LES of direct-fired oxy-combustion in sCO2 power systems

PI: Lee Shunn (shunn@cascadetech.com)
Award: DE-SC0017230

2019 UTSR Project Review Meeting

CASCADE TECHNOLOGIES

Project personnel

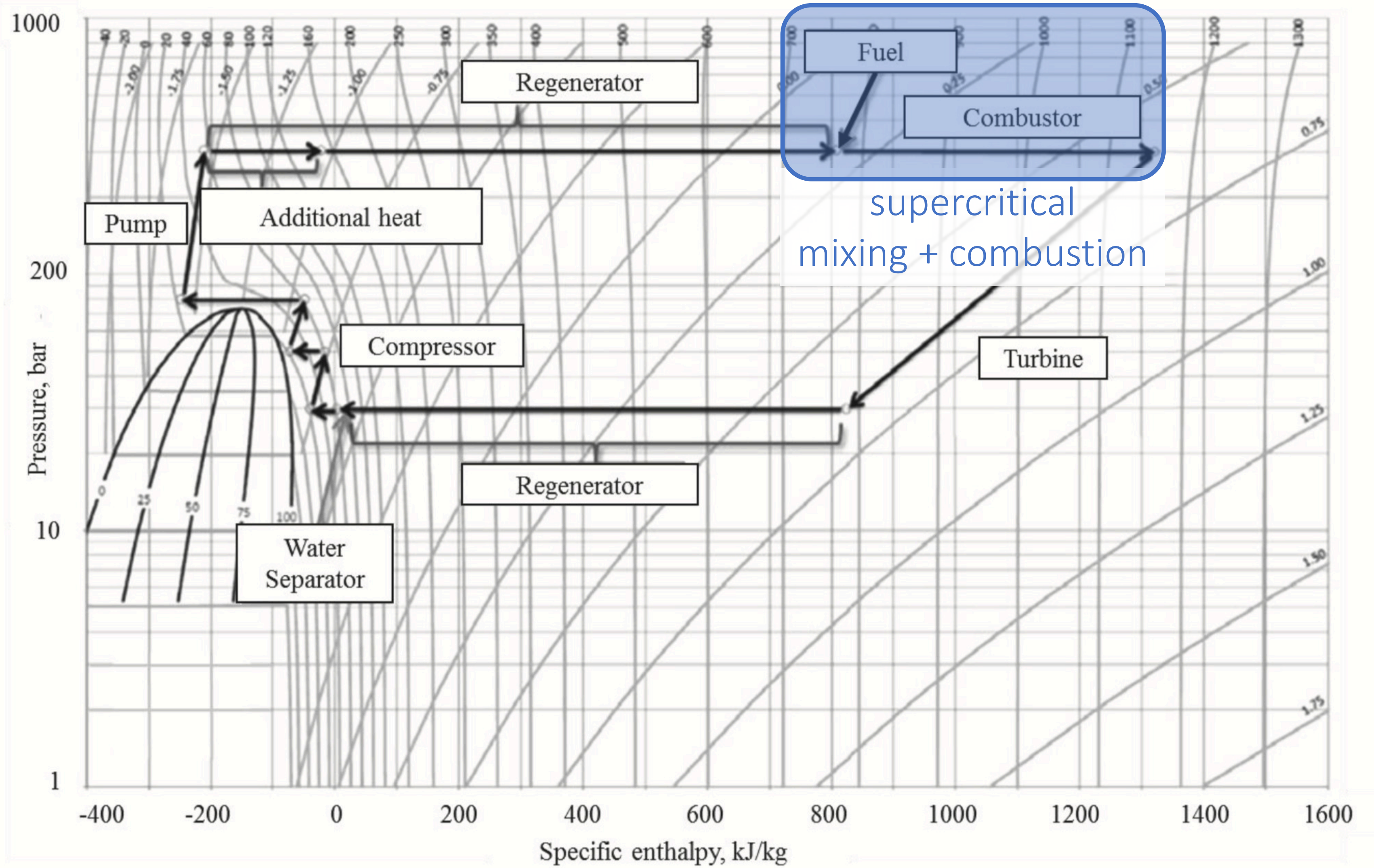
- Cascade Technologies
  - Combustion: Lee Shunn (PI)
  - Real-fluid CFD: Daniel Banuti*
  - Numerical Analysis: Sanjeeb Bose
- Consultants
  - Javier Urzay, Stanford CTR
  - Lluis Jofre, Stanford CTR
  - Subith Vasu, UCF
- Acknowledgements
  - Jacob Delimont, SwRI
  - Mark Freeman, NETL

* Currently Assistant Prof of ME at UNM, Albuquerque NM

Project overview

- Objective: Develop numerical methods and CFD models for oxy-fuel combustion in direct-fired sCO2 power systems
- Phase I (Mar 2017-Feb 2018)
  - Proof-of-concept for CFD "building blocks" (i.e. real-fluid thermodynamics, numerical methods, combustion models)
- Phase II (Jun 2018-May 2020)
  - Implement models and methods from Phase I
  - Demonstrate utility for scientific discovery and design exploration in practical sCO2 systems

