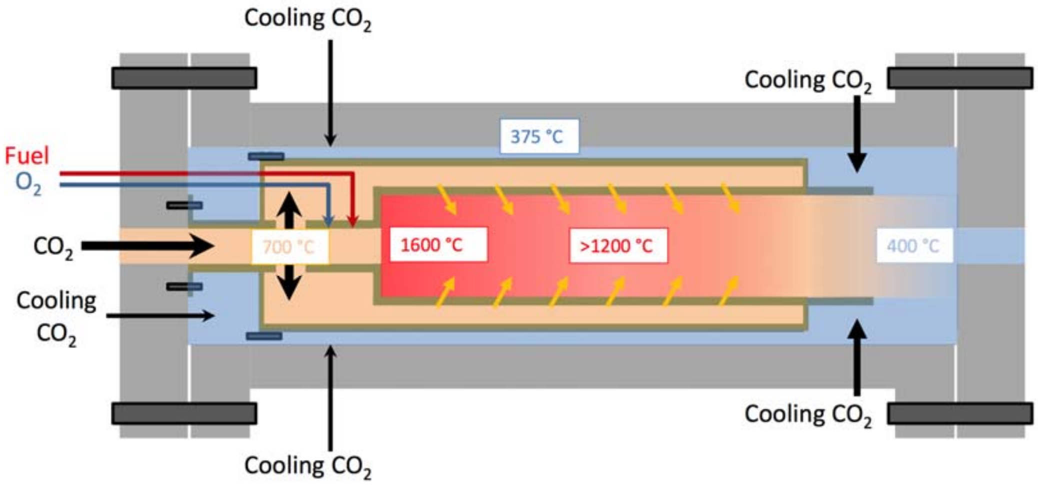


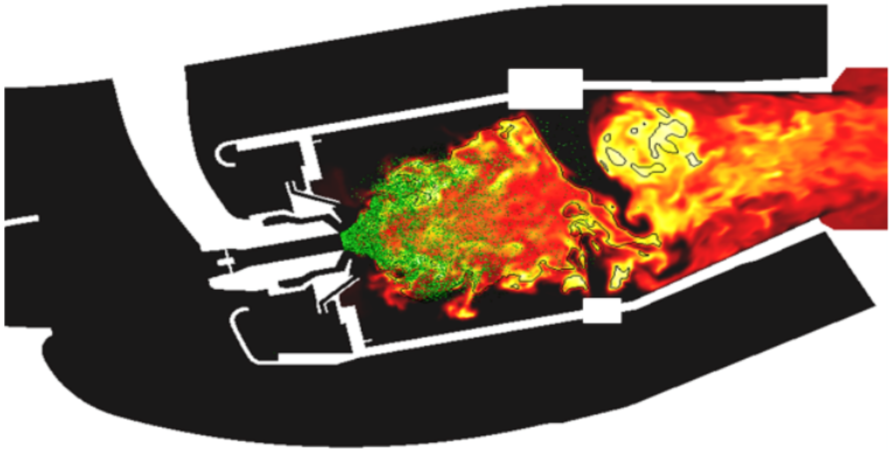
Swirl injector in liner
(Delimont et al. UTSR 2017)



Coaxial injectors
(Strakey UTSR 2017)

Combustor concept from SwRI



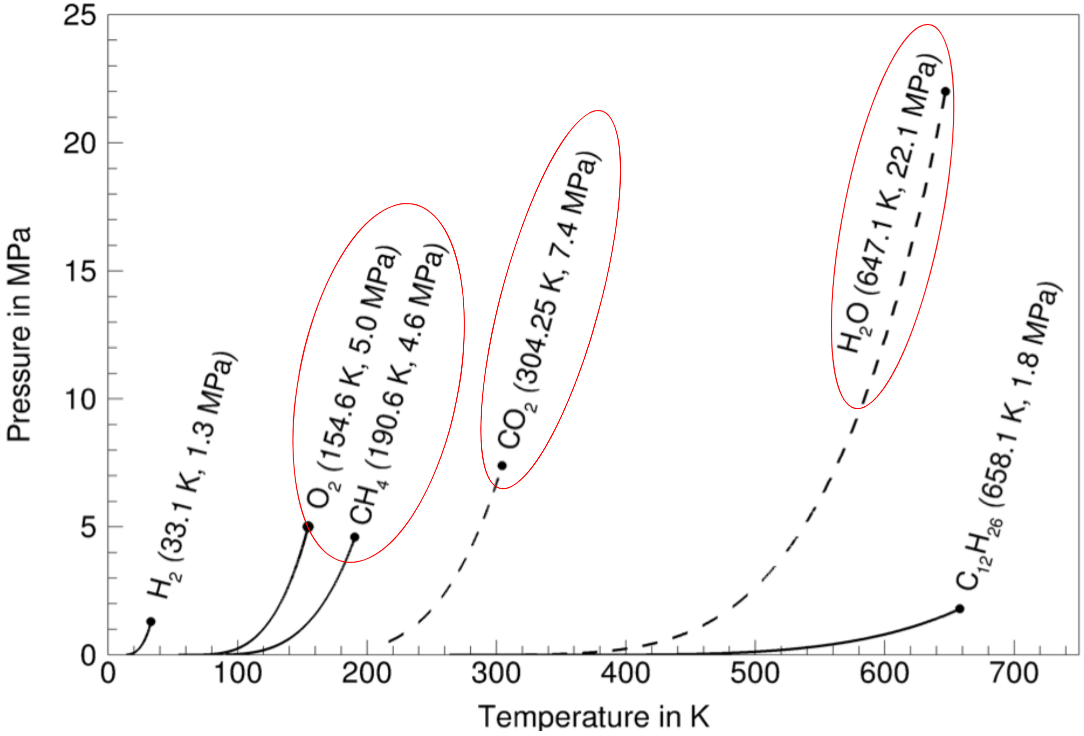


Component	Mass flow in kg/s
CH_4	0.02
O_2	0.08
CO_2 combustor	0.626
CO_2 bypass	0.899
Total	1.625

p > 200 bar

Delimont et al. 2017

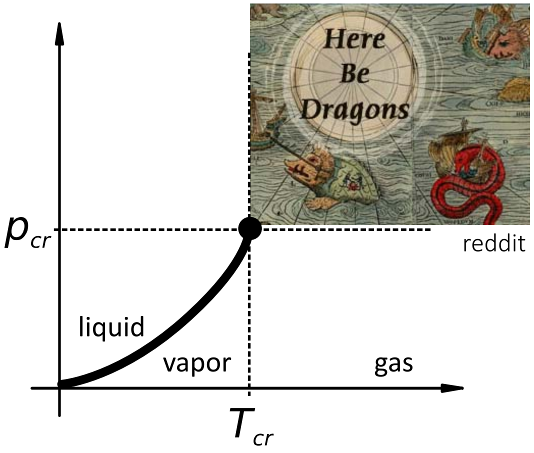
Thermophysical Properties at High Pressures



- Anticipated combustor conditions:
  - T = 1000-2000K,
  - p = 200-300 bar
- Mixtures are supercritical with respect to:
  CH4, O2, CO2, H2O

Objectives

What is ‘supercritical’ anyway?

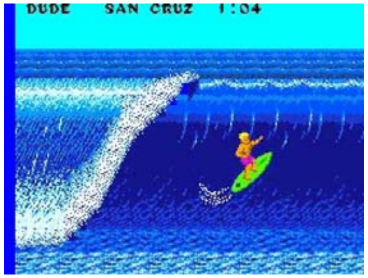


reddit

Identify and analyze model

reddit

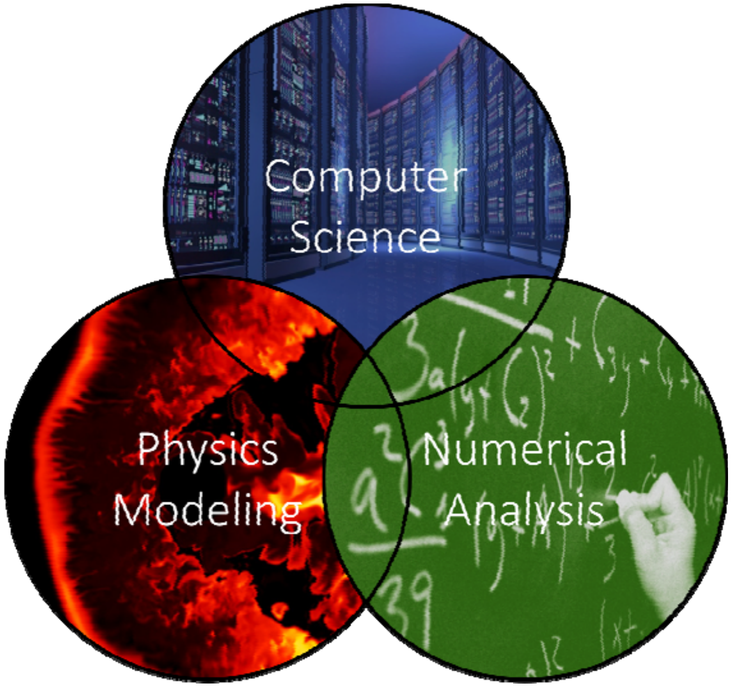
Perform simulations



california games

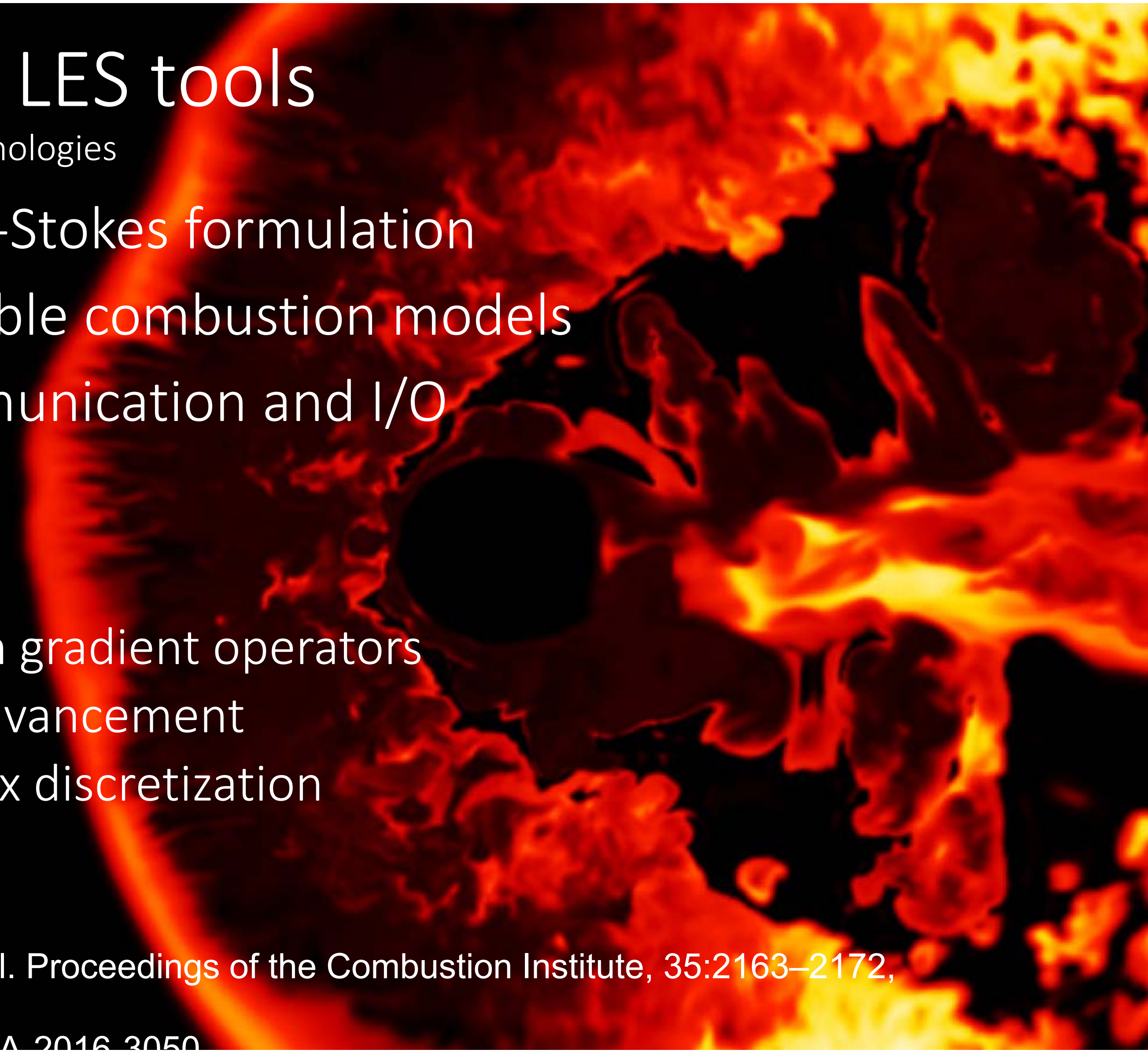
Cascade Background

- Founded in 1997 to support technology transfer from Stanford University's Center for Turbulence Research to industry
- Located in Palo Alto, CA
- Since 2007, Cascade has developed and licensed multi-physics Large Eddy Simulation (LES) tools tailored for high-performance and extreme scalability
- Cascade's LES software is developed and supported by a growing team of full-time professionals with expertise in physics modeling, computer science, and numerical analysis



CHARLES™ suite of LES tools

Developed and licensed by Cascade Technologies



- Compressible FV Navier-Stokes formulation
- Flamelet/progress-variable combustion models
- Massively-parallel communication and I/O

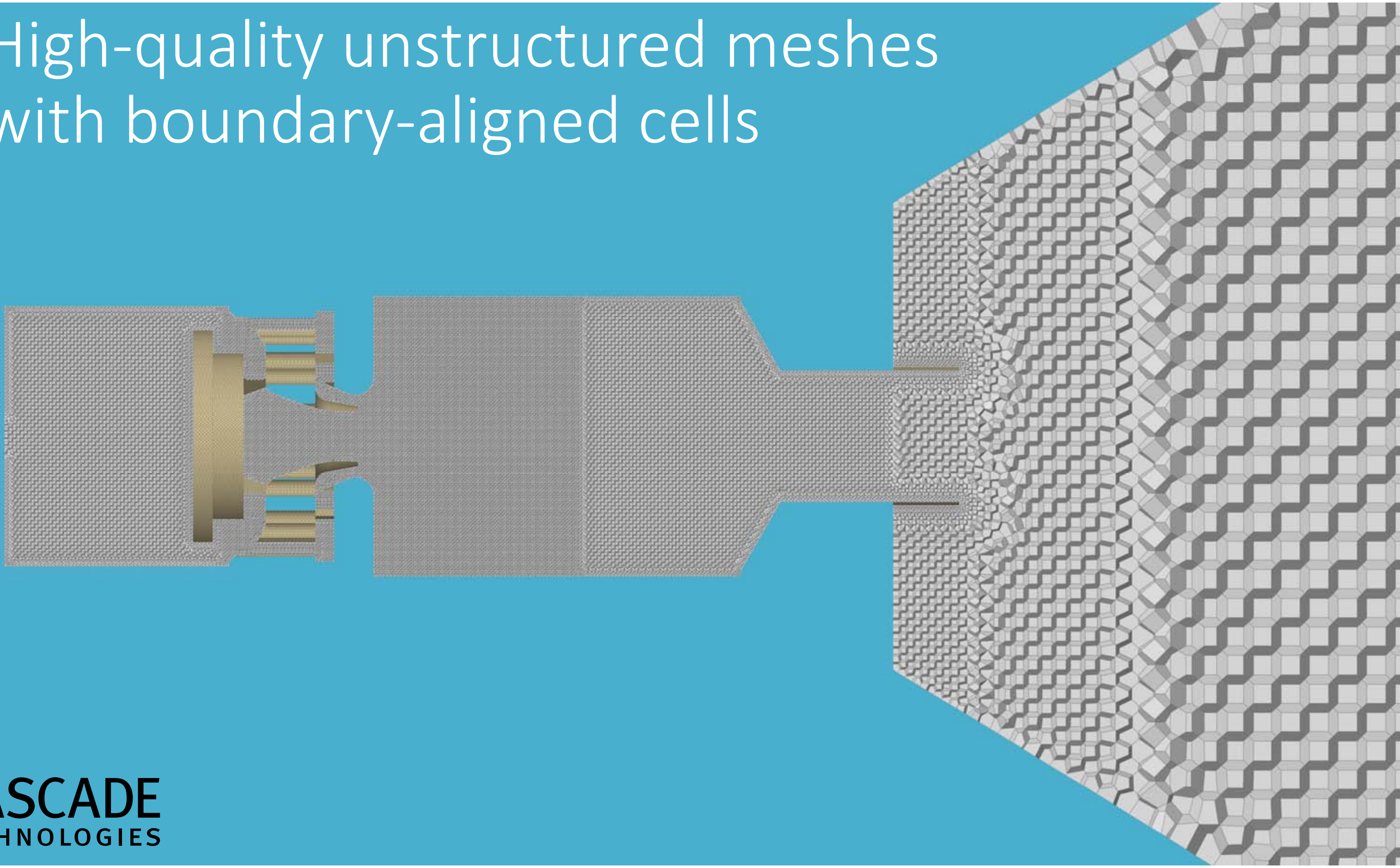
- Numerical method
  - 2nd-order low-dissipation gradient operators
  - 3rd-order explicit time advancement
  - ‘KEEP’ entropy-stable flux discretization

CASCADE TECHNOLOGIES

A. Saghafian et al. Proceedings of the Combustion Institute, 35:2163–2172, 2015

G. Brès et al. AIAA 2016 3050

High-quality unstructured meshes with boundary-aligned cells



CASCADE TECHNOLOGIES

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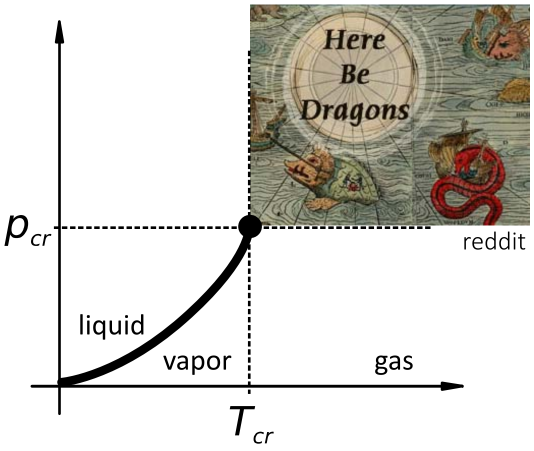

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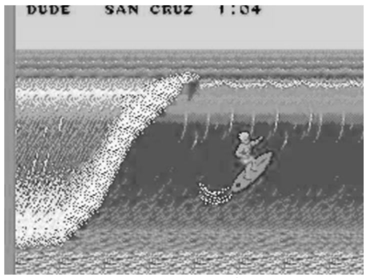

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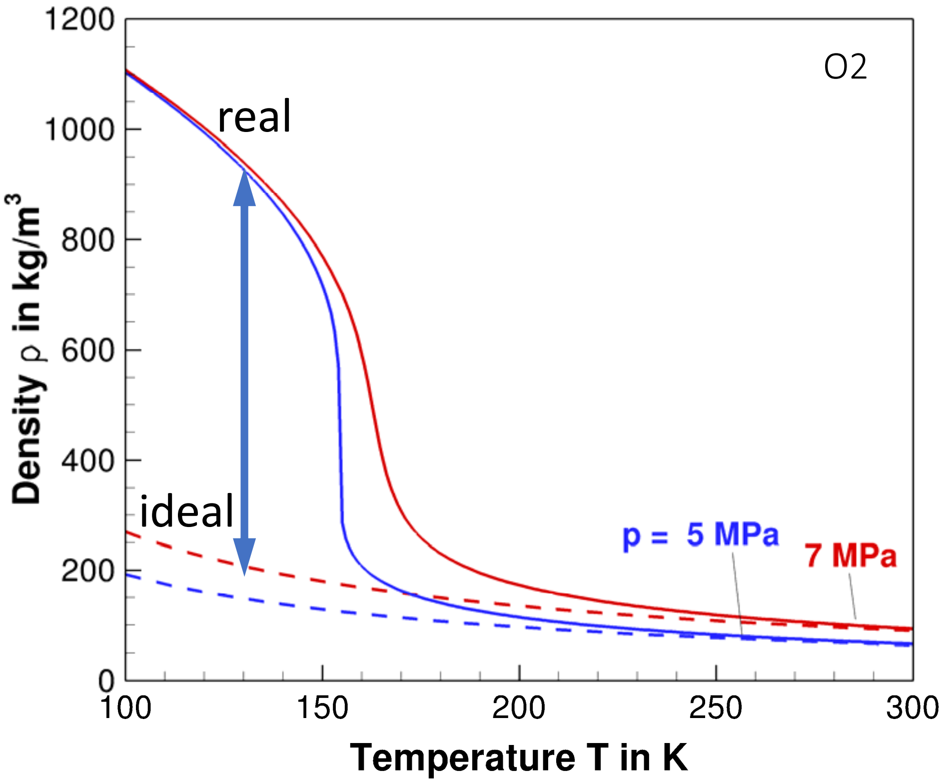
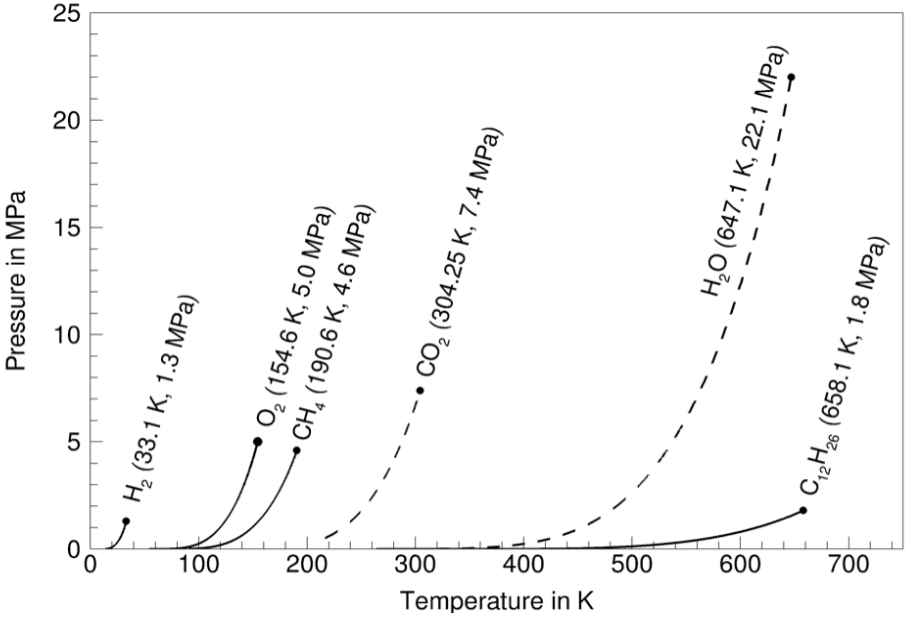
What is the difference between real and ideal gases?



$$p = \frac{RT}{v \underbrace{- b}_{\text{molecular volume}}} \underbrace{- \frac{a}{v^2}}_{\text{intermolecular attraction}}$$

The supercritical state space



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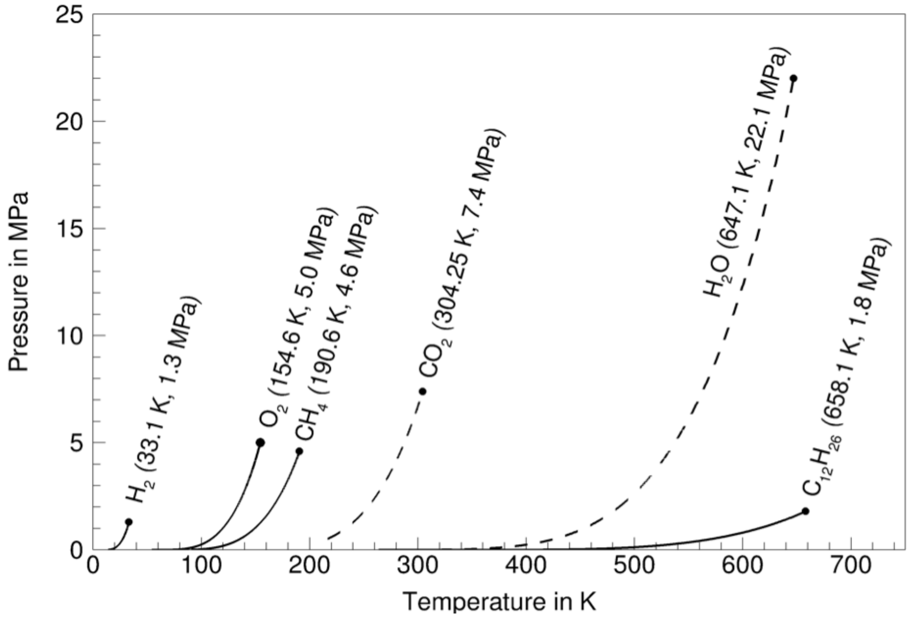
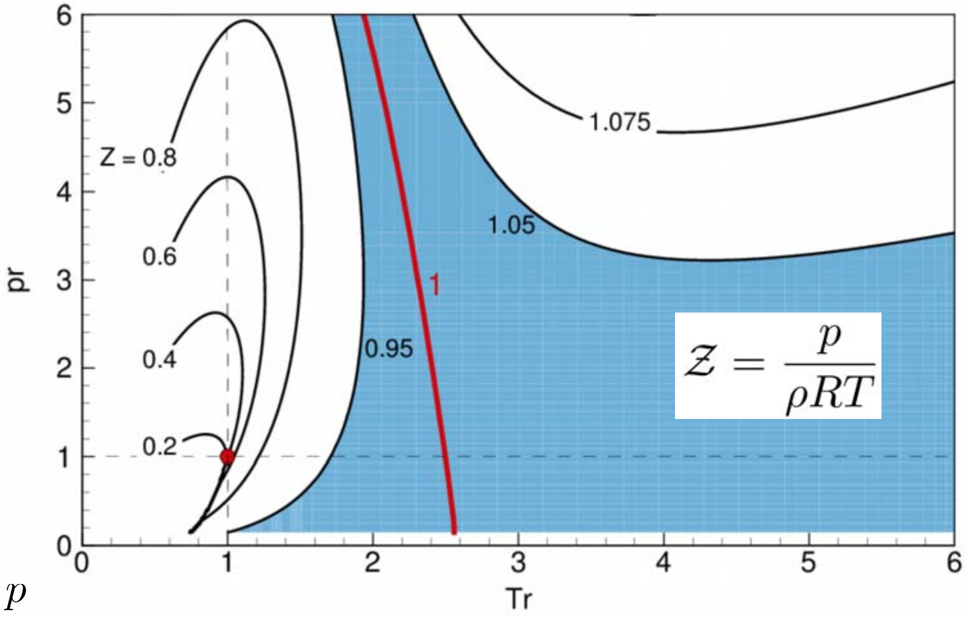




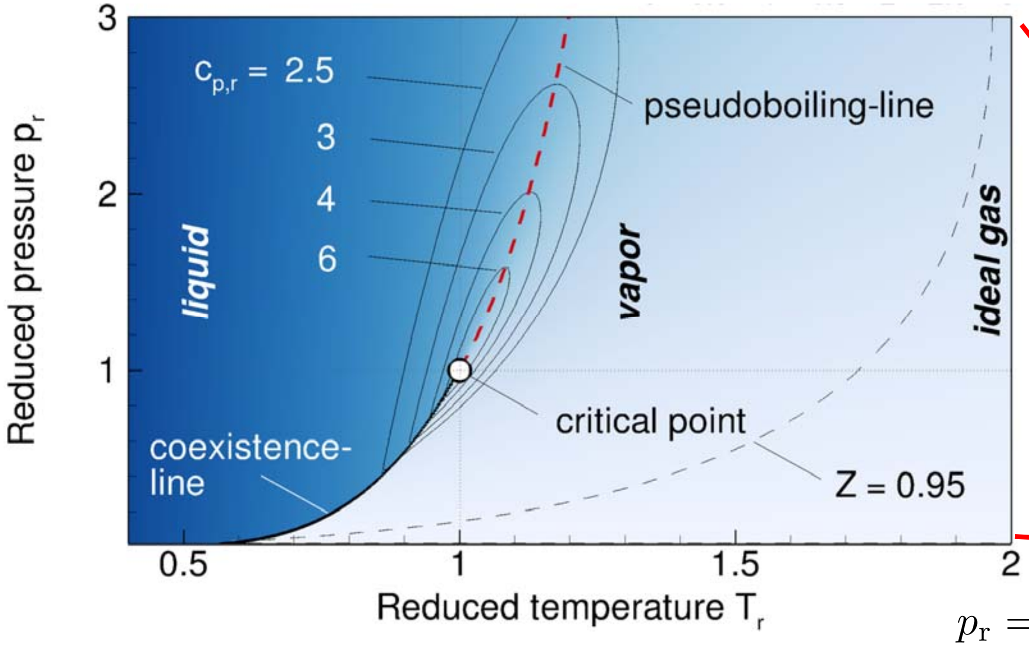
$$\mathcal{Z} = \frac{p}{\rho R T}$$

$$p_\mathrm{r} = \frac{p}{p_\mathrm{cr}}$$

$$T_\mathrm{r} = \frac{T}{T_\mathrm{cr}}$$

Banuti et al. CnF 2016

The supercritical state space



Banuti et al. PRE 2017

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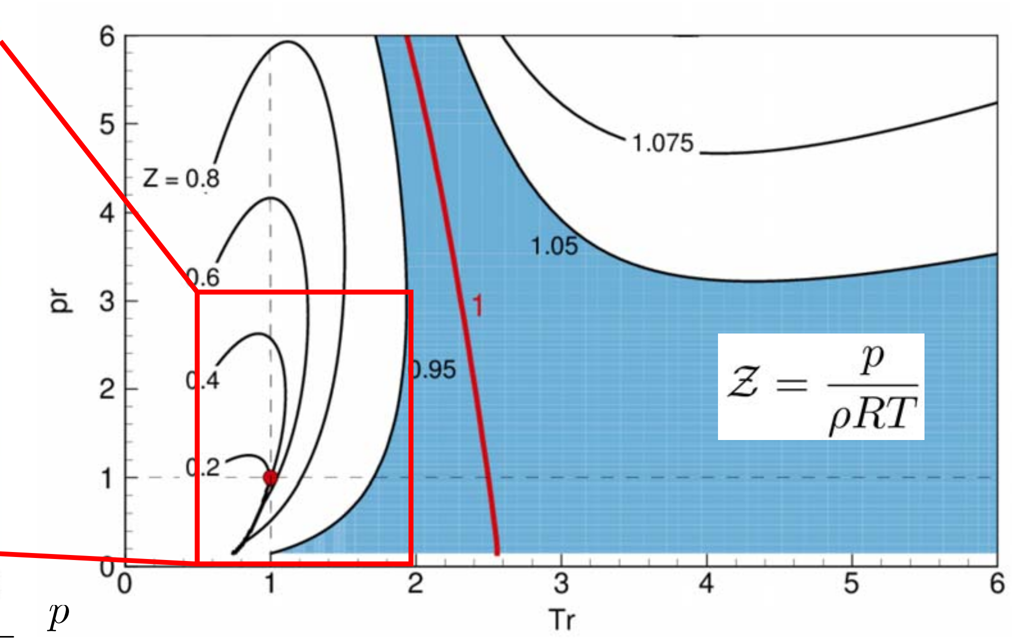

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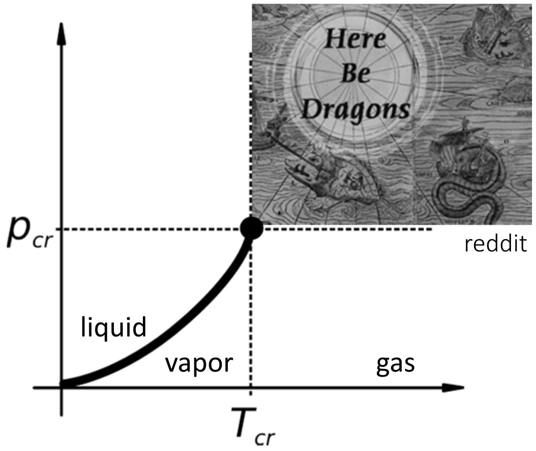

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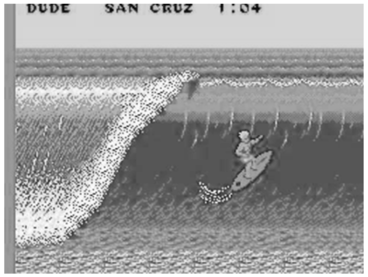

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Real fluid thermodynamics for mixtures

Peng-Robinson equation of state:

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

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

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

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

One fluid mixing model

Peng-Robinson equation of state:

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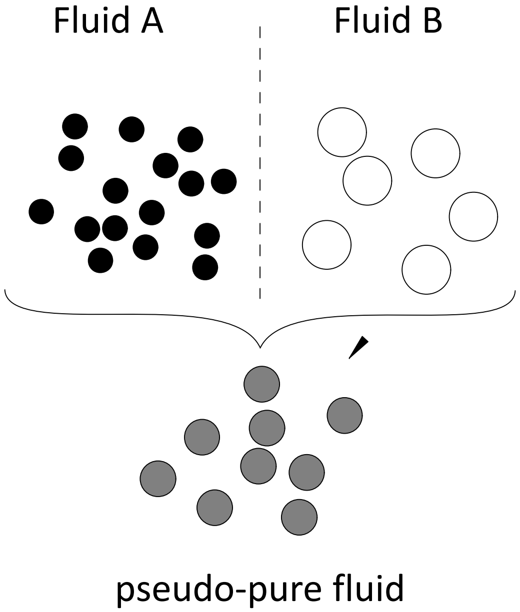

Oefelein and Yang (1998)

One fluid mixing model

Peng-Robinson equation of state:

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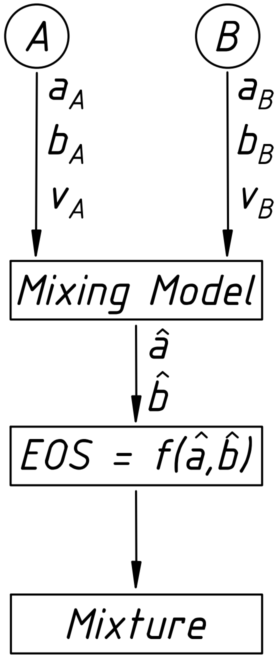


Oefelein and Yang (1998)

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

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

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

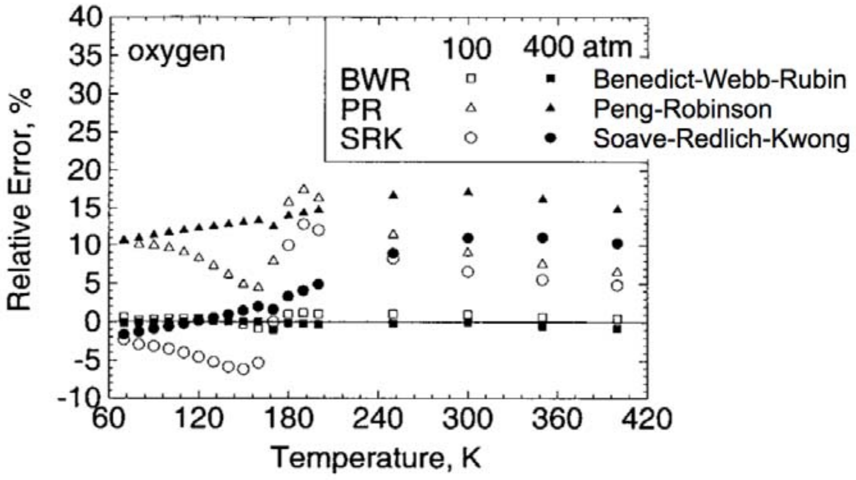
$$Z_{\mathrm{cr},i,j} = \frac{1}{2}\left(Z_{\mathrm{cr},i} + Z_{\mathrm{cr},j}\right),$$