sCO2 Allam cycle

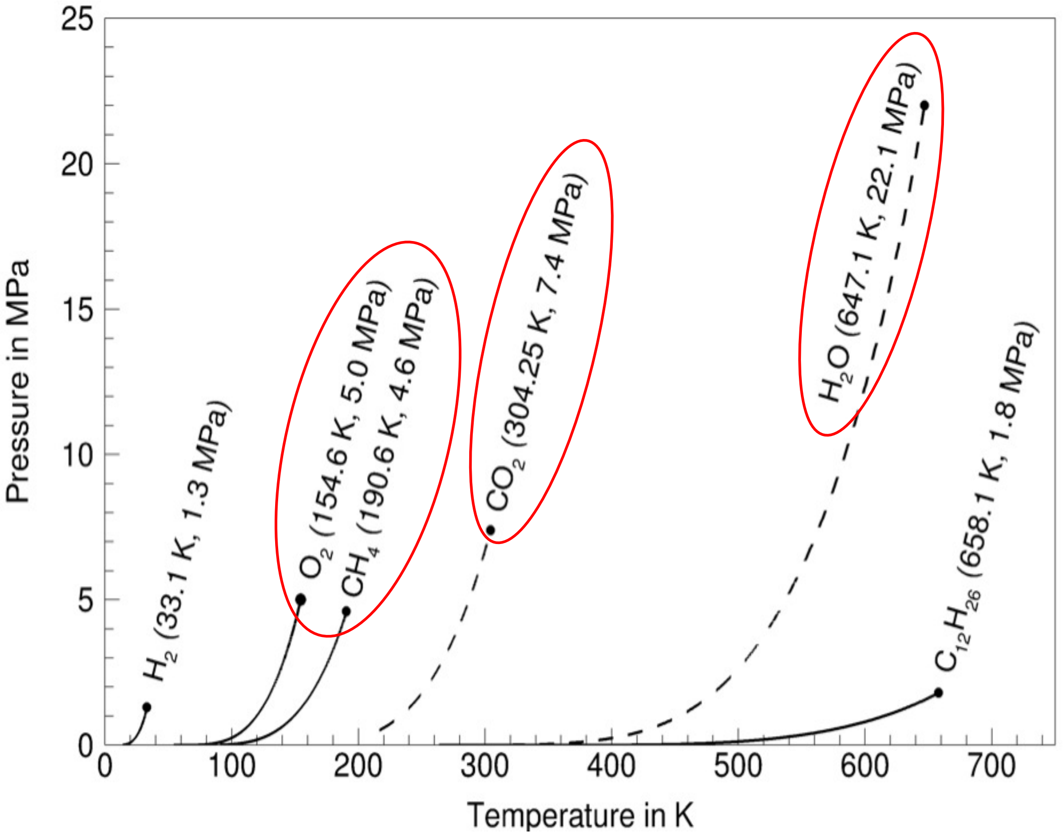


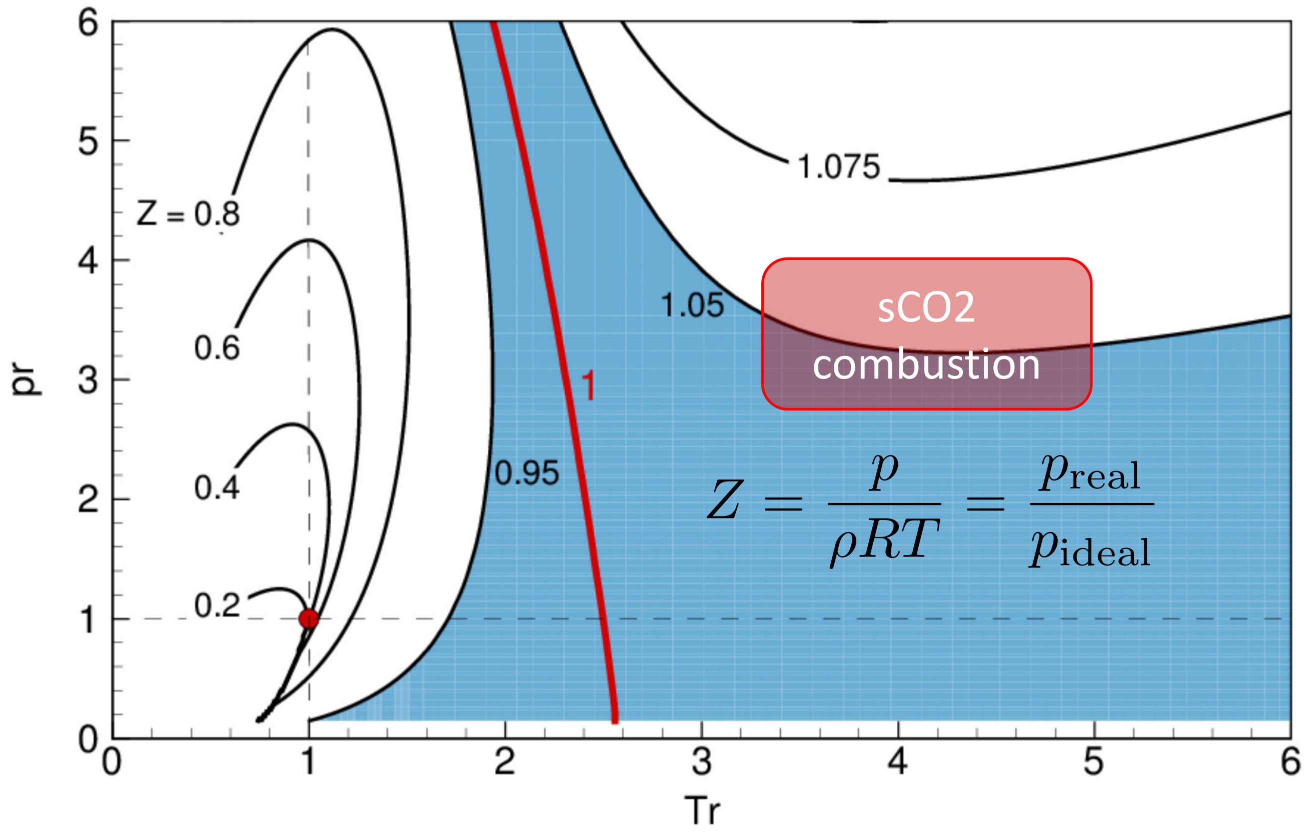
- High-pressure (~30 MPa)
- CO_2 is mostly recycled, remainder is captured at high pressure
- Compact footprint
- Reduced emissions
- Improved efficiency
- Heat added by oxy-fuel combustion (e.g. CH_4+O_2)

adapted from: Zaryankin et al, AIP Conf Proc 2047, 020026 (2018)

Thermophysical properties at sCO2 conditions

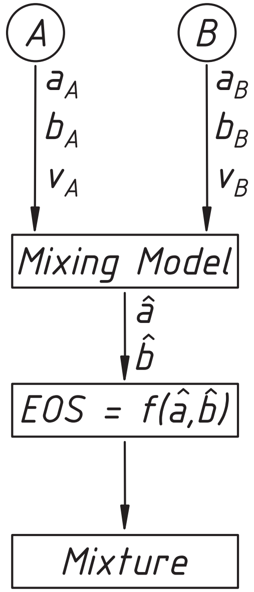
- Combustor conditions: T = 1000-1500K, P = 20-30 MPa
- Mixtures are supercritical with respect to: CH4, O2, CO2, H2O





models & numerical methods

Cubic EOS
for multicomponent mixtures



$$b_i = C_b \frac{RT_{c,i}}{P_{c,i}}$$

$$P = \frac{RT}{V-b} - \frac{a}{V^2 + ubV + vb^2}$$

$$a_i = C_a \frac{R^2 T_{c,i}^2}{P_{c,i}} \alpha_i(T)$$

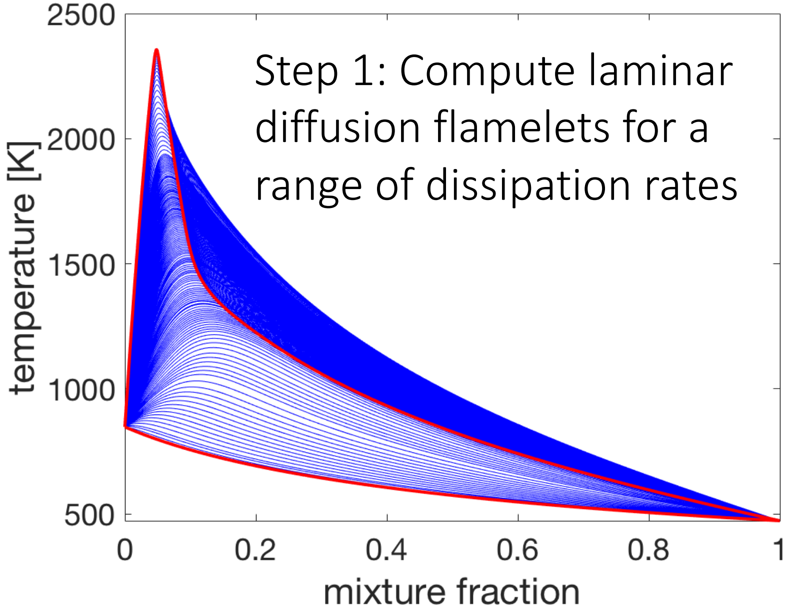
$$a = \sum_i \sum_j X_i X_j \sqrt{a_i a_j}\,(1-\bar{k}_{ij})\,, \quad b = \sum_i X_i b_i$$

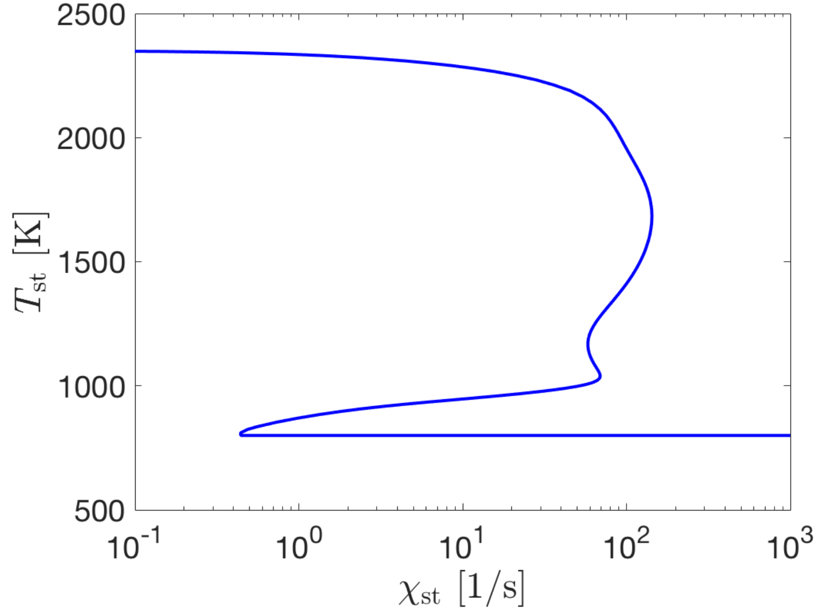
$$\alpha_i(T) = \left[1 + f_\omega\left(1 - \sqrt{T/T_{c,i}}\right)\right]^2$$

equation	u	v	C_b	C_a	f_ω
van der Waals	0	0	1/8	27/64	0
Redlich-Kwong	1	0	0.08664	0.42748	$[(T/T_{c,i})^{-1/4} - 1]/[1 - (T/T_{c,i})^{1/2}]$
Soave-Redlich-Kwong	1	0	0.08664	0.42748	$0.48 + 1.574\omega - 0.176\omega^2$
Peng-Robinson	2	-1	0.07780	0.45724	$0.37464 + 1.54226\omega - 0.26992\omega^2$