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

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

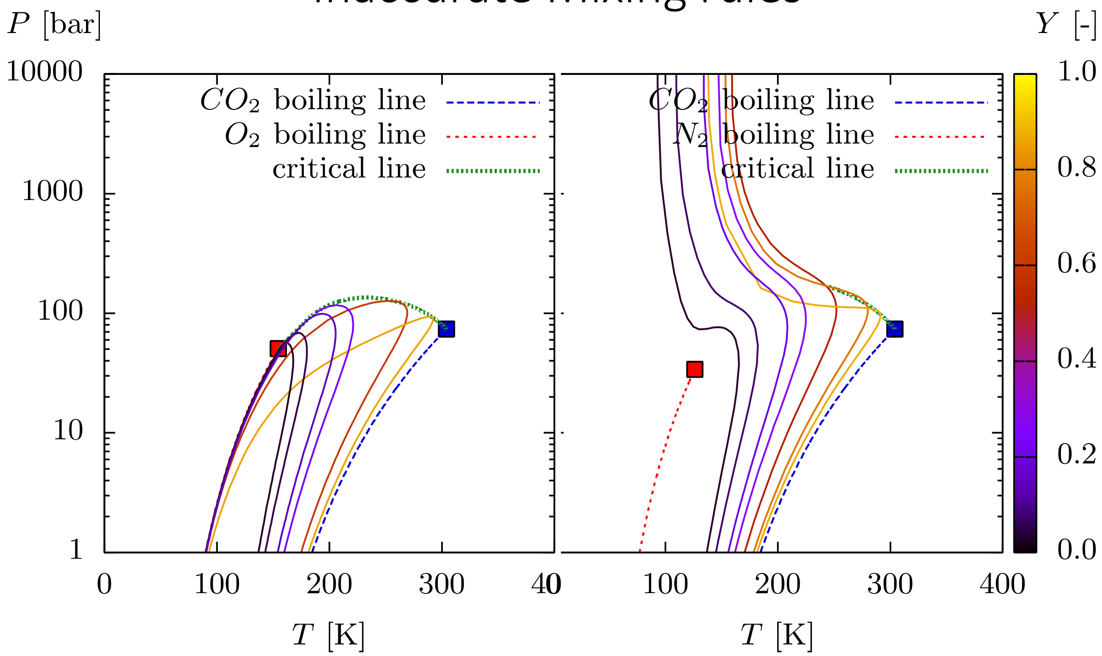
Main Deficiencies

Inaccurate EOS



Yang 2000

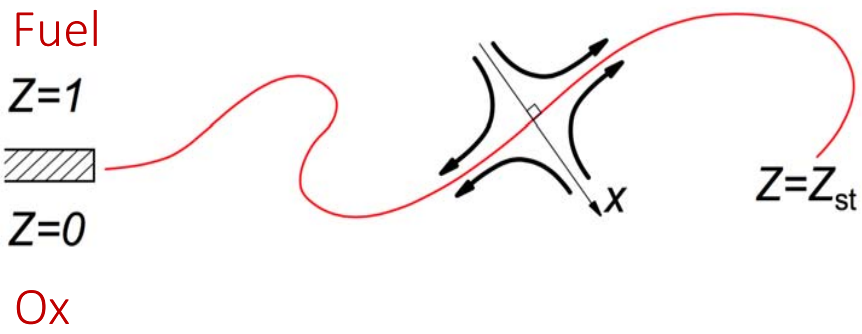
Inaccurate Mixing rules



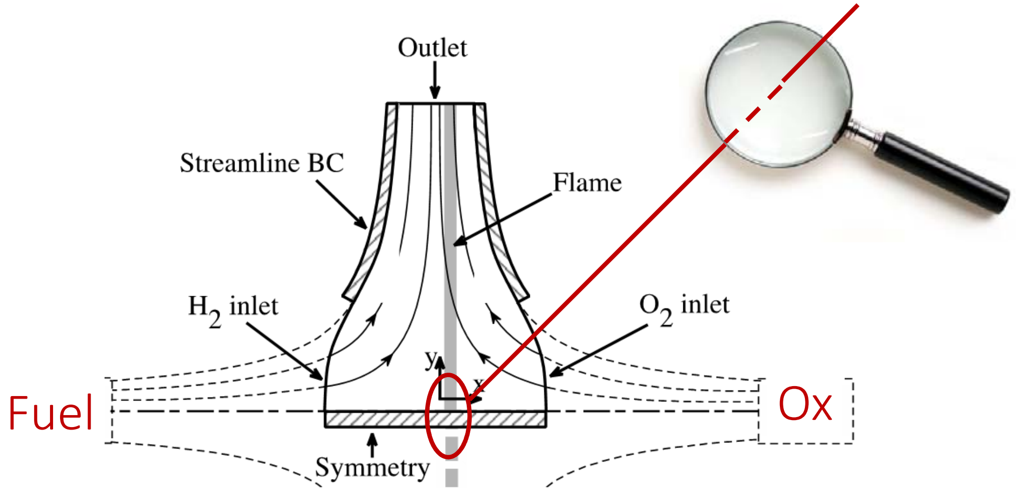
vdW mixing rules always assume Type I mixture

Not applicable for many technical mixtures

1D flame representation - flamelet

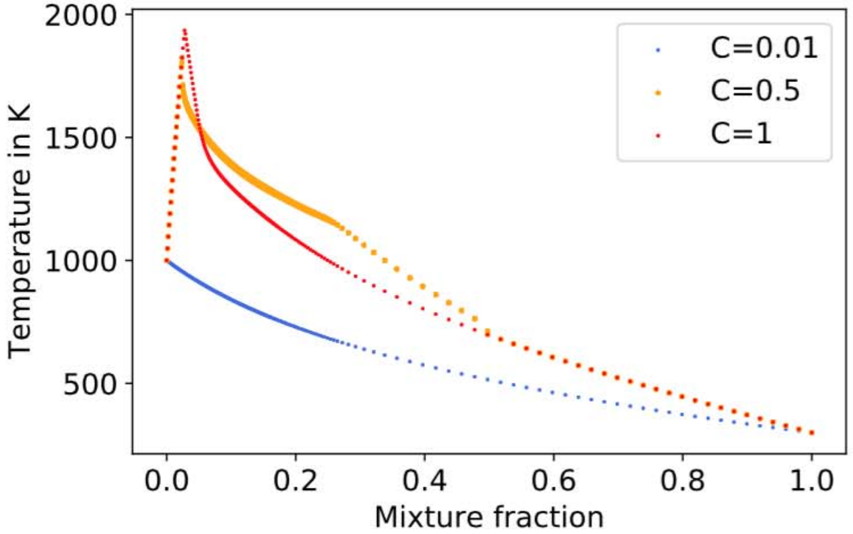


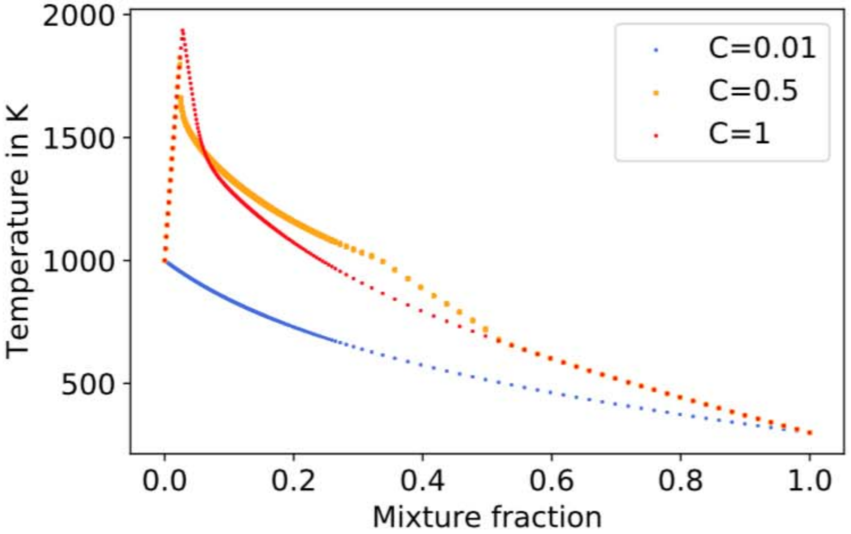
‘Mixture fraction’ as variable transformation



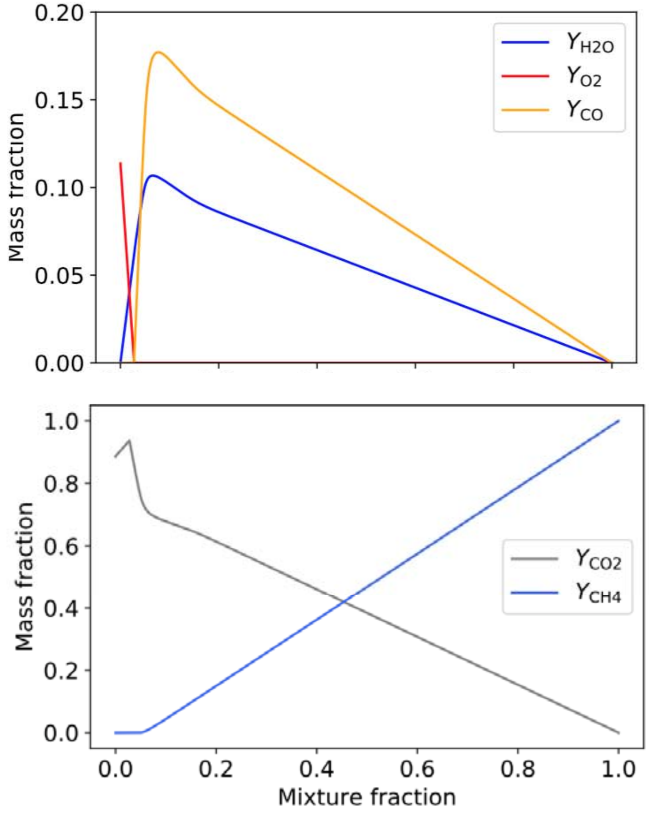
Lacaze & Oefelein CnF 2012

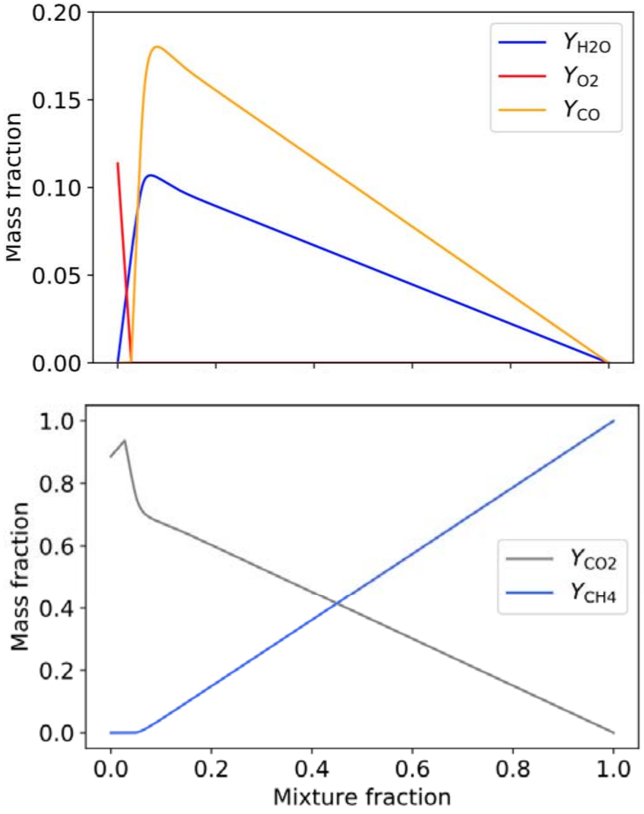
1D flame profiles


GRI 3.0

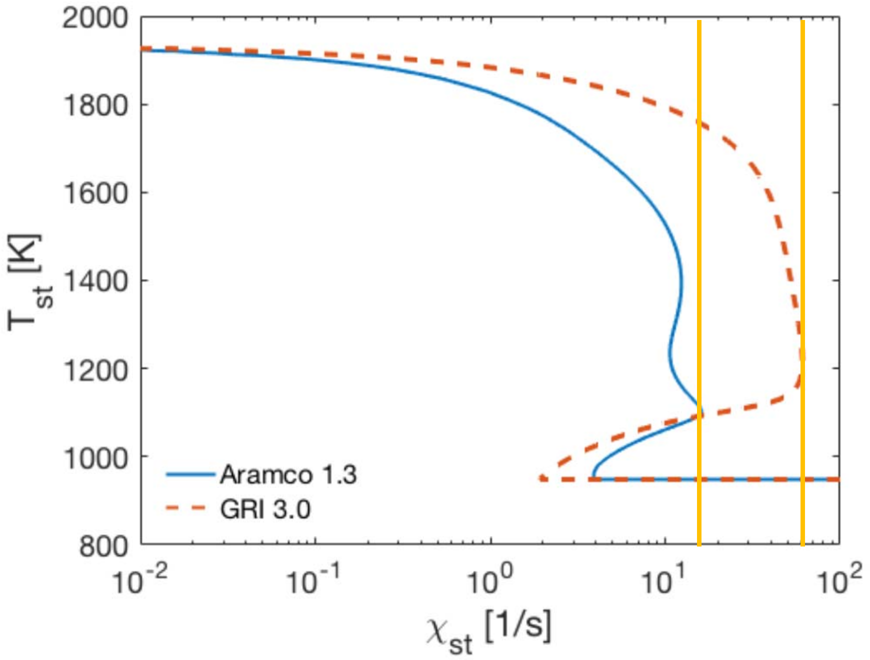

Aramco 1.3

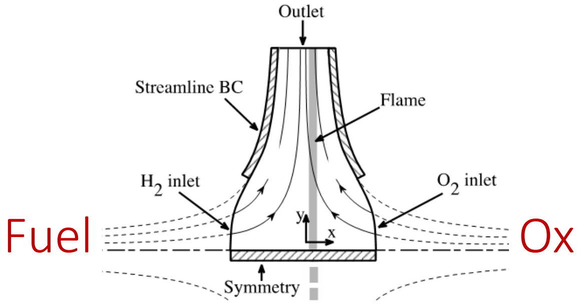
Species distributions


GRI 3.0


Aramco 1.3

Main differences between mechanisms





Signficant discrepancy in maximum strain rate introduced uncertainty for injector studies

Flame thickness

- Decreases with pressure
- Deviation between models for pressures > 10 bar

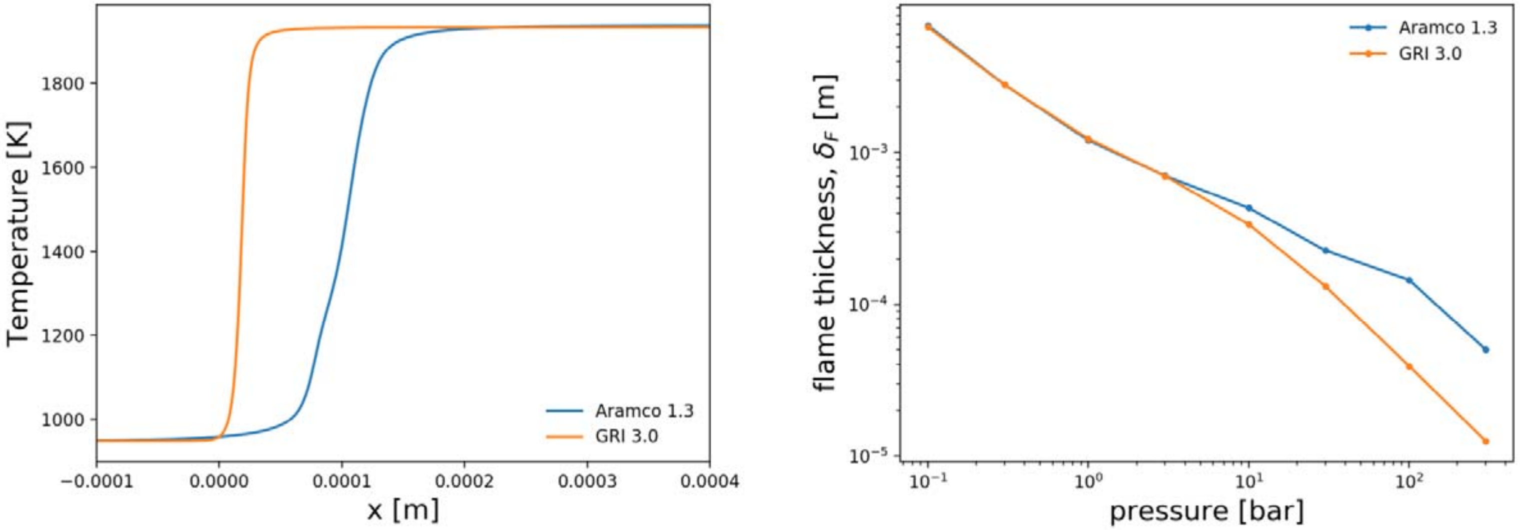
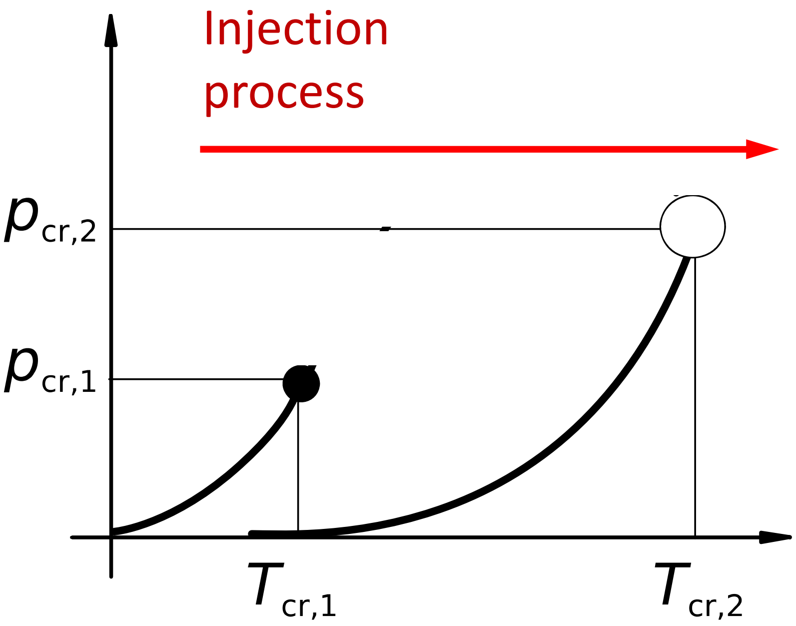
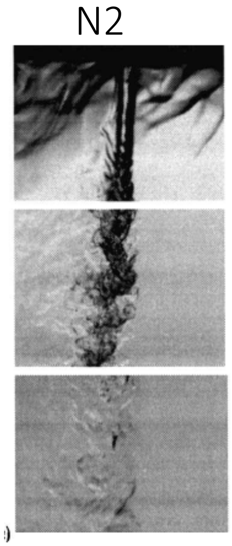


Figure 11: Laminar premixed flames in a stoichiometric mixture of CH_4-O_2-CO_2 using two different kinetic mechanisms. (left) Flame structure at 300 bar and (right) laminar flame thickness, δ_F, versus pressure.