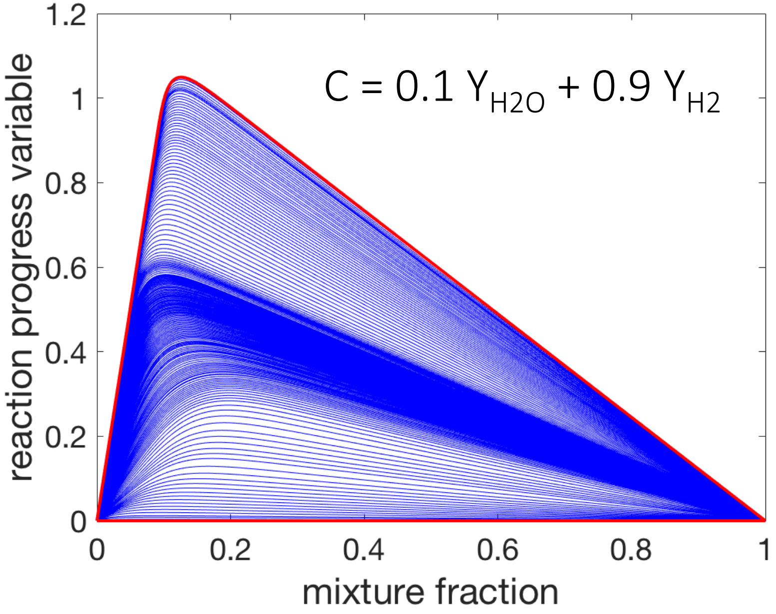
Flamelet/progress-variable (FPV) combustion model

Step 1: Compute laminar diffusion flamelets for a range of dissipation rates



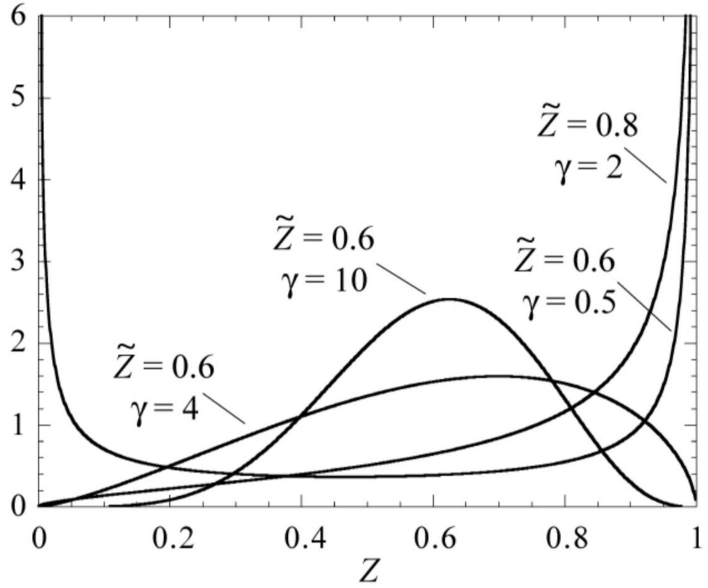


Step 2: Define a reaction progress variable and map flamelets to (Z, C)

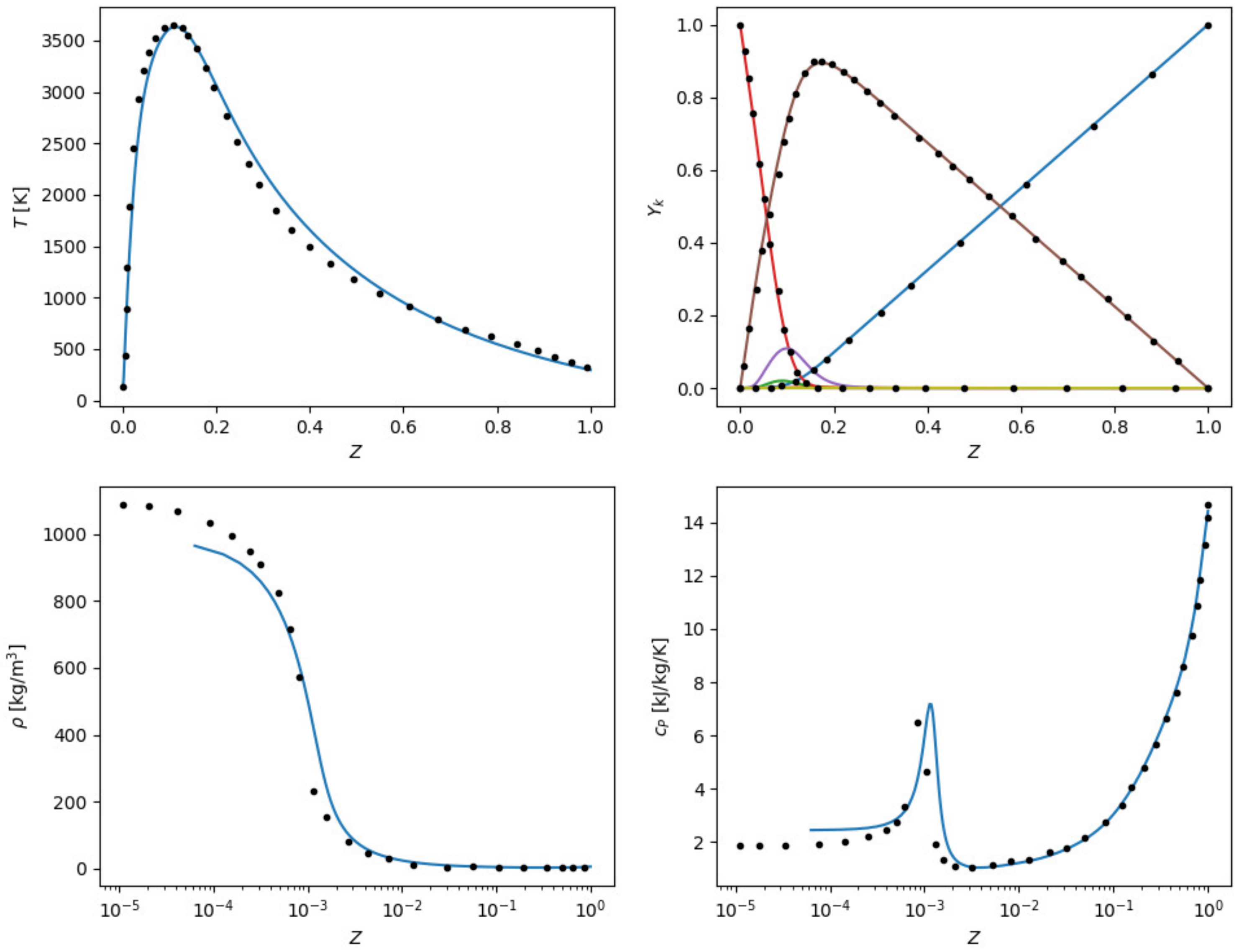


Step 3: Assume PDF closure for SGS turbulence-chemistry interactions

$$\widetilde{\psi} = \int \int \psi(z, \Lambda)\widetilde{P}(z)\widetilde{P}(\Lambda)\mathrm{d}z\mathrm{d}\Lambda$$



1D counterflow diffusion flame



- ● Lacaze & Oefelein 2012
- — Current flamelet solver (built on Cantera libs)

P = 7 MPa
Fuel: H_2 @ 295K
Oxid: O_2 @ 120K

Mixture fraction formulation
with real-fluid properties from cubic EOS

$$\frac{\partial \psi}{\partial t} = \frac{\chi}{2} \frac{\partial^2 \psi}{\partial Z^2} + \Omega$$