Assess relevance of real fluid effects



Nitrogen into



Mayer et al. (1998)

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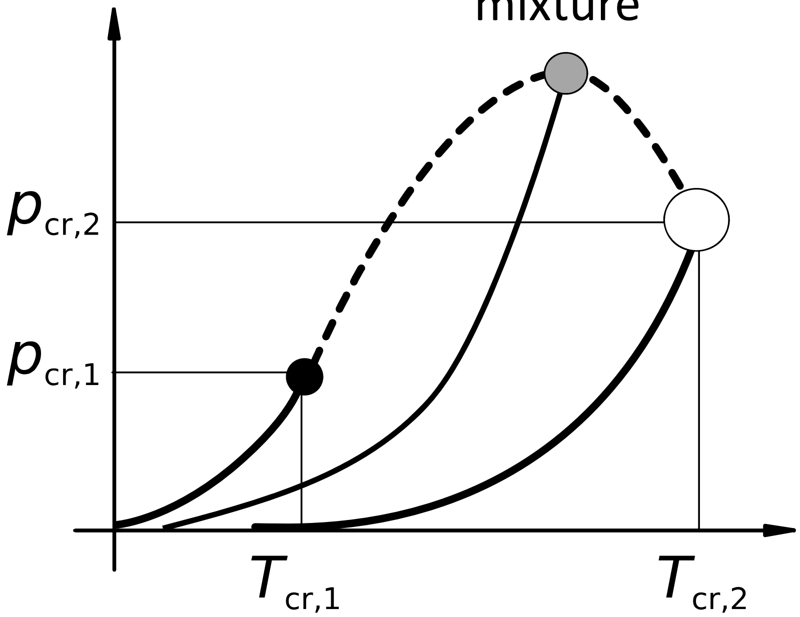

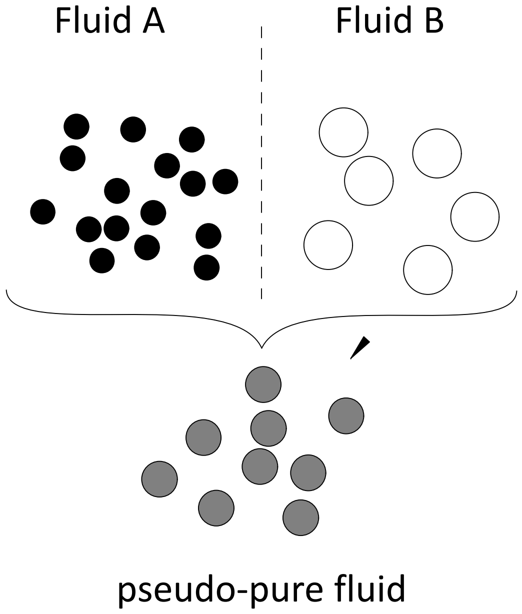

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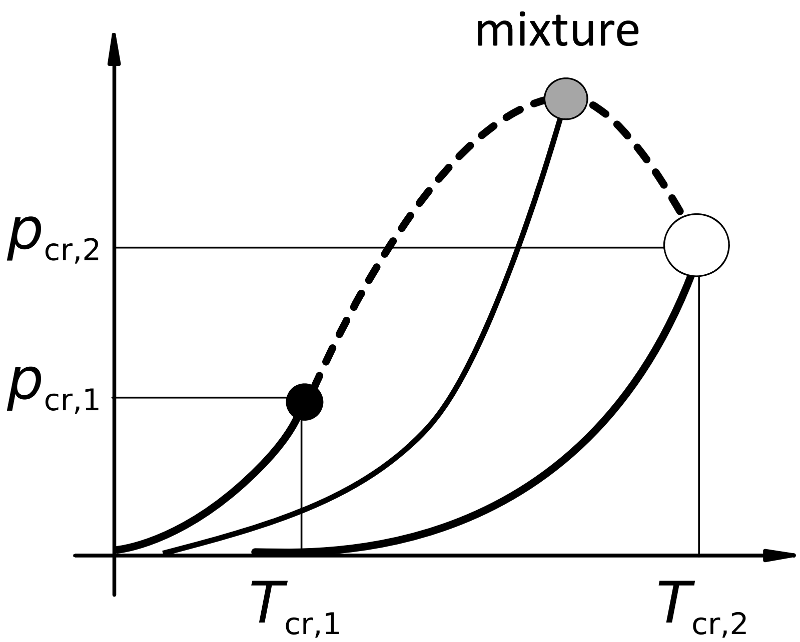
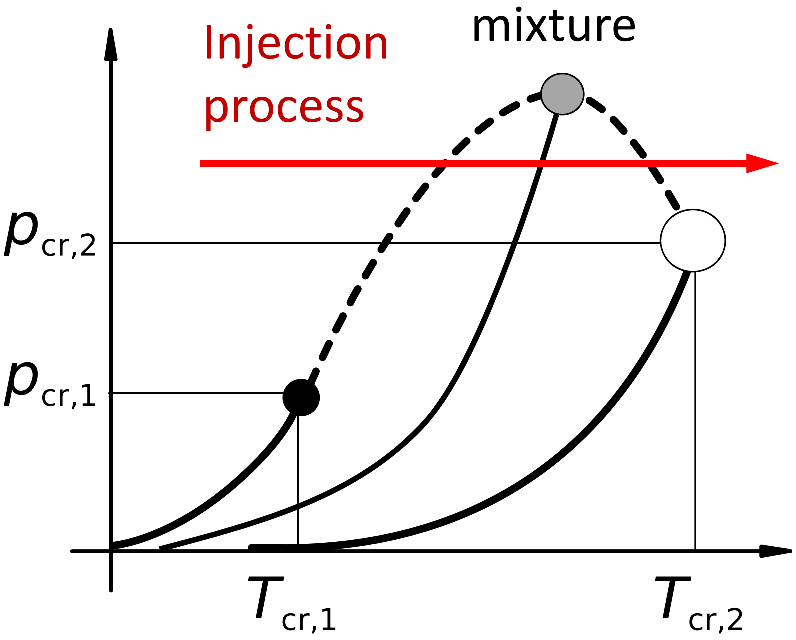


Reid et al. 1987

$$T_{\mathrm{mix,cr}} = \sum_{\alpha=1}^{N_S} X_\alpha T_{\alpha,\mathrm{cr}},$$

$$p_{\mathrm{mix,cr}} = \frac{R T_{\mathrm{mix,cr}} \sum_{\alpha=1}^{N_S} X_\alpha Z_{\alpha,\mathrm{cr}}}{\sum_{\alpha=1}^{N_S} X_\alpha v_{\alpha,\mathrm{cr}}}.$$

Assess relevance of real fluid effects



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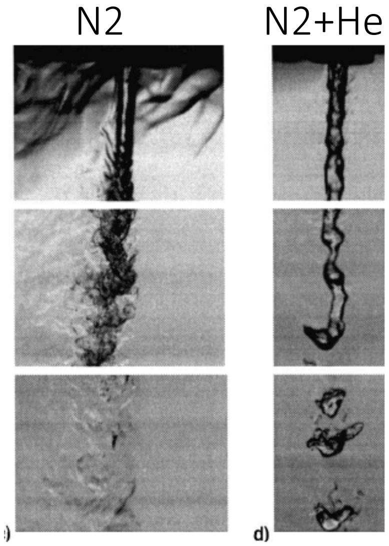
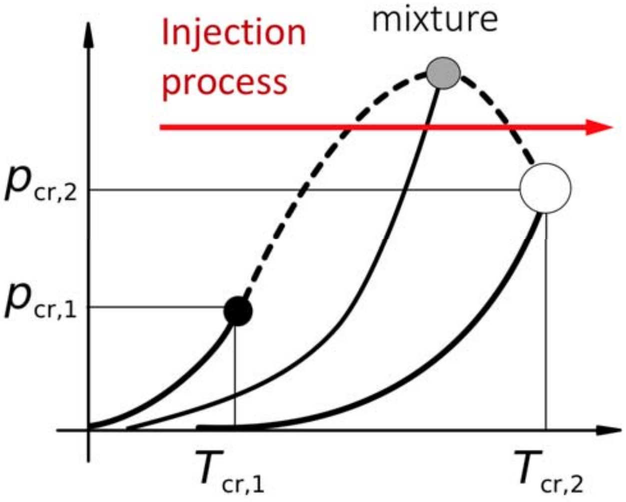
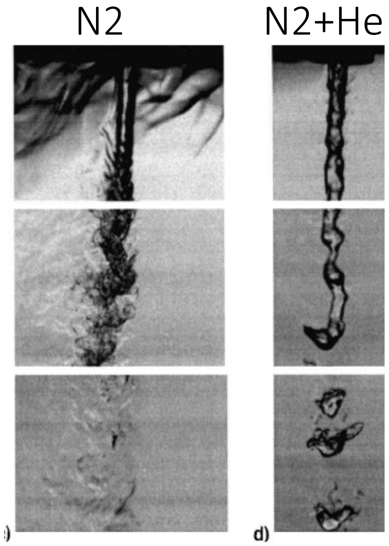


Mayer et al.
(1998)

Assess relevance of real fluid effects

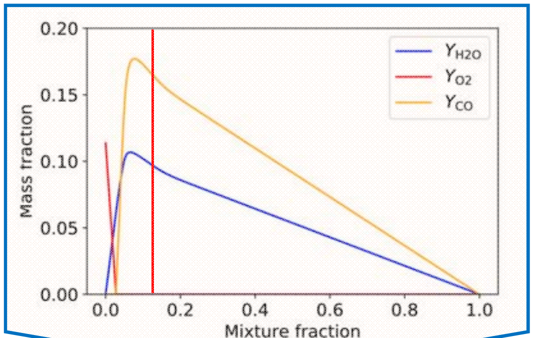


Nitrogen into



Mayer et al.
(1998)

Thermodynamic flame trajectory



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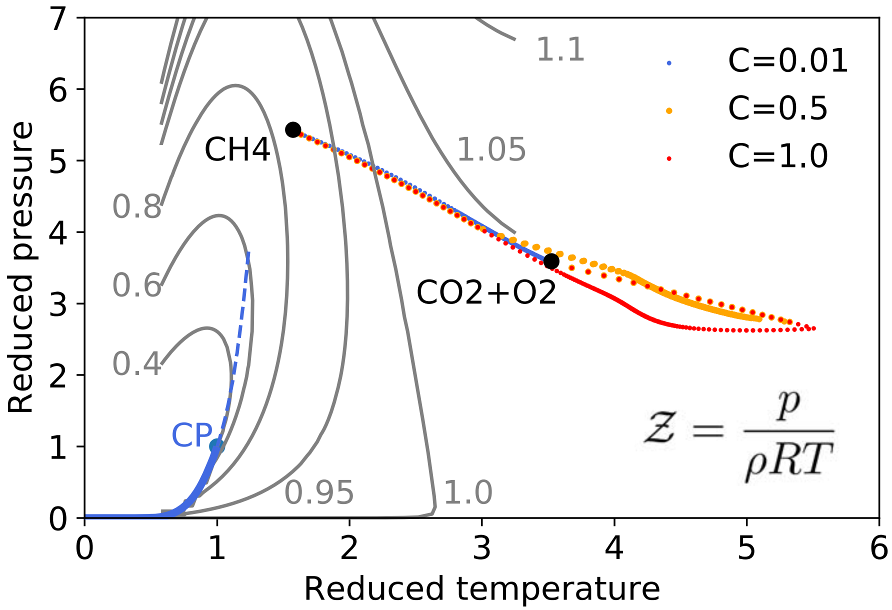
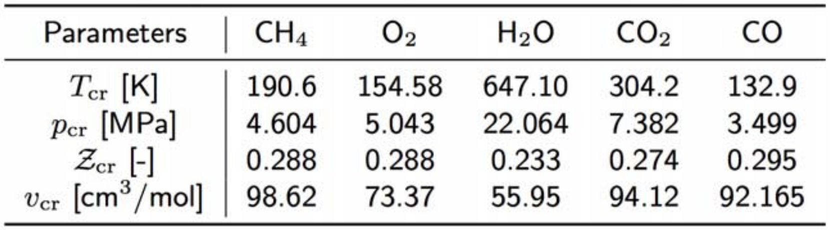
$$p_\mathrm{r} = \frac{p}{p_\mathrm{cr}} \qquad T_\mathrm{r} = \frac{T}{T_\mathrm{cr}}$$

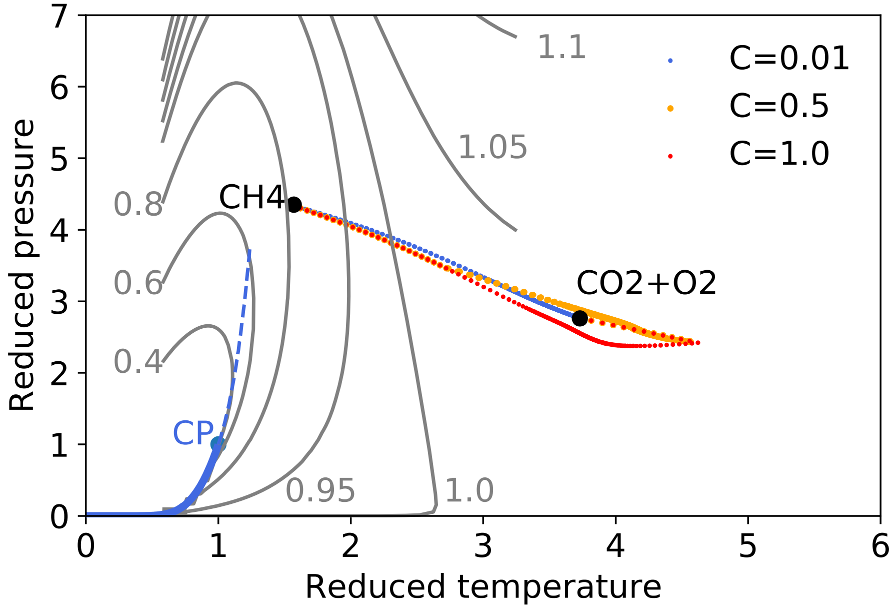
Banuti et al. AIAA 2016-4789





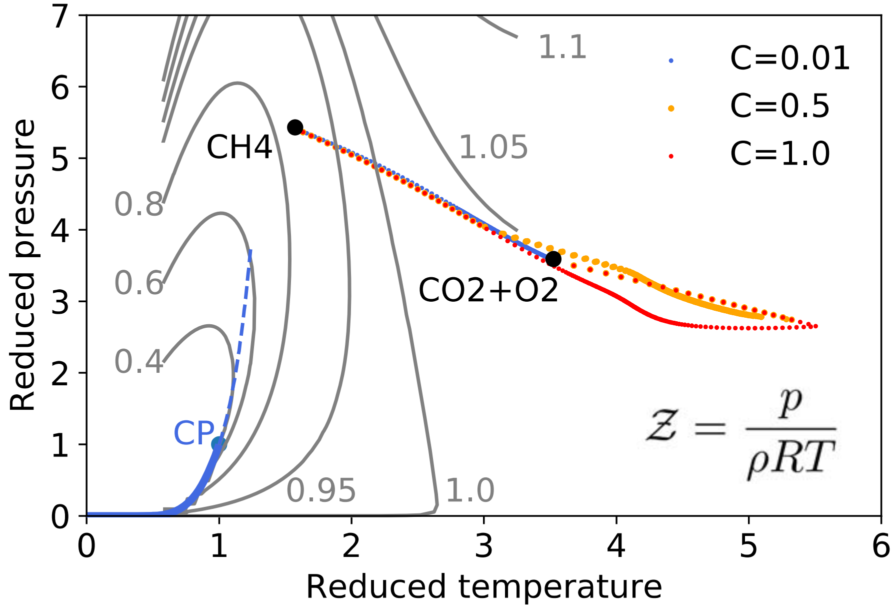
Parameters	CH_4	O_2	H_2O	CO_2	CO
T_{cr} [K]	190.6	154.58	647.10	304.2	132.9
p_{cr} [MPa]	4.604	5.043	22.064	7.382	3.499
$\mathcal{Z}_{\mathrm{cr}}$ [-]	0.288	0.288	0.233	0.274	0.295
v_{cr} [cm^3/mol]	98.62	73.37	55.95	94.12	92.165

Impact of operating conditions



p = 20 MPa
TFu = 300K
TOx = 1100K
YO2 = 0.05
YCO2 = 0.95

Chong et al.
AIAA 2017-0141



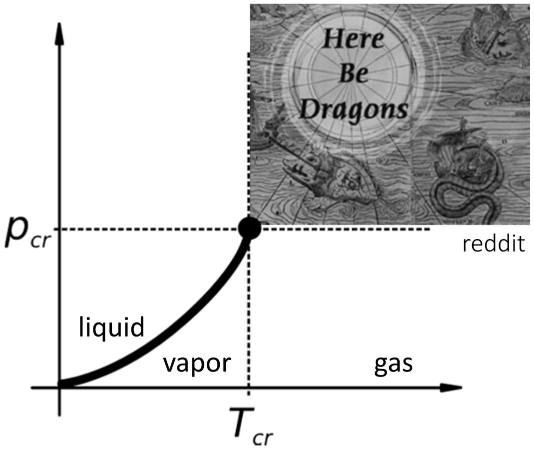
$$\mathcal{Z} = \frac{p}{\rho R T}$$

p = 25 MPa
TFu = 300K
TOx = 1000K
XO2= 0.15
XCO2 = 0.85

~Delimont UTSR 2017

Objectives

What is ‘supercritical’ anyway?