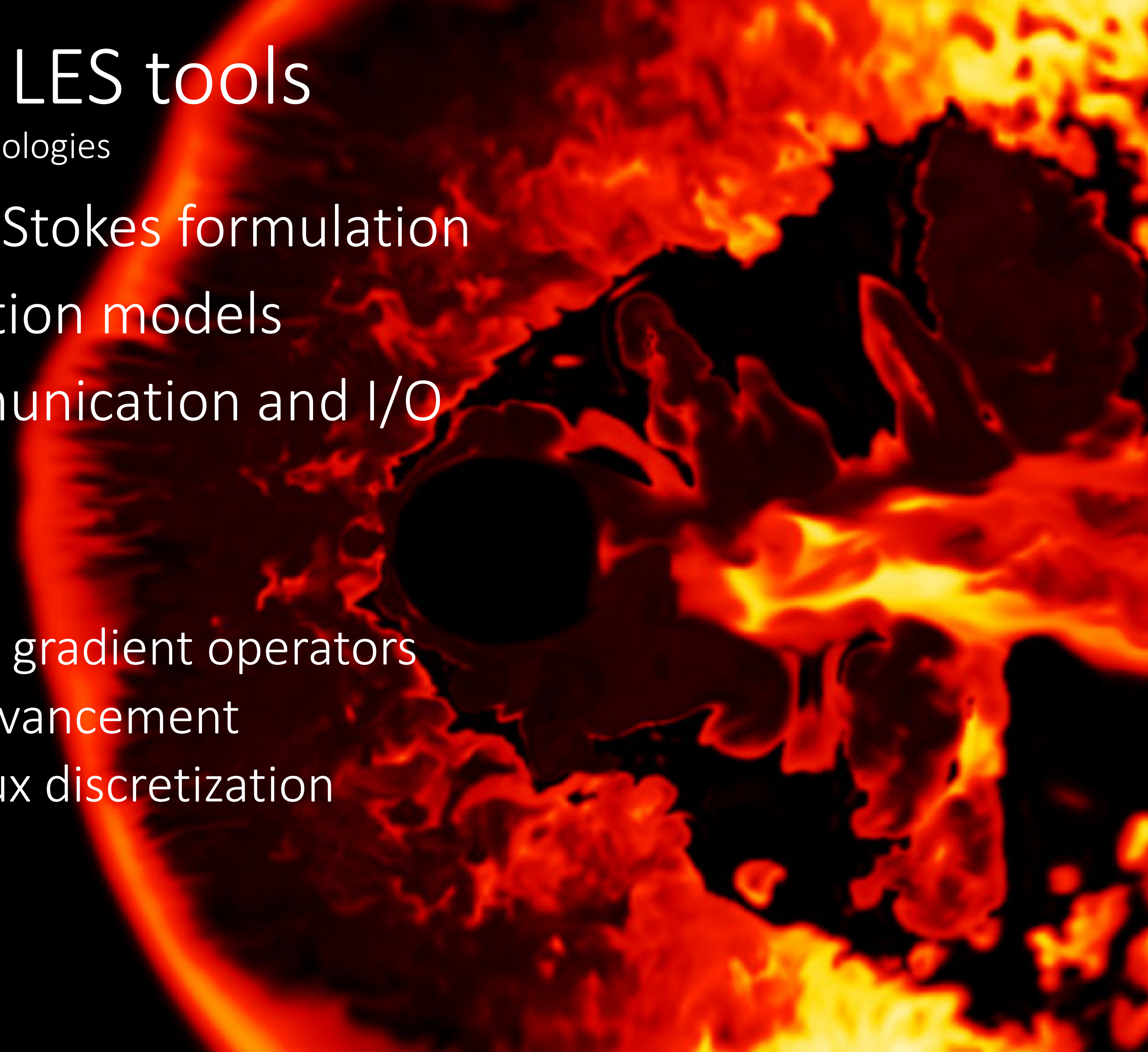
$$\chi \equiv 2D \left| \nabla Z \right|^2$$

CHARLES™ suite of LES tools

Developed and licensed by Cascade Technologies

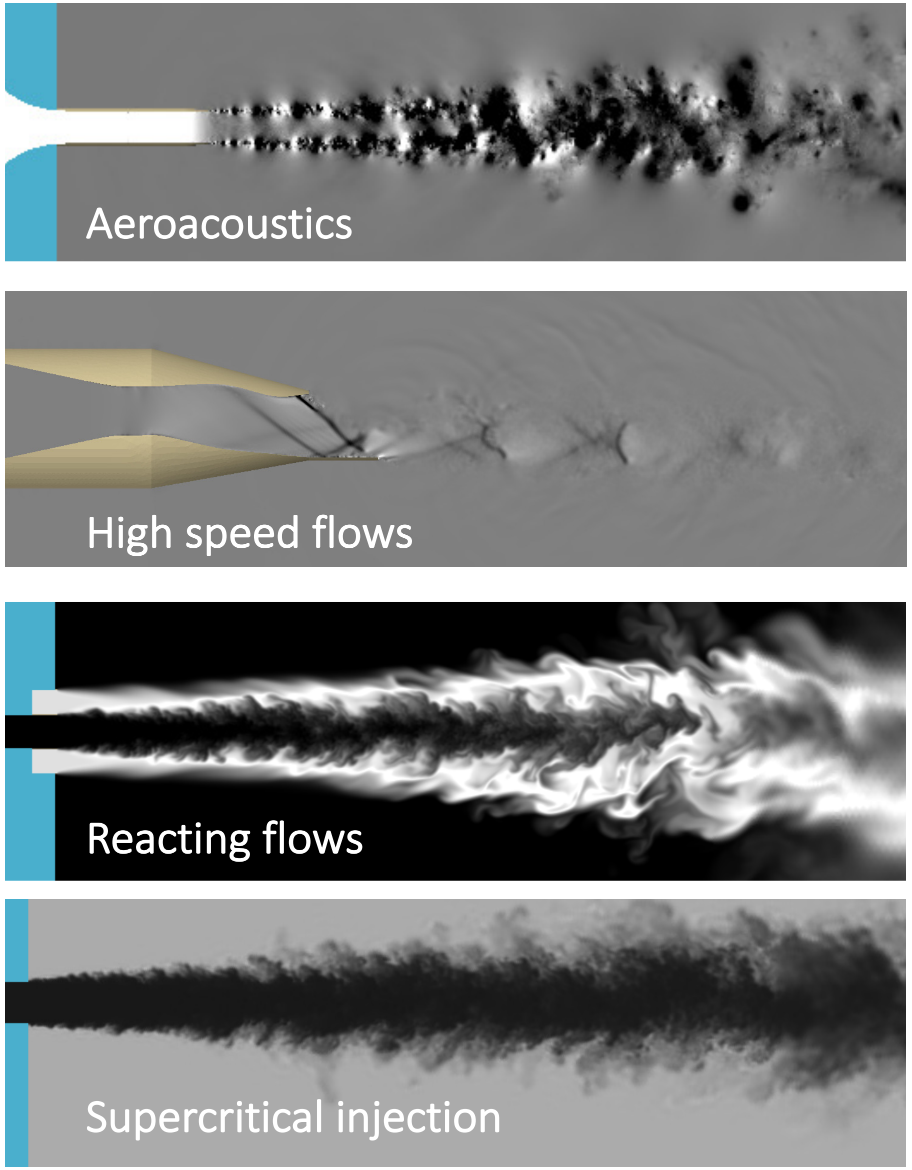
- Compressible FV Navier-Stokes formulation
- Flamelet-based combustion models
- Massively-parallel communication and I/O

- Numerical method
  - 2^{nd}-order low-dissipation gradient operators
  - 3^{rd}-order explicit time advancement
  - “KEEP” entropy-stable flux discretization



CASCADE TECHNOLOGIES

Stability from physics, not dissipation



Kinetic energy, entropy preserving (KEEP) operators

- 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

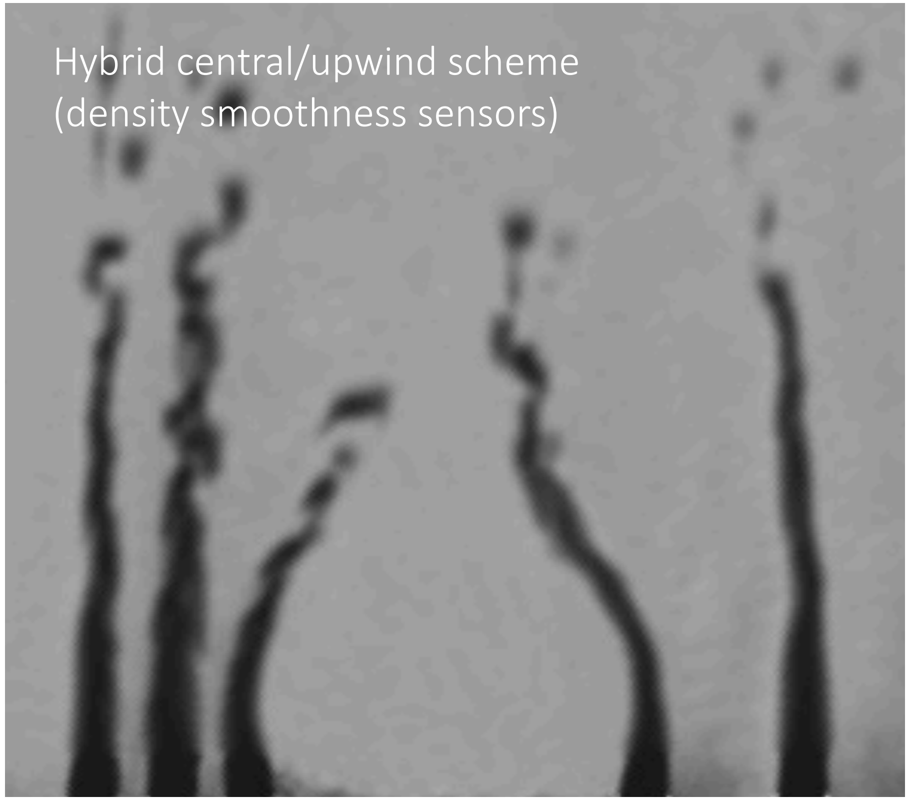
Stability conditions based on discrete satisfaction of Gibbs-Duhem condition (2nd law of thermodynamics)

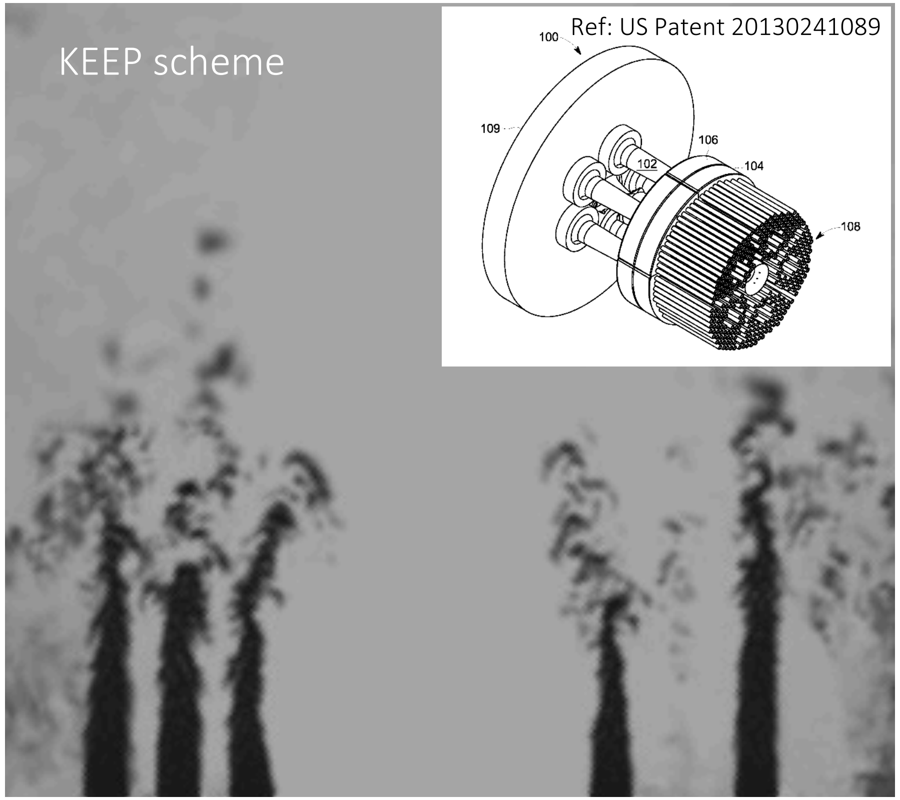
$$d\left(\rho s\right) = \frac{1}{T} d\left(\rho E\right) - \frac{u}{T} d\left(\rho u\right) + \left(s + \frac{u^2}{2T} - \frac{h}{T}\right) d\rho$$

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

KEEP schemes drastically improve solution quality and numerical stability

Example: Premixed combustion in industrial multi-element combustor





System level LES calculations necessarily result in coarsely resolved structures

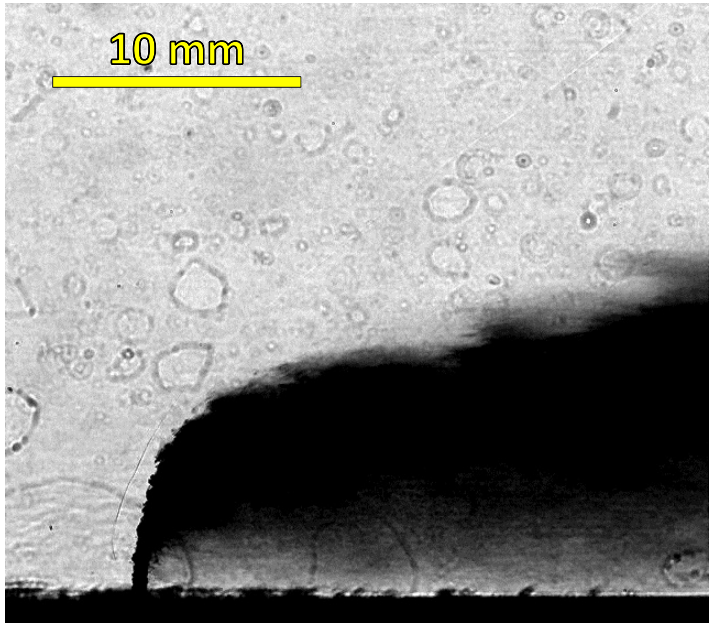
- KEEP schemes improve accuracy (e.g., flame length consistent with experiments)
- Simulations are more robust and less sensitive to mesh resolution and transitions

model validation

High-fidelity primary atomization in multiphase flows

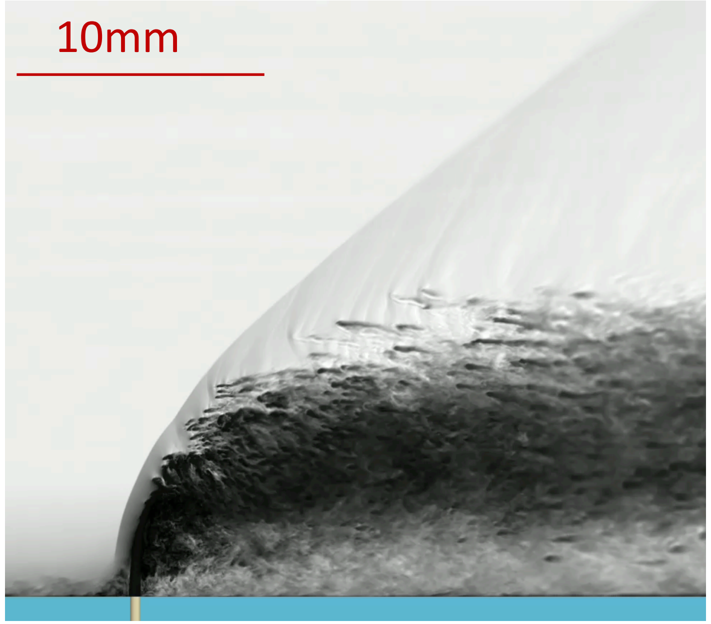
liquid jet in supersonic gas flow of Ma=1.94 (Lin et al. AIAA 2018)