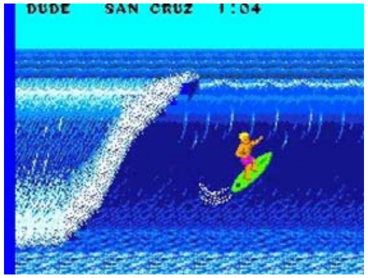


reddit

Identify and analyze model

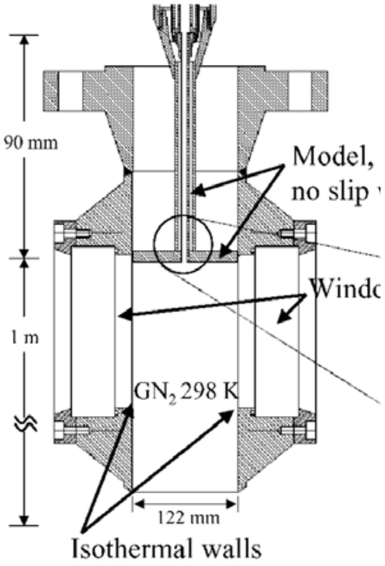
reddit

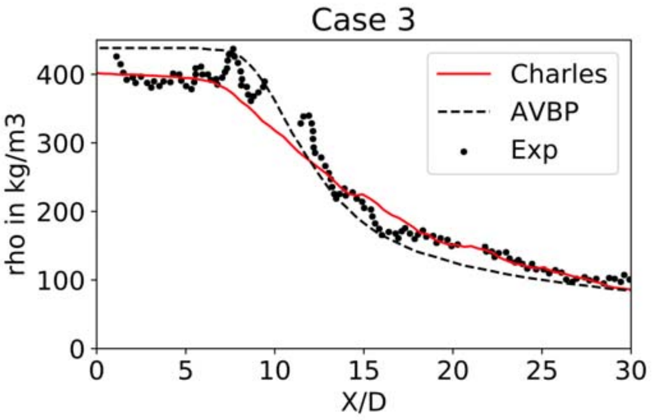
Perform simulations!

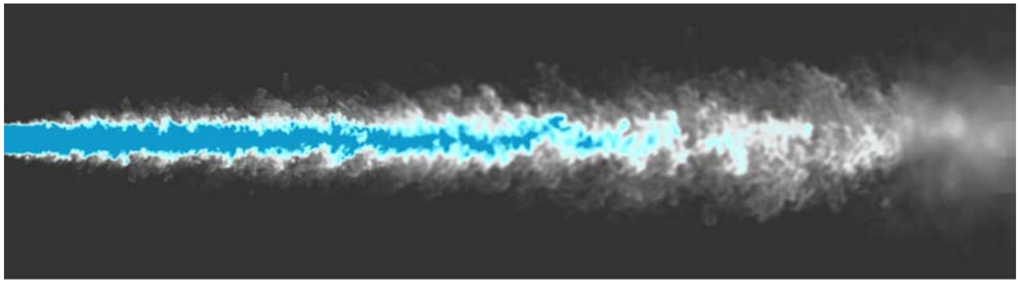


california games

Transcritical nitrogen injection



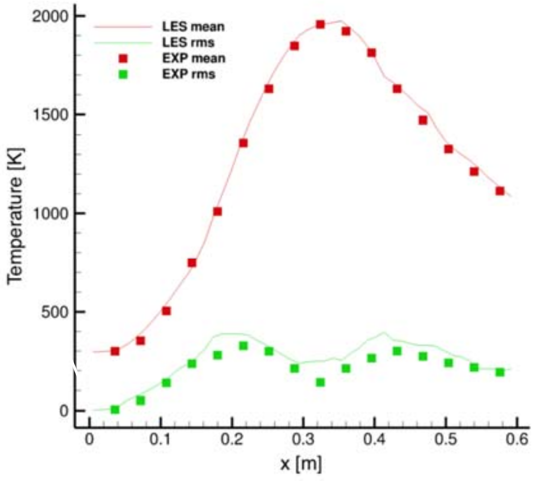




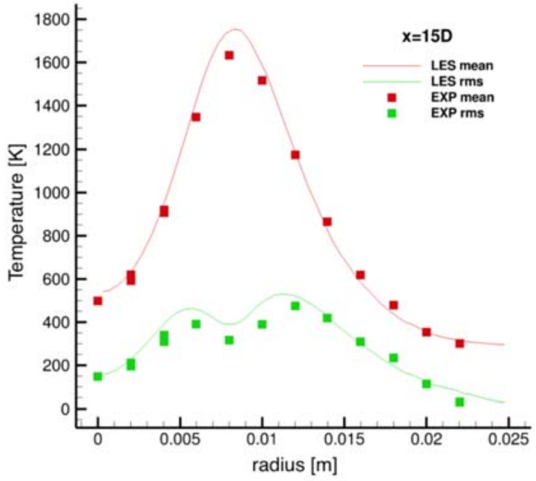
Pure real fluid injection

- Mayer & Branam 2003
- Test EOS implementation
- Test real fluid dynamics & numerics
- No mixture models
- Agreement very good

Sandia Flame D



(a) centerline temperature



(b) radial temperature at $x/D = 15$

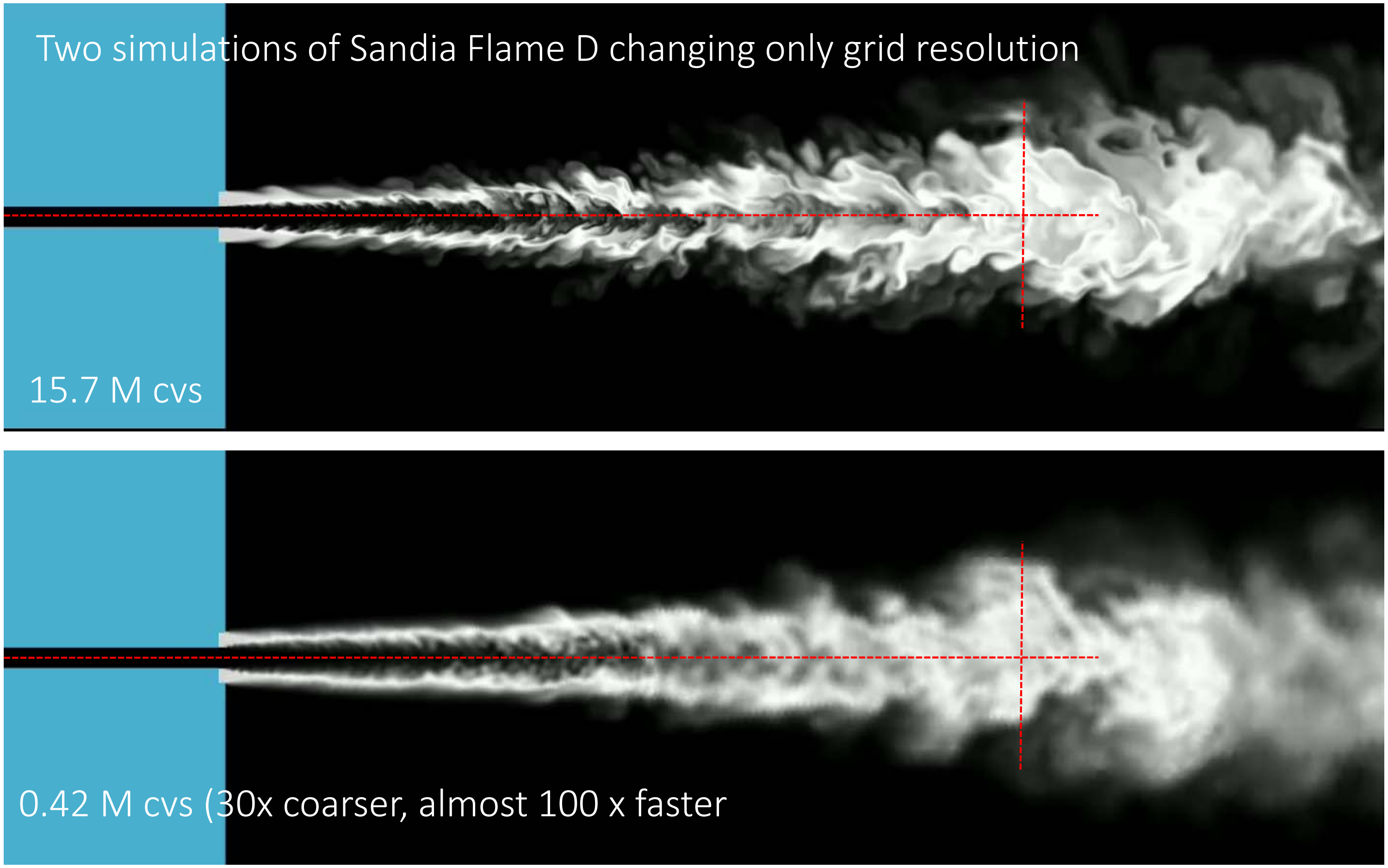
Reactive mixture

- Barlow et al. 2005
- Multispecies transport
- Partially premixed
- Flamelet progress variable approach
- Agreement very good

Jet: CH4/Air
Co-flow: C2H2, H2, air, CO, and N2

Quantitative impact of entropy-preserving schemes (I)

Application to Sandia Flame D



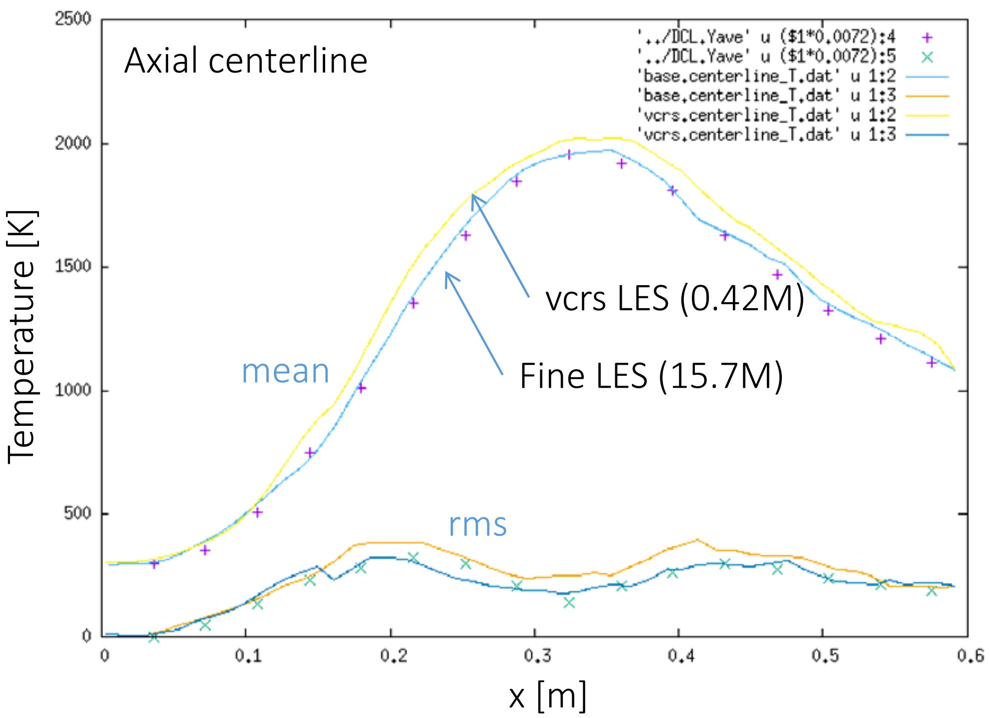
Two simulations of Sandia Flame D changing only grid resolution

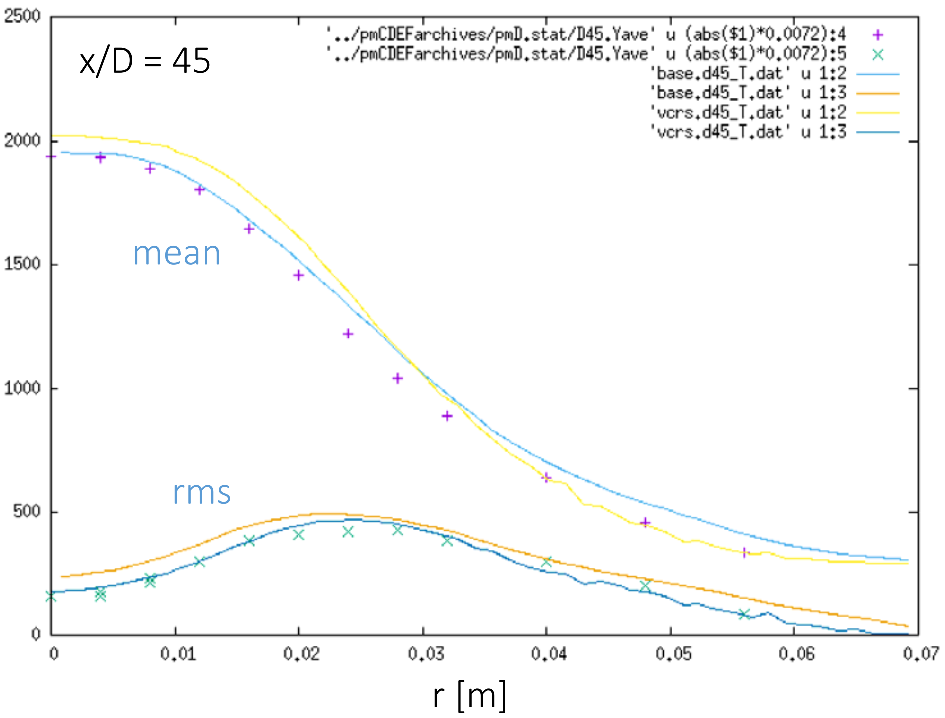
Compare temperature profiles for axial centerline and radial profiles where the centerline temperature peaks

Both locations are sensitive to the addition of numerical dissipation – either from spurious diffusion of hot products or spurious entrainment of the surrounding air

Quantitative impact of entropy-preserving schemes (II)

Application to Sandia Flame D

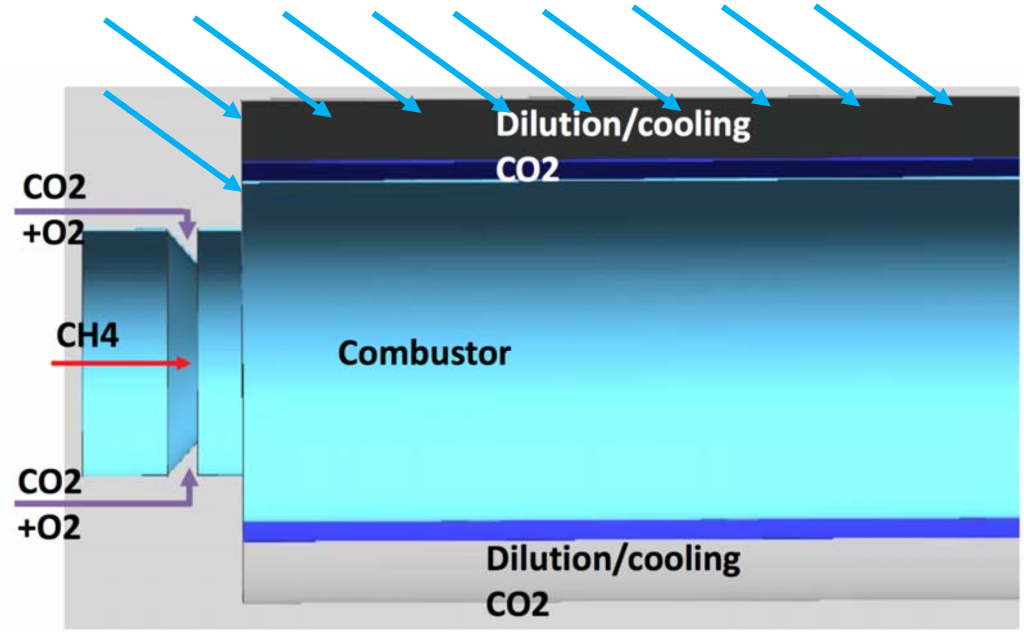




LES statistics compare remarkably well with experiment from both “fine” and *very* “coarse” LES