Shadowgraph images (AFRL)



2017 data
50K fps recording
10 fps playback
0.159 μs exposure
44.3 (W) × 43.3 (V) μm/pixel

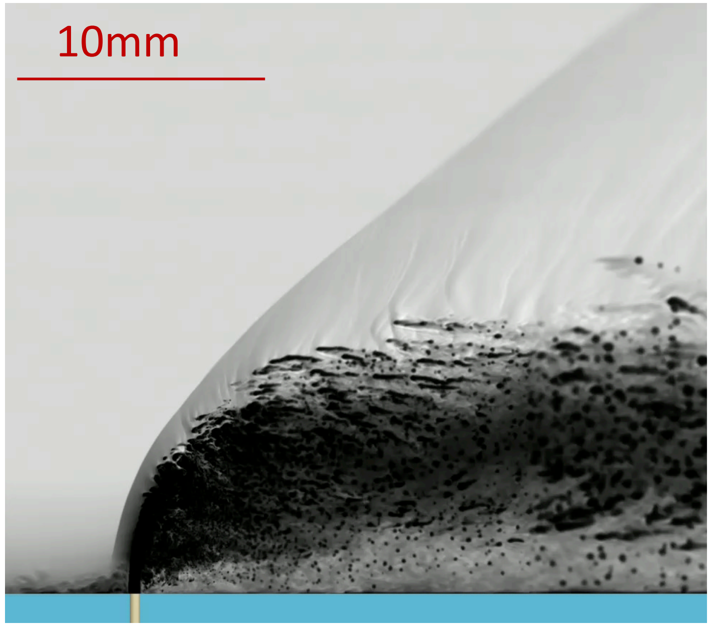
Velocity magnitude contours at y=0



contour levels
- white: 700m/s
- black: 0m/s

(stiffened gas EOS)

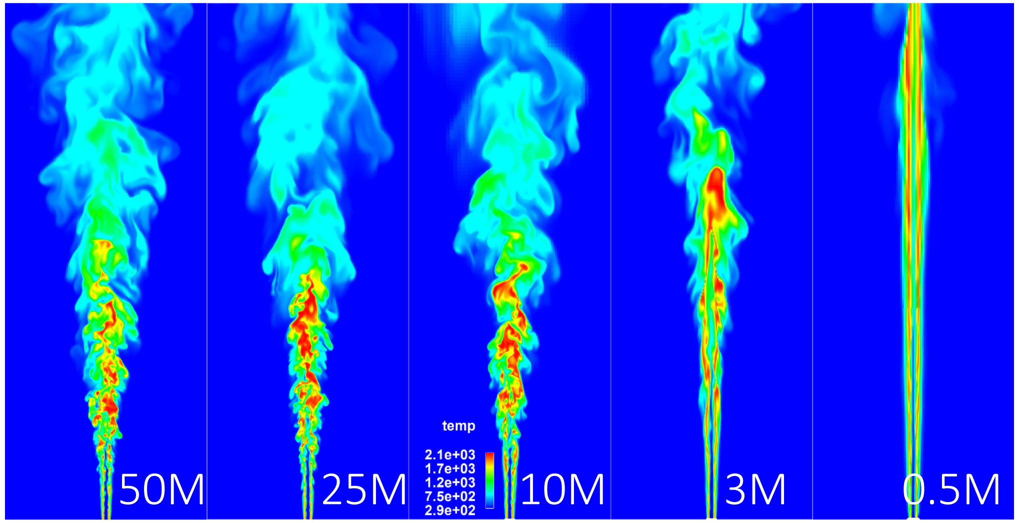
Ma contours at y=0

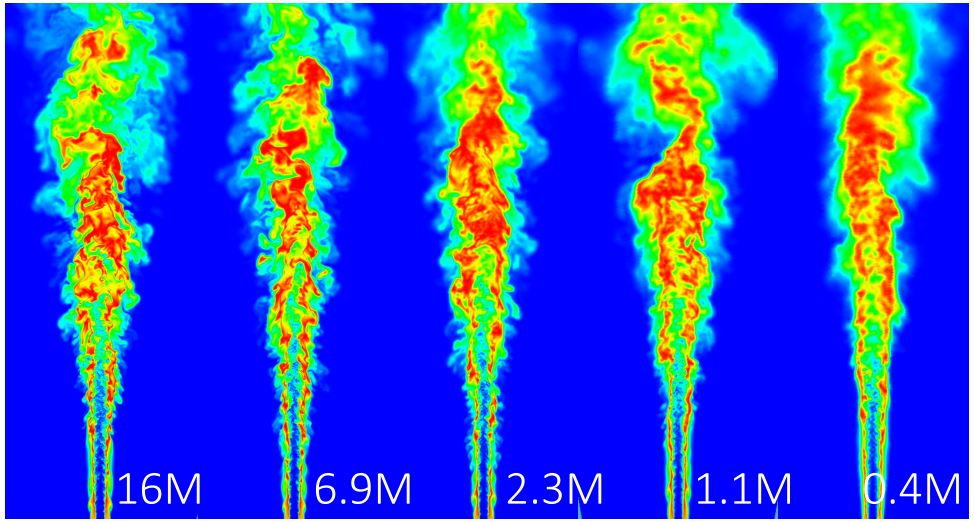


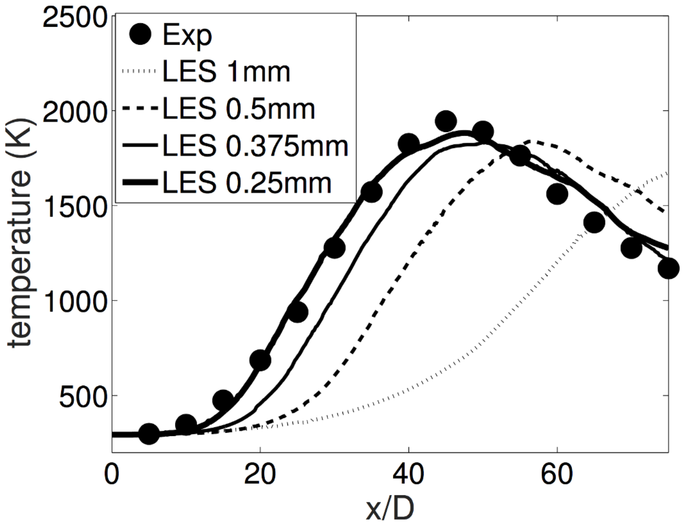
contour levels (not fixed...)
- white: 2
- black: 0

Turbulent combustion validation: Sandia Flame D

KEEP scheme + robust physics models = improved stability, reduced mesh sensitivity

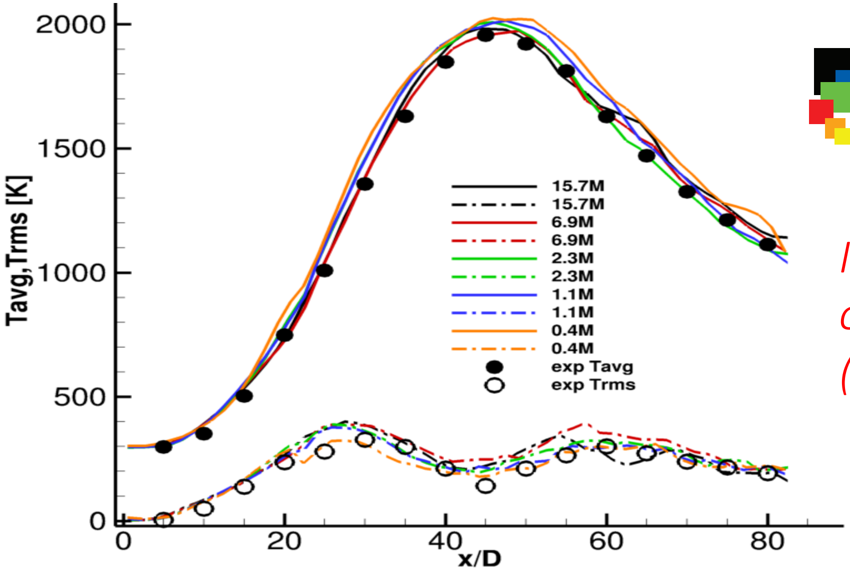






CONVERGE CFD SOFTWARE

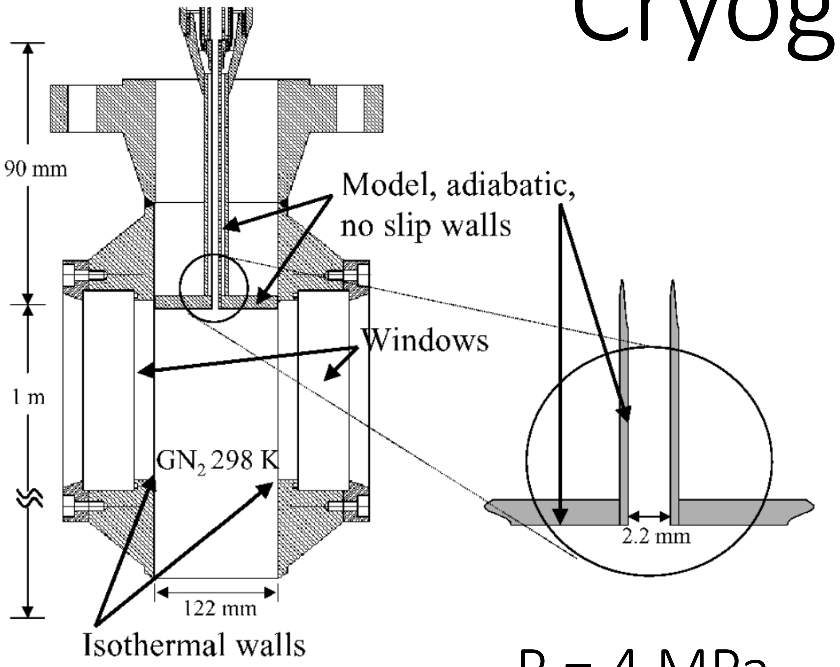
Liu et al, 2018, AIAA



CASCADE TECHNOLOGIES

Improved accuracy on coarse grids (>50x less cost)