SwRI sCO2 Swirl Combustor

Effusion cooling: constant mass flux bypass

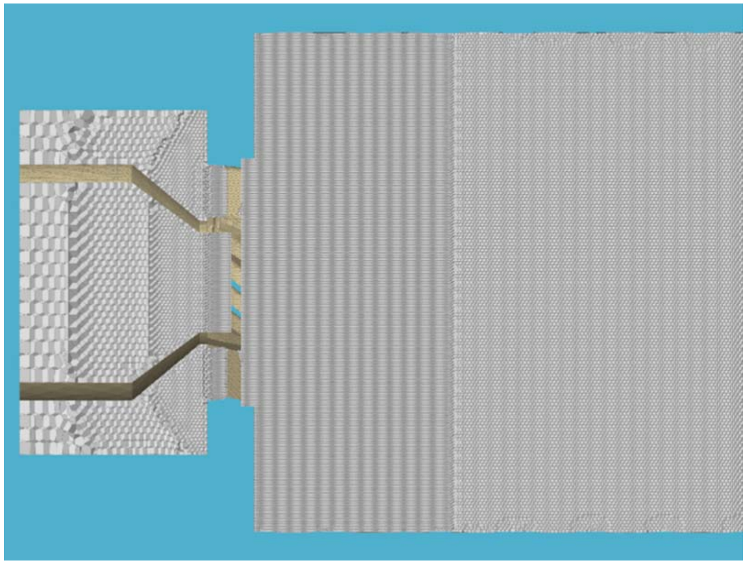


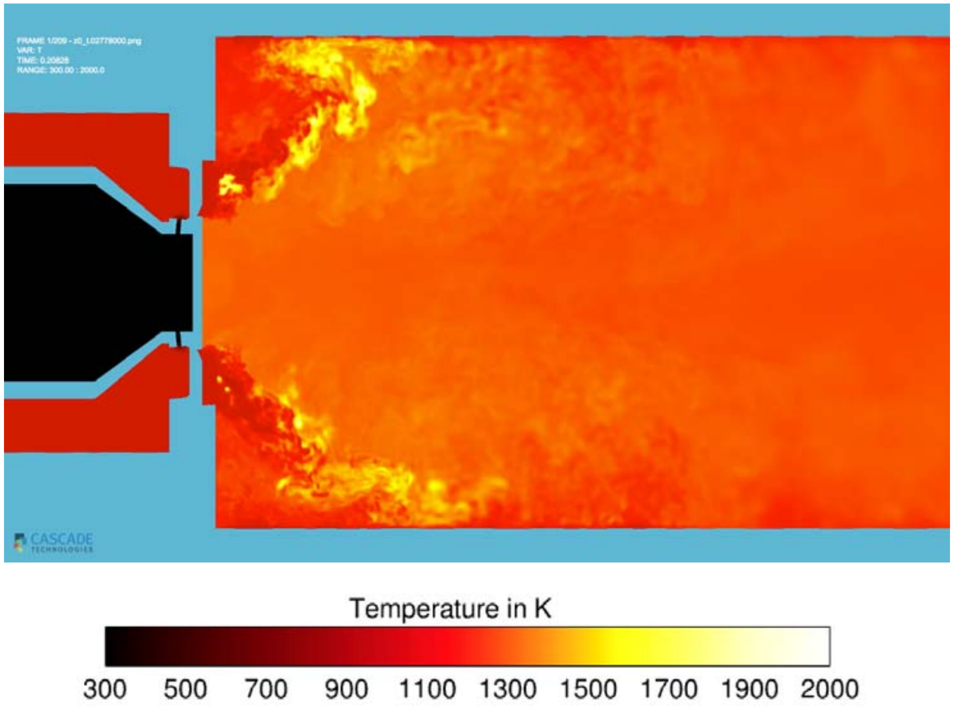
Delimont UTSR 2017

Component	Mass flow in kg/s
CH_4	0.02
O_2	0.08
CO_2 combustor	0.626
CO_2 bypass	0.899
Total	1.625

SwRI sCO2 Swirl Combustor

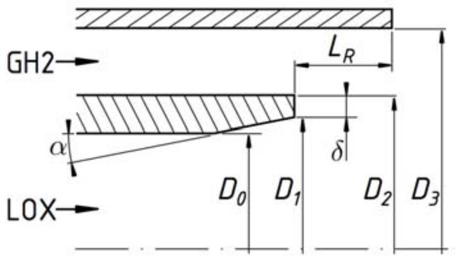
Delimont 2017



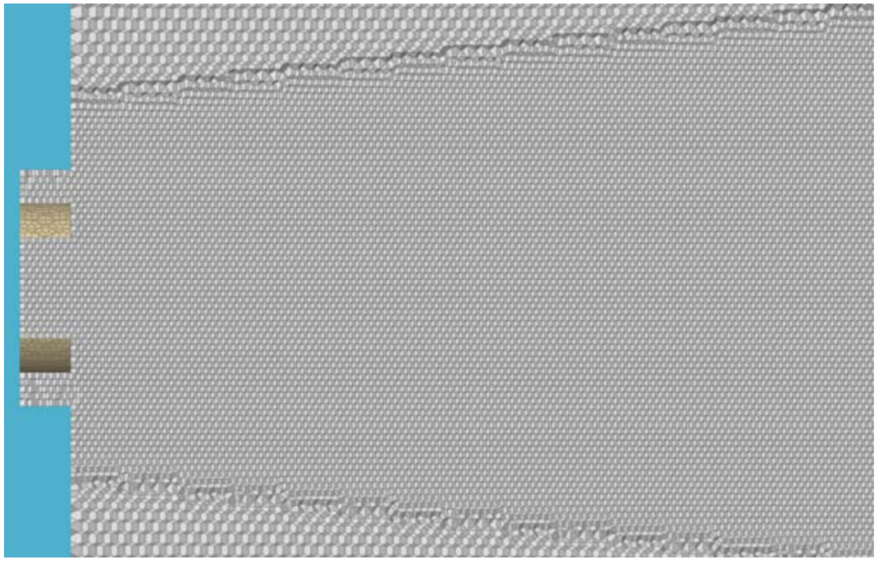


Component	$\dot{m}$ in kg/s	T_{in} in K	ρ_{in} in kg/m^3	X_i	Position
CH_4	0.02	300	186.3	1.0	center
O_2	0.08	1000	90.23	0.15	annulus
CO_2	0.626	1000	125.0	0.85	annulus

Coaxial injector – reduce wall heat loads

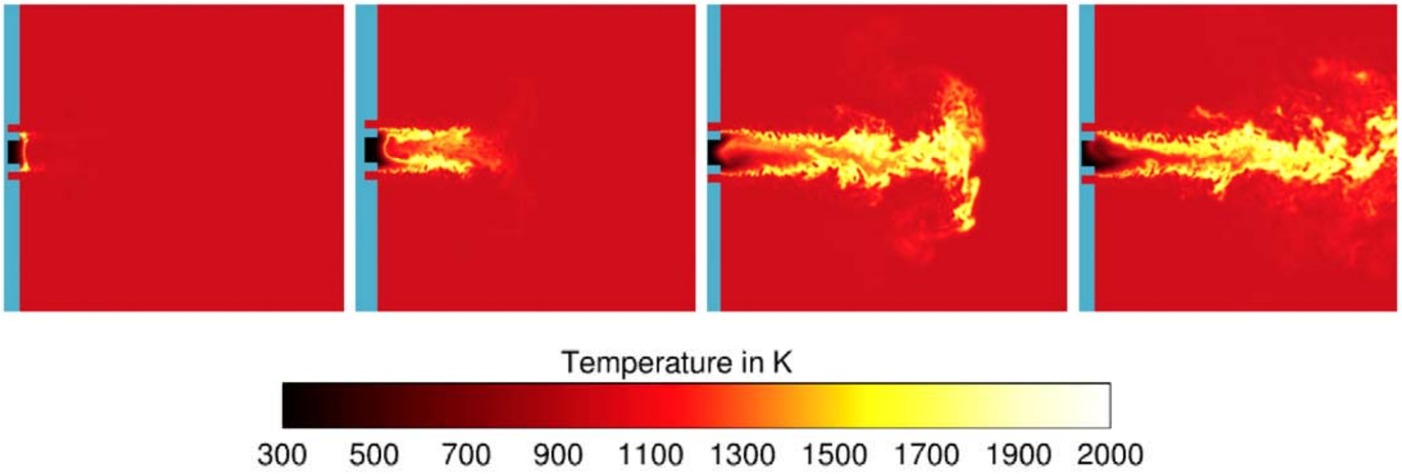


D_0	D_2	D_3	α	L_R	D
0.003	0.005	0.007	0	0	0.0508



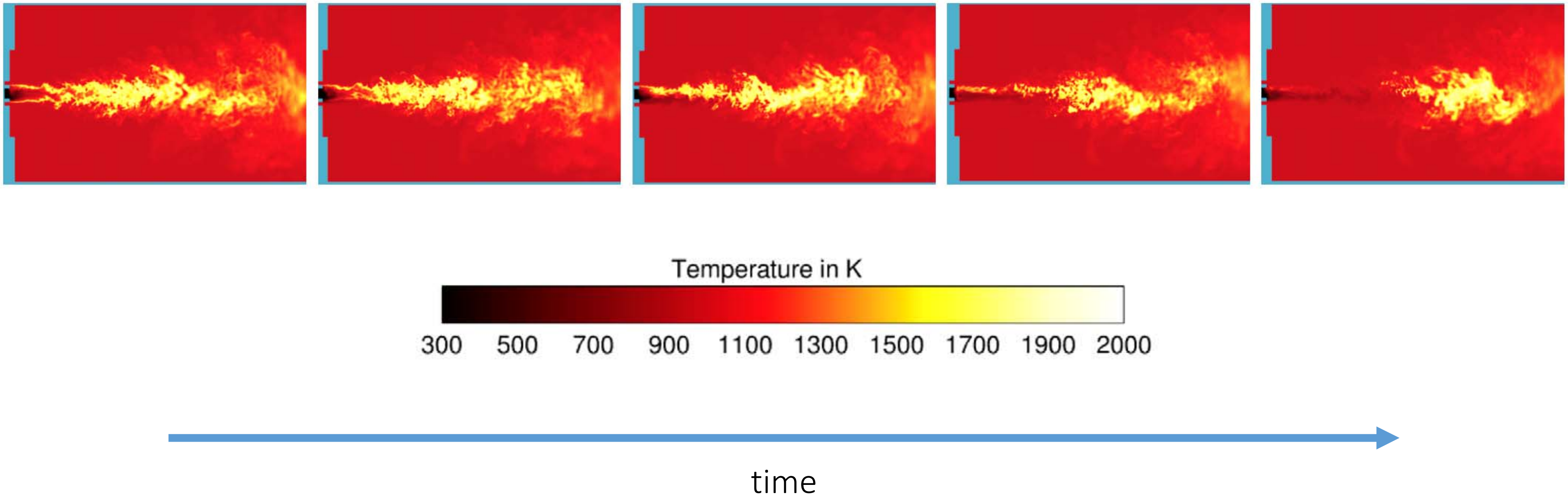
Component	$\dot{m}$ in kg/s	T_{in} in K	ρ_{in} in kg/m^3	X_i	Position
CH_4	0.02	300	186.3	1.0	center
O_2	0.08	1000	90.23	0.15	annulus
CO_2	0.626	1000	125.0	0.85	annulus

Transients – start up

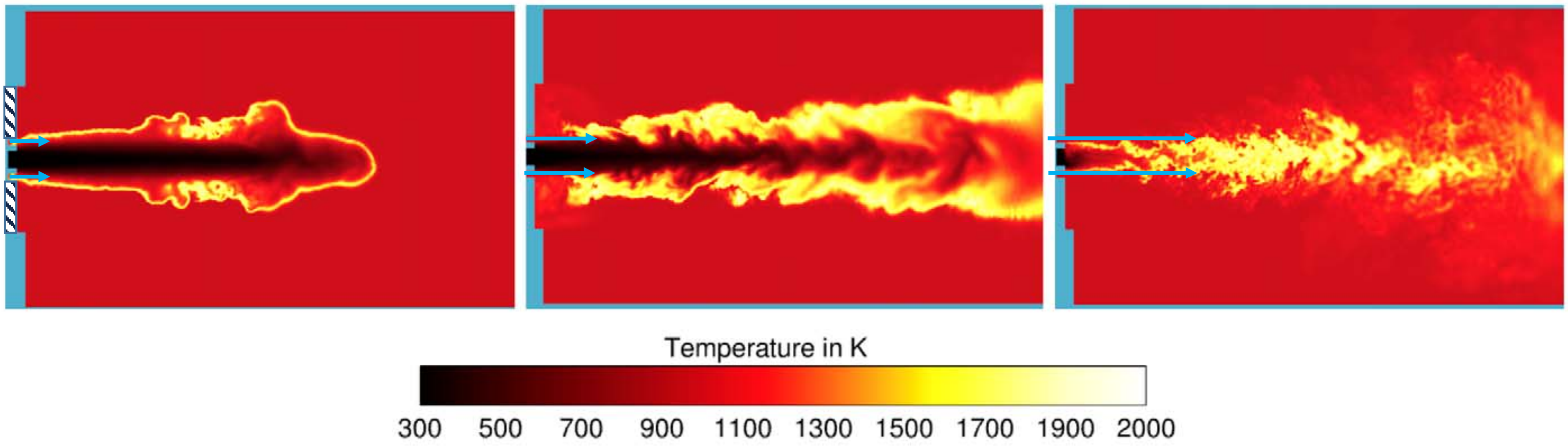


time

Transients – blow out



Different mixing regimes



Essentially laminar CH4 jet, insufficient mixing

Flame anchored in Recirculation zone

Flame blowout due to too high shear

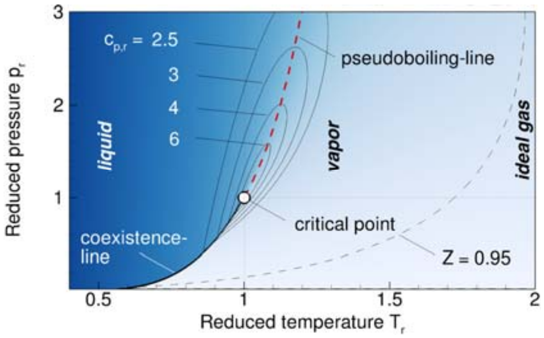
Increasing co-flow mass flow

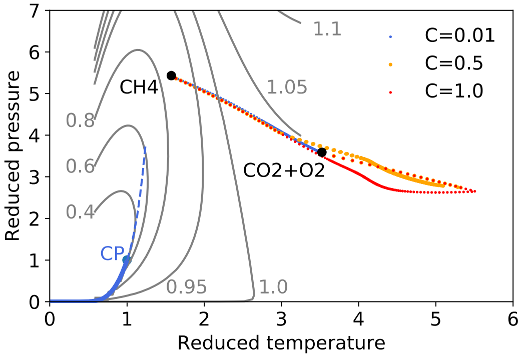
Conclusions

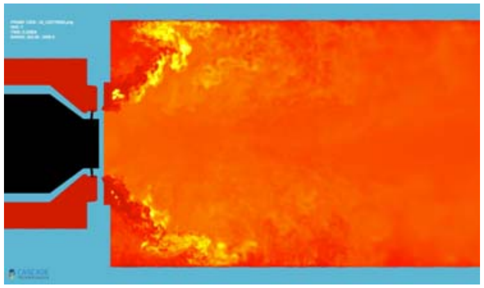
- Goal: develop HPC CFD for sCO2 combustion
- Supercritical fluids can be ideal gases, subcritical gases can be real fluids
- In sCO2 combustion, even hot reaction gases may exhibit real fluid properties
- Solver validated for pure real fluids and combustion
- Preliminary ideal gas sCO2 results promising
- Next step: reactive real fluids

- Q: Why not burn pure CH4+O2, and dilute later?

dbanuti@cascadetechnologies.com







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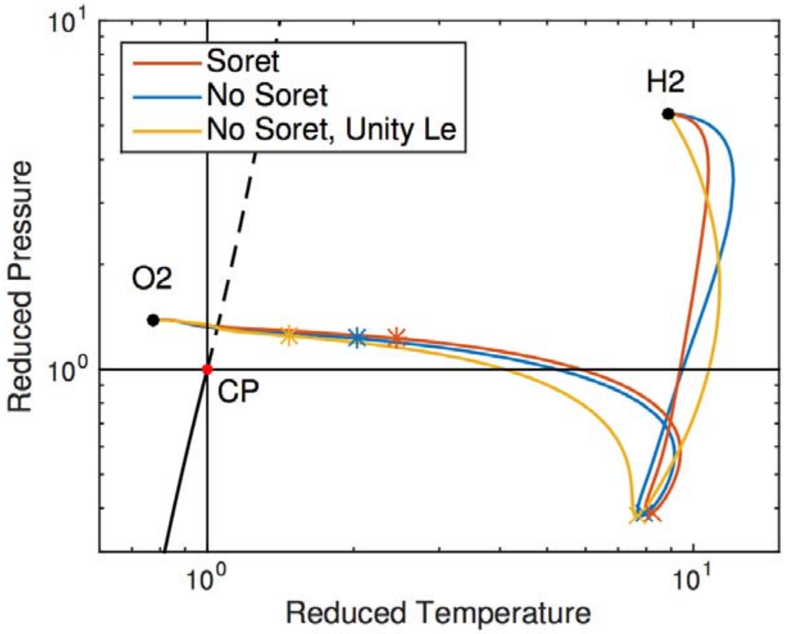
TECHNOLOGIES

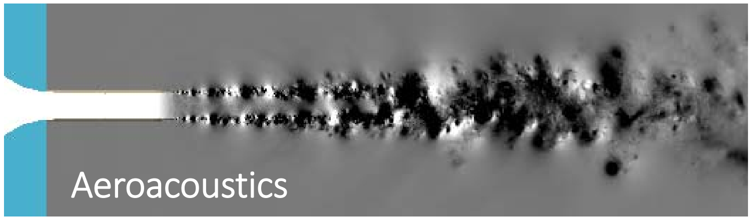
Discovery through simulation

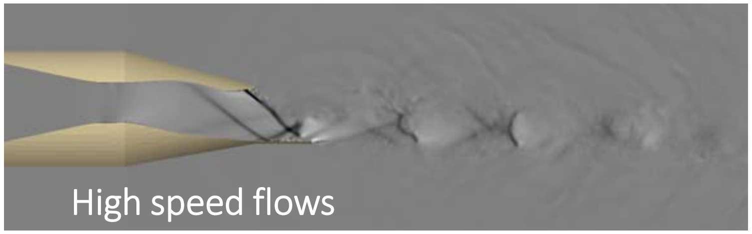
LOX/GH2 flame trajectory - transport



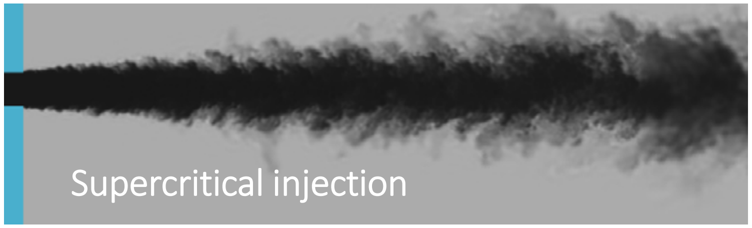
- End points and flame not affected
- Reduced diffusion in real fluid makes trajectory more horizontal

Stability using physics, not dissipation!


Aeroacoustics


High speed flows


Reacting flows


Supercritical injection

Kinetic energy, entropy preserving (KEEP) schemes

- Discrete entropy framework used to develop low dissipation fluxes has been generalized to treat a variety of flow regimes (e.g., high speed flows, reacting flows, real gas effects)
- Leads to a stable, homogenous flux discretization without complex sensors, upwinding hybridization, or tuning of coefficients for stability

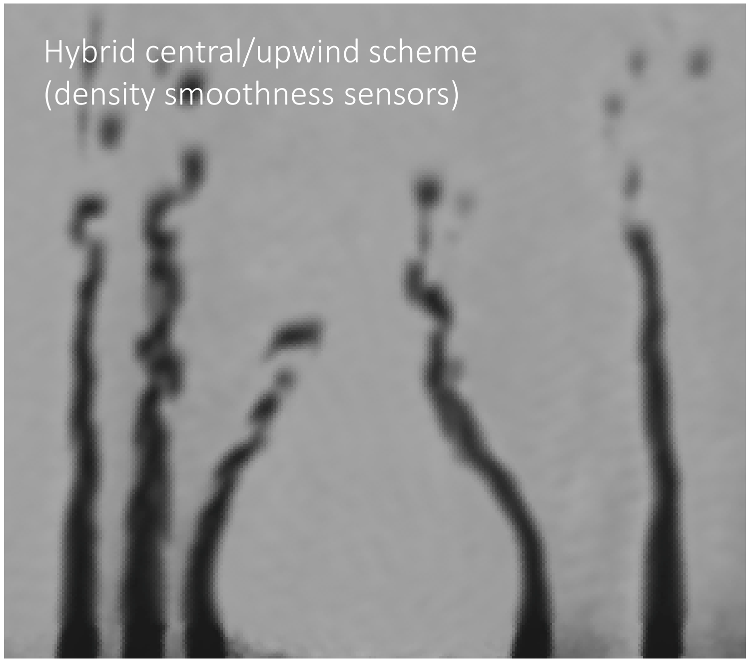
Stability conditions based on discrete satisfication of Gibbs-Duhem condition (2nd law of thermodynamics)

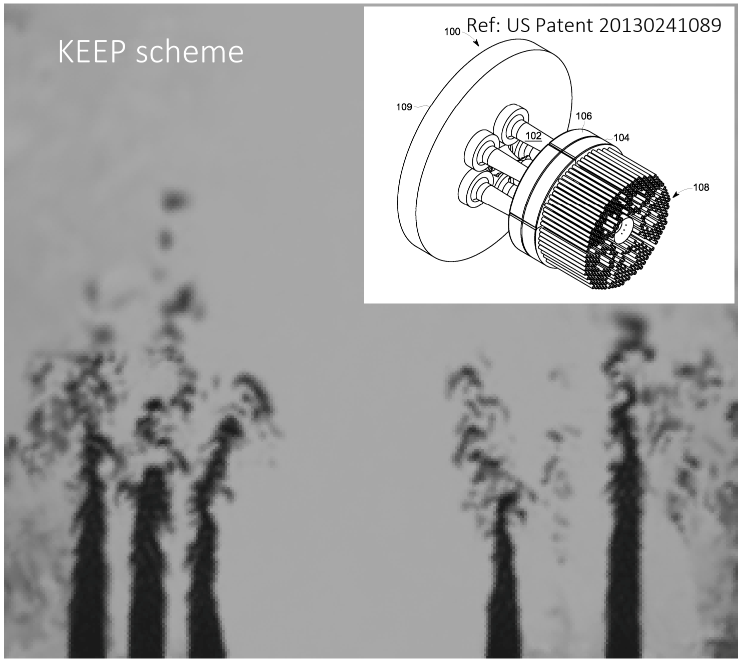
$$d(\rho s) = \frac{1}{T} d(\rho E) - \frac{u}{T} d(\rho u) + \left(s + \frac{u^2}{2T} - \frac{h}{T} \right) d\rho$$

$$\Delta w_i f_i + \Delta(\rho u) = 0; w_i = \nabla_\phi(\rho s)$$

KEEP schemes drastically improve solution quality and numerical stability

Example: Premixed combustion in industrial multi-element combustor


Hybrid central/upwind scheme
(density smoothness sensors)


KEEP scheme

Ref: US Patent 20130241089

System level LES calculations necessarily result in coarsely resolved structures

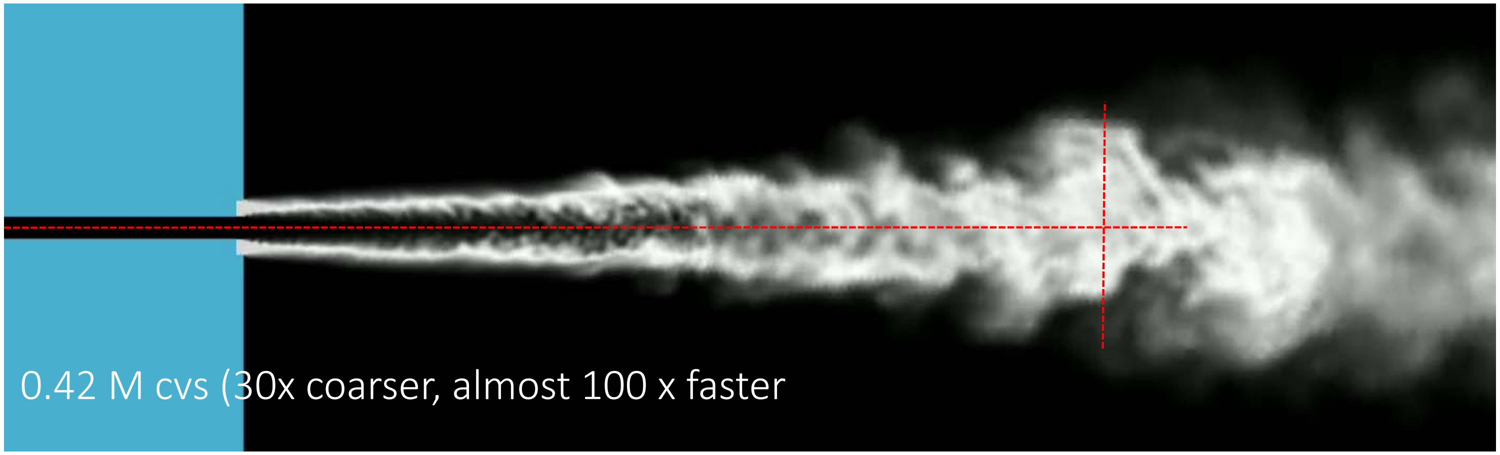
- KEEP schemes improve accuracy (e.g., flame length consistent with experiments)
- Simulations are more robust and less sensitive to mesh resolution and transitions

Quantitative impact of entropy-preserving schemes (I)

Application to Sandia Flame D

Two simulations of Sandia Flame D changing only grid resolution

15.7 M cvs



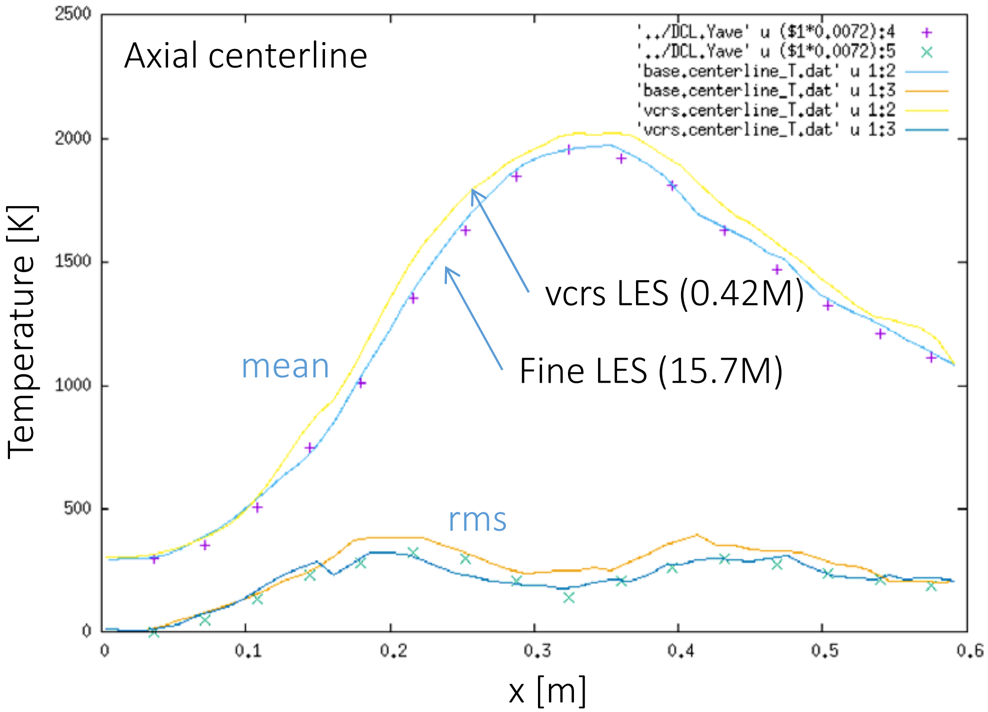
0.42 M cvs (30x coarser, almost 100 x faster

Compare temperature profiles for axial centerline and radial profiles where the centerline temperature peaks

Both locations are sensitive to the addition of numerical dissipation – either from spurious diffusion of hot products or spurious entrainment of the surrounding air

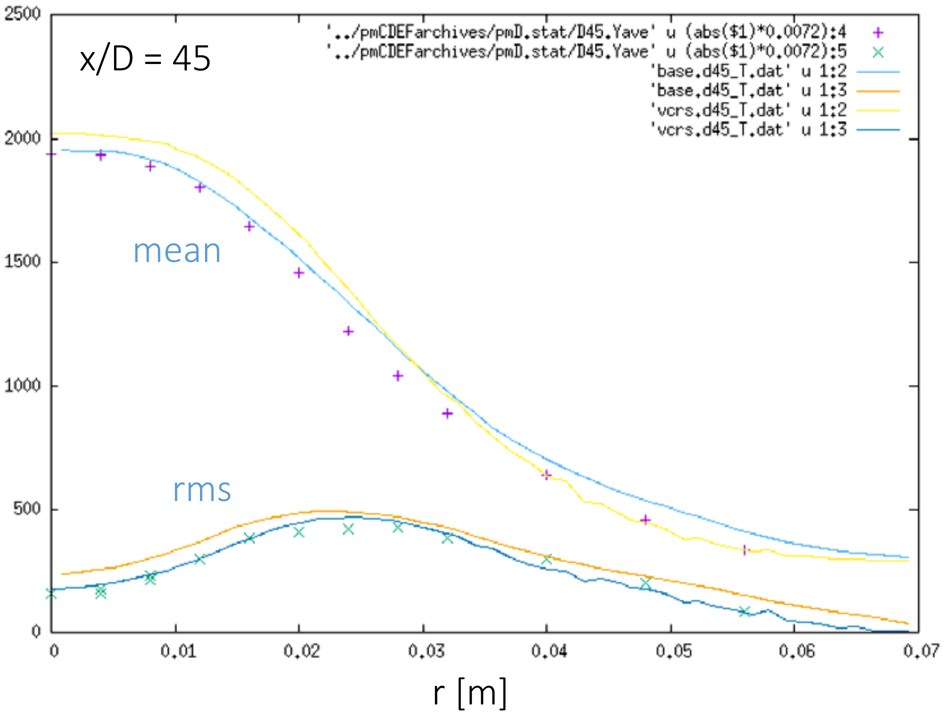
Quantitative impact of entropy-preserving schemes (II)

Application to Sandia Flame D



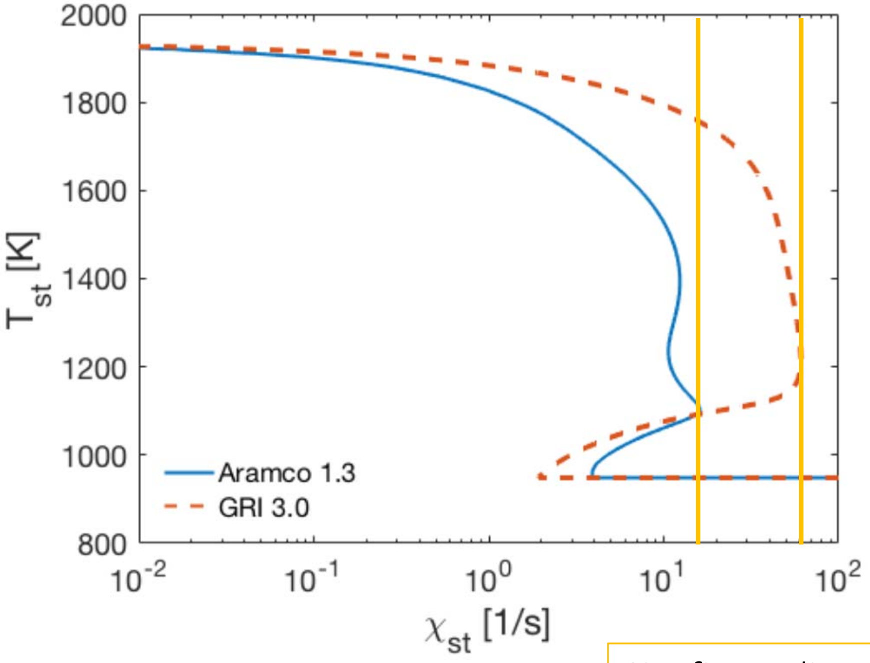
vcrs LES (0.42M)

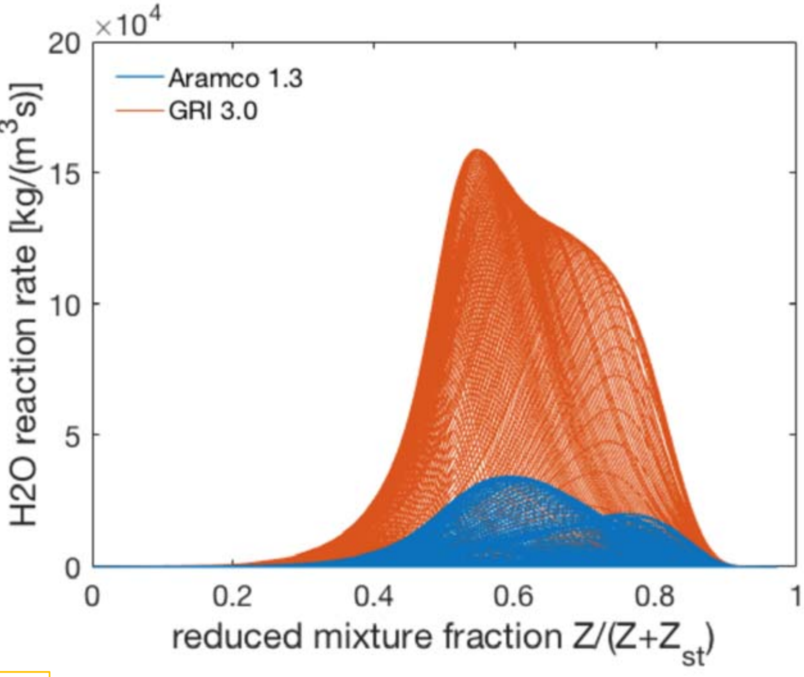
Fine LES (15.7M)



LES statistics compare remarkably well with experiment from both “fine” and *very* “coarse” LES

Main differences between mechanisms

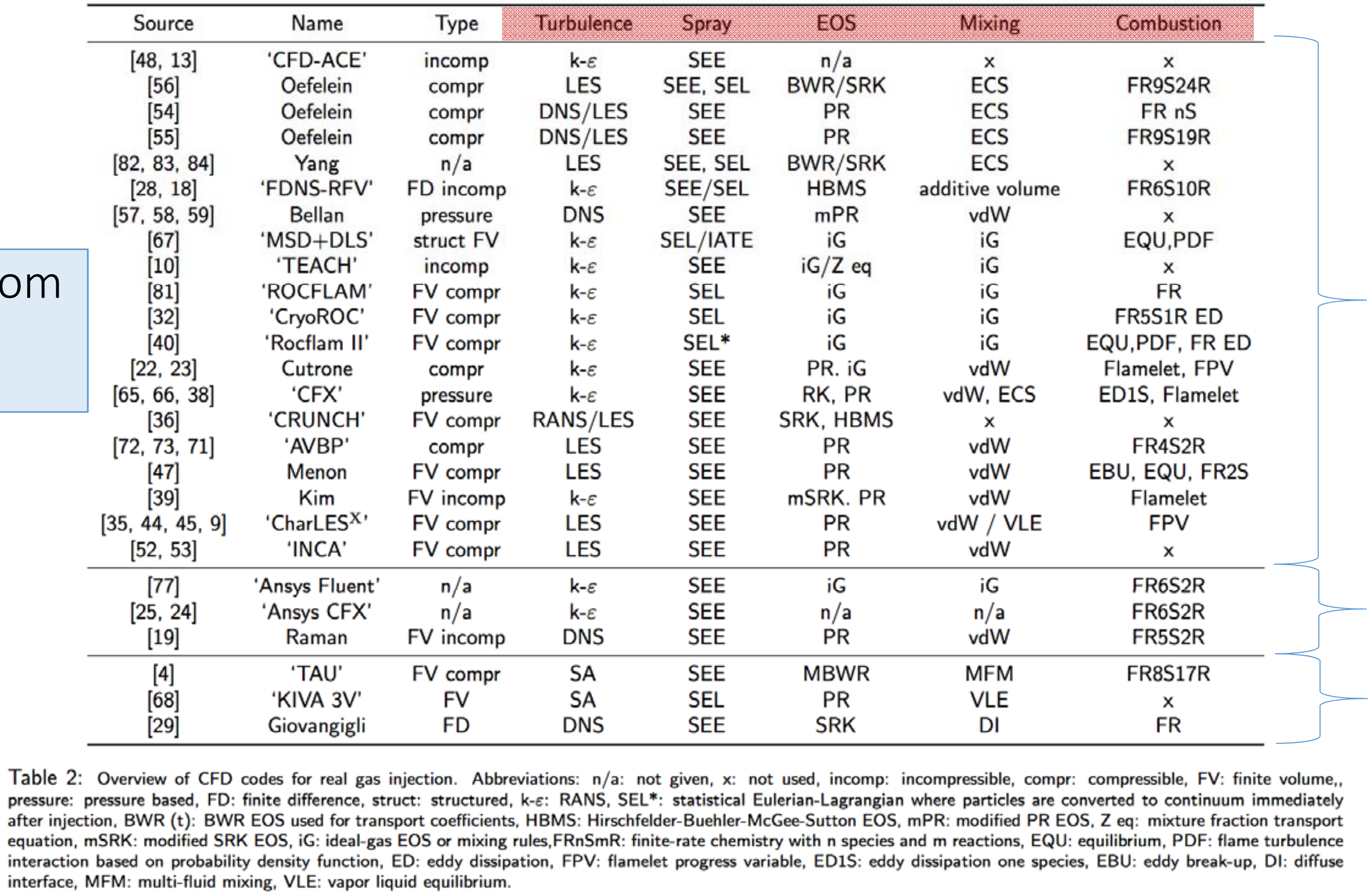




Signficant discrepancy in maximum strain rate introduced uncertainty for injector studies

Literature review

+40 papers from
+20 groups



Source	Name	Type	Turbulence	Spray	EOS	Mixing	Combustion
[48, 13]	'CFD-ACE'	incomp	k-ε	SEE	n/a	x	x
[56]	Oefelein	compr	LES	SEE, SEL	BWR/SRK	ECS	FR9S24R
[54]	Oefelein	compr	DNS/LES	SEE	PR	ECS	FR nS
[55]	Oefelein	compr	DNS/LES	SEE	PR	ECS	FR9S19R
[82, 83, 84]	Yang	n/a	LES	SEE, SEL	BWR/SRK	ECS	x
[28, 18]	'FDNS-RFV'	FD incomp	k-ε	SEE/SEL	HBMS	additive volume	FR6S10R
[57, 58, 59]	Bellan	pressure	DNS	SEE	mPR	vdW	x
[67]	'MSD+DLS'	struct FV	k-ε	SEL/IATE	iG	iG	EQU,PDF
[10]	'TEACH'	incomp	k-ε	SEE	iG/Z eq	iG	x
[81]	'ROCFLAM'	FV compr	k-ε	SEL	iG	iG	FR
[32]	'CryoROC'	FV compr	k-ε	SEL	iG	iG	FR5S1R ED
[40]	'Rocflam II'	FV compr	k-ε	SEL*	iG	iG	EQU,PDF, FR ED
[22, 23]	Cutrone	compr	k-ε	SEE	PR. iG	vdW	Flamelet, FPV
[65, 66, 38]	'CFX'	pressure	k-ε	SEE	RK, PR	vdW, ECS	ED1S, Flamelet
[36]	'CRUNCH'	FV compr	RANS/LES	SEE	SRK, HBMS	x	x
[72, 73, 71]	'AVBP'	compr	LES	SEE	PR	vdW	FR4S2R
[47]	Menon	FV compr	LES	SEE	PR	vdW	EBU, EQU, FR2S
[39]	Kim	FV incomp	k-ε	SEE	mSRK. PR	vdW	Flamelet
[35, 44, 45, 9]	'CharLES^X'	FV compr	LES	SEE	PR	vdW / VLE	FPV
[52, 53]	'INCA'	FV compr	LES	SEE	PR	vdW	x
[77]	'Ansys Fluent'	n/a	k-ε	SEE	iG	iG	FR6S2R
[25, 24]	'Ansys CFX'	n/a	k-ε	SEE	n/a	n/a	FR6S2R
[19]	Raman	FV incomp	DNS	SEE	PR	vdW	FR5S2R
[4]	'TAU'	FV compr	SA	SEE	MBWR	MFM	FR8S17R
[68]	'KIVA 3V'	FV	SA	SEL	PR	VLE	x
[29]	Giovangigli	FD	DNS	SEE	SRK	DI	FR

Table 2: Overview of CFD codes for real gas injection. Abbreviations: n/a: not given, x: not used, incomp: incompressible, compr: compressible, FV: finite volume,, pressure: pressure based, FD: finite difference, struct: structured, k-ε: RANS, SEL*: statistical Eulerian-Lagrangian where particles are converted to continuum immediately after injection, BWR (t): BWR EOS used for transport coefficients, HBMS: Hirschfelder-Buehler-McGee-Sutton EOS, mPR: modified PR EOS, Z eq: mixture fraction transport equation, mSRK: modified SRK EOS, iG: ideal-gas EOS or mixing rules,FRnSmR: finite-rate chemistry with n species and m reactions, EQU: equilibrium, PDF: flame turbulence interaction based on probability density function, ED: eddy dissipation, FPV: flamelet progress variable, ED1S: eddy dissipation one species, EBU: eddy break-up, DI: diffuse interface, MFM: multi-fluid mixing, VLE: vapor liquid equilibrium.

standard

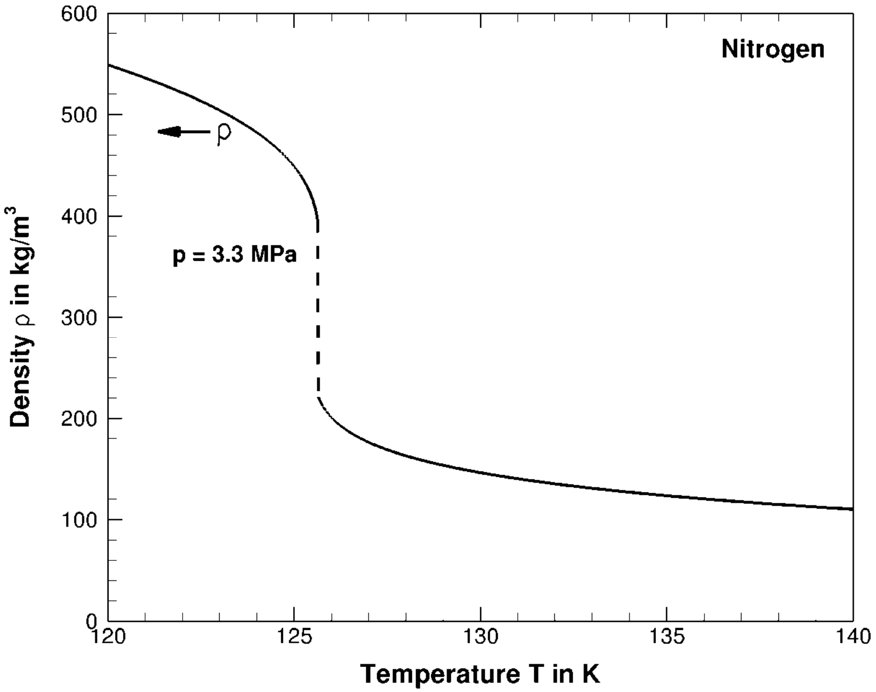
sCO2

alternative
mixing

What happens at the supercritical transition?

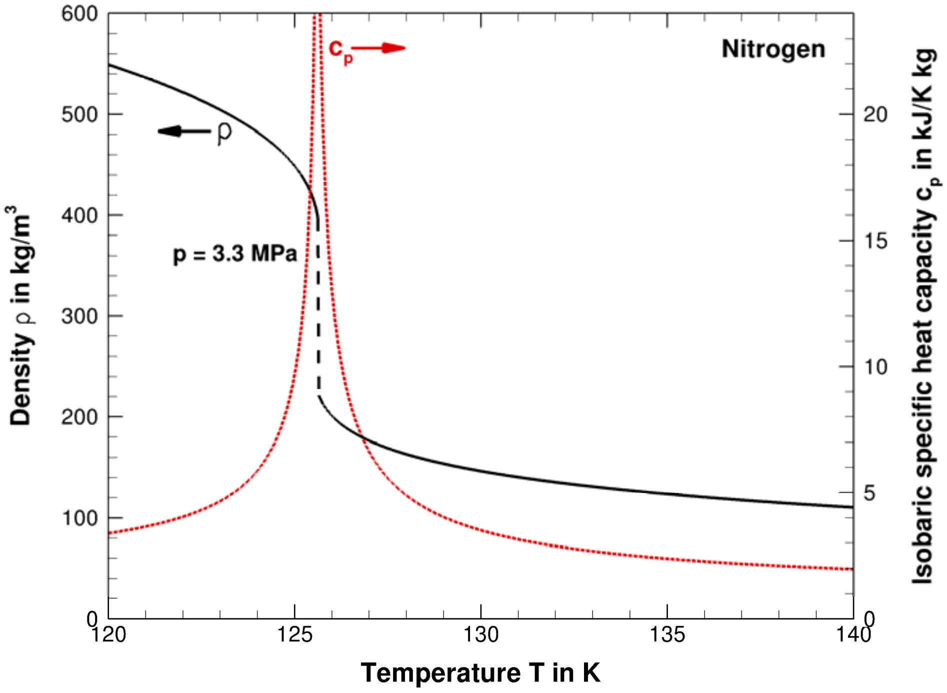
Are supercritical fluids insensitive to dp, dT?

Sub- and supercritical phase transitions



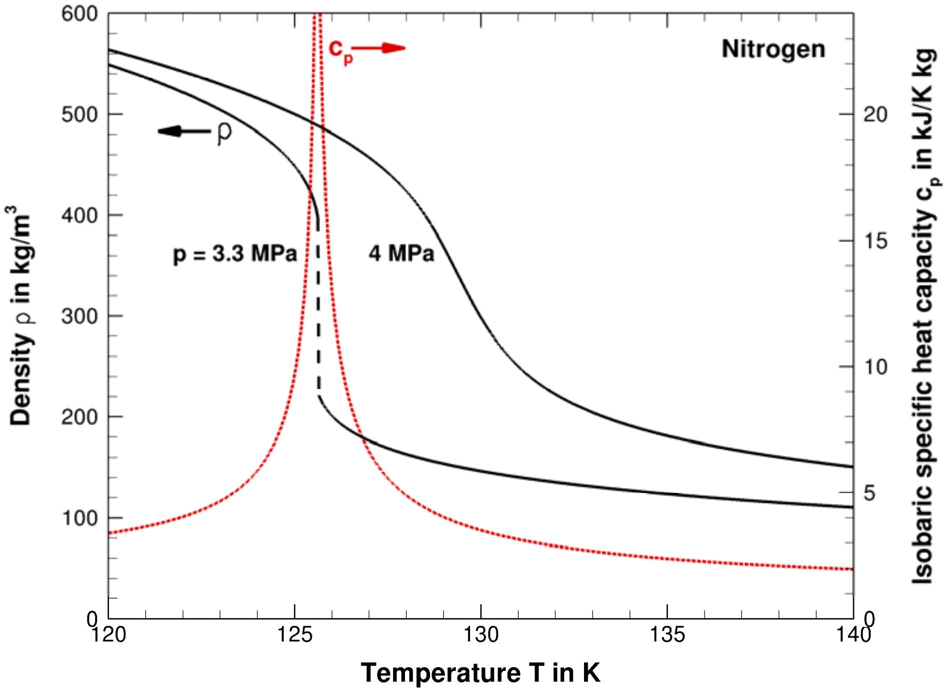
Banuti and Hannemann PoF 2016

Sub- and supercritical phase transitions



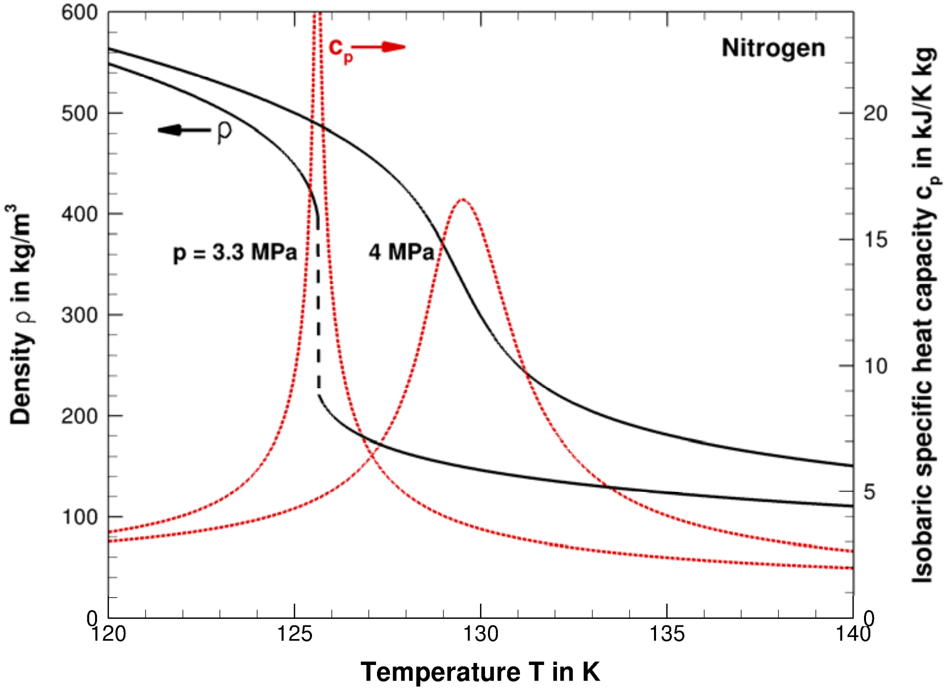
Banuti and Hannemann PoF 2016

Sub- and supercritical phase transitions



Banuti and Hannemann PoF 2016

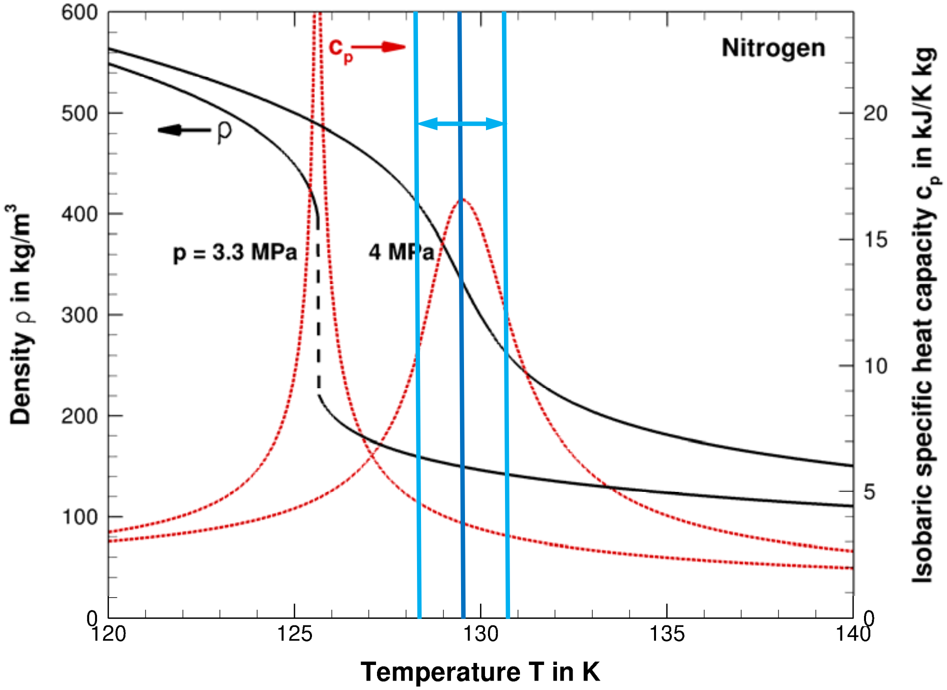
Sub- and supercritical phase transitions: pseudoboiling



Banuti and Hannemann PoF 2016

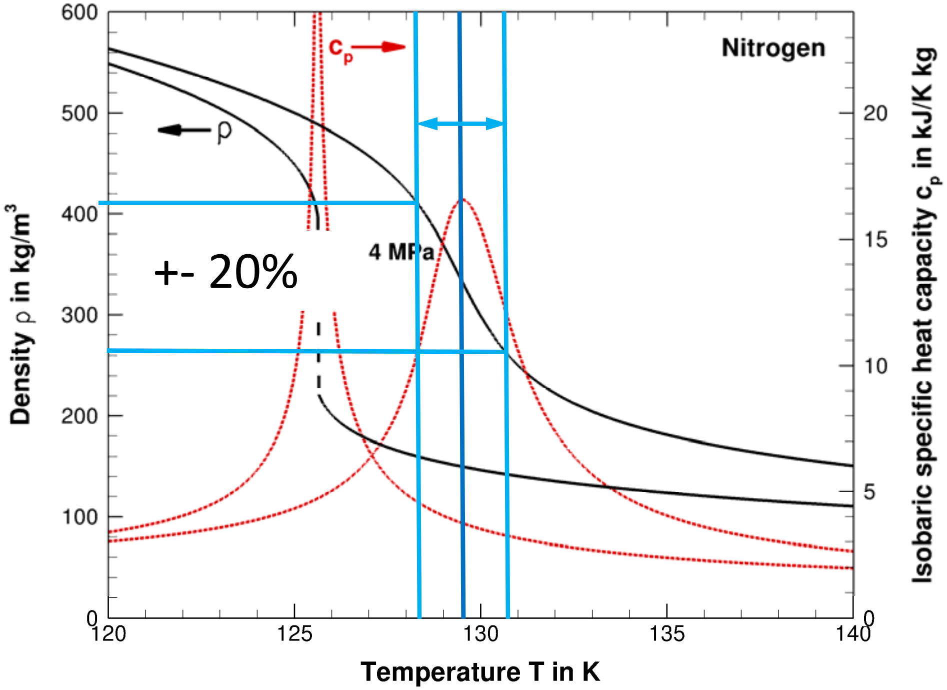
Sub- and supercritical phase transitions: pseudoboiling

+- 1% T



Banuti and Hannemann PoF 2016

Sub- and supercritical phase transitions: pseudoboiling



+- 1% T

+- 20%

Banuti and Hannemann PoF 2016