Cryogenic nitrogen injection

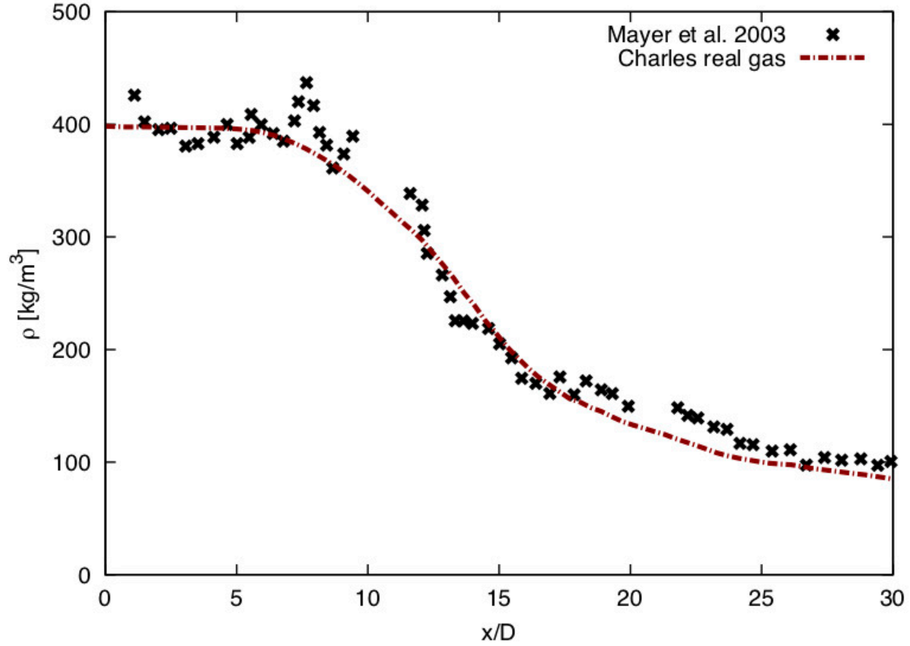


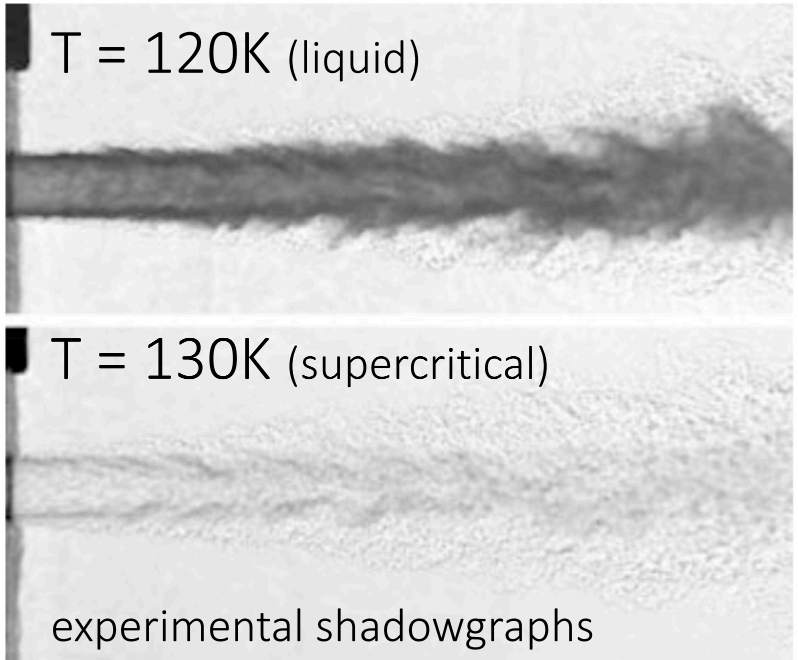
P = 4 MPa

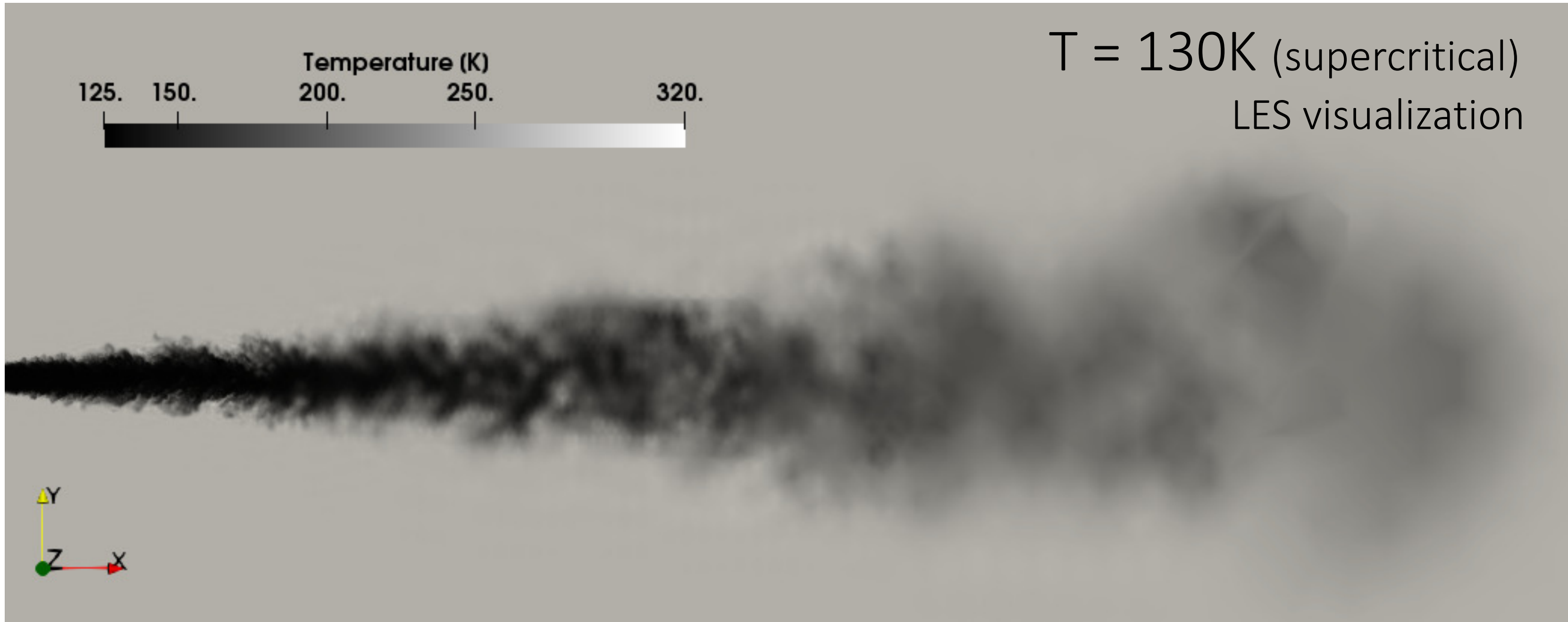
Mayer & Branam 2003

Cryogenic N2 jet into Gaseous N2 chamber

– T_C = 126.2 K
– P_C = 3.396 MPa







Penn State GH2/GO2 coaxial combustor

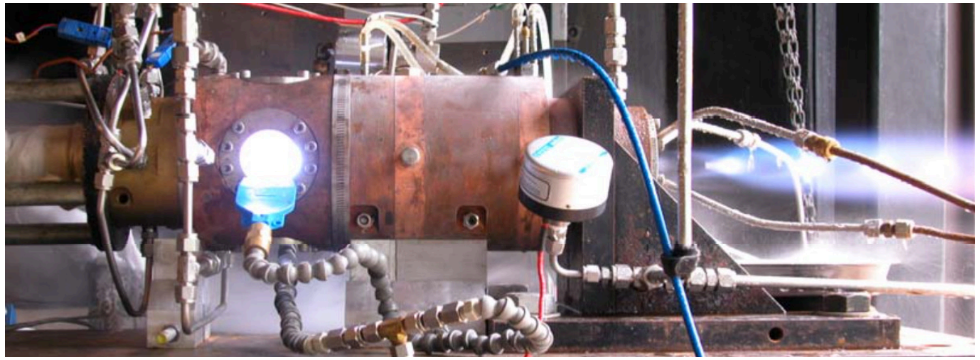
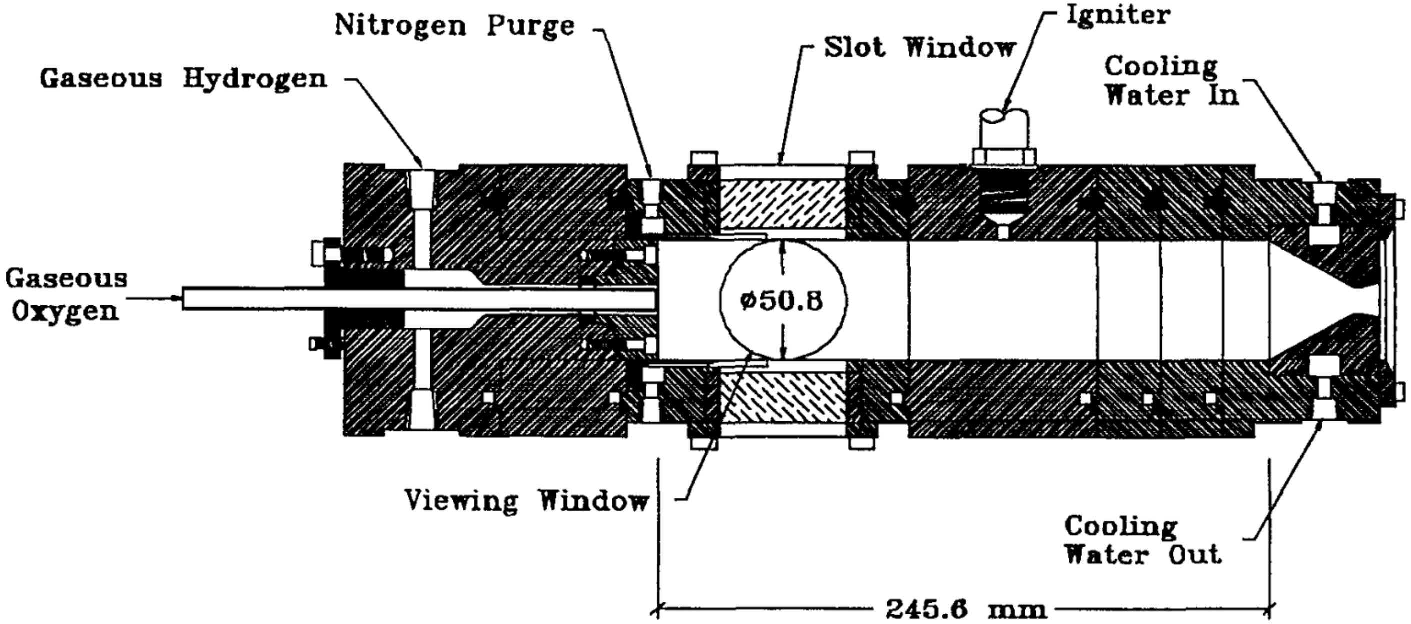


Table 1: Rocket Chamber Conditions.

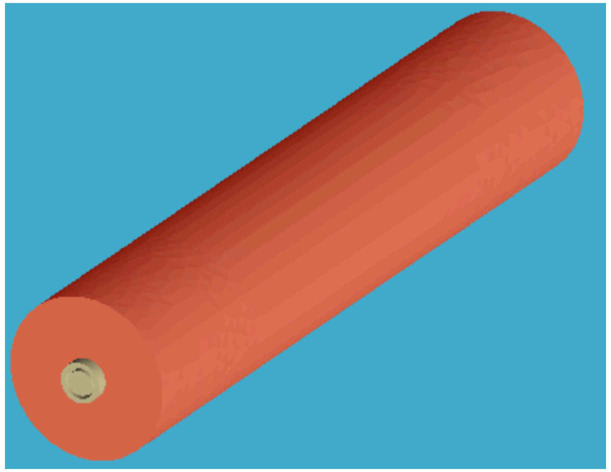
GH_2 Mass Flow Rate	1.03×10^{-2} kg/s
GO_2 Mass Flow Rate	4.2×10^{-2} kg/s
GO_2/GH_2 Mass Flow Ratio	4.0
GN_2 Mass Flow Rate (Purge)	0.01 kg/s
GH_2 Injector Velocity	177 m/s
GO_2 Injector Velocity	51 m/s
GO_2/GH_2 Velocity Ratio	0.29
Inlet Gas Temperature	297 K
Chamber Pressure	1.29 MPa
c^* Efficiency (with GN_2 purge) (without GN_2 purge)	 0.90 0.99



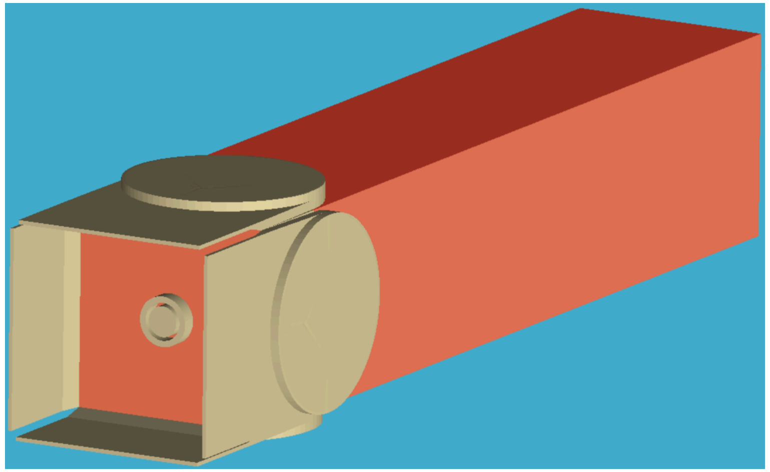
Square cross-section 50.8mm x 50.8mm

Foust et al 1996

Assessed sensitivity to chamber geometry and inlet BC



Cylinder



Square w/ purge

Simplified vs "full" geometry

Different papers, different conditions reported (~10%)

Table 1: Rocket Chamber Conditions.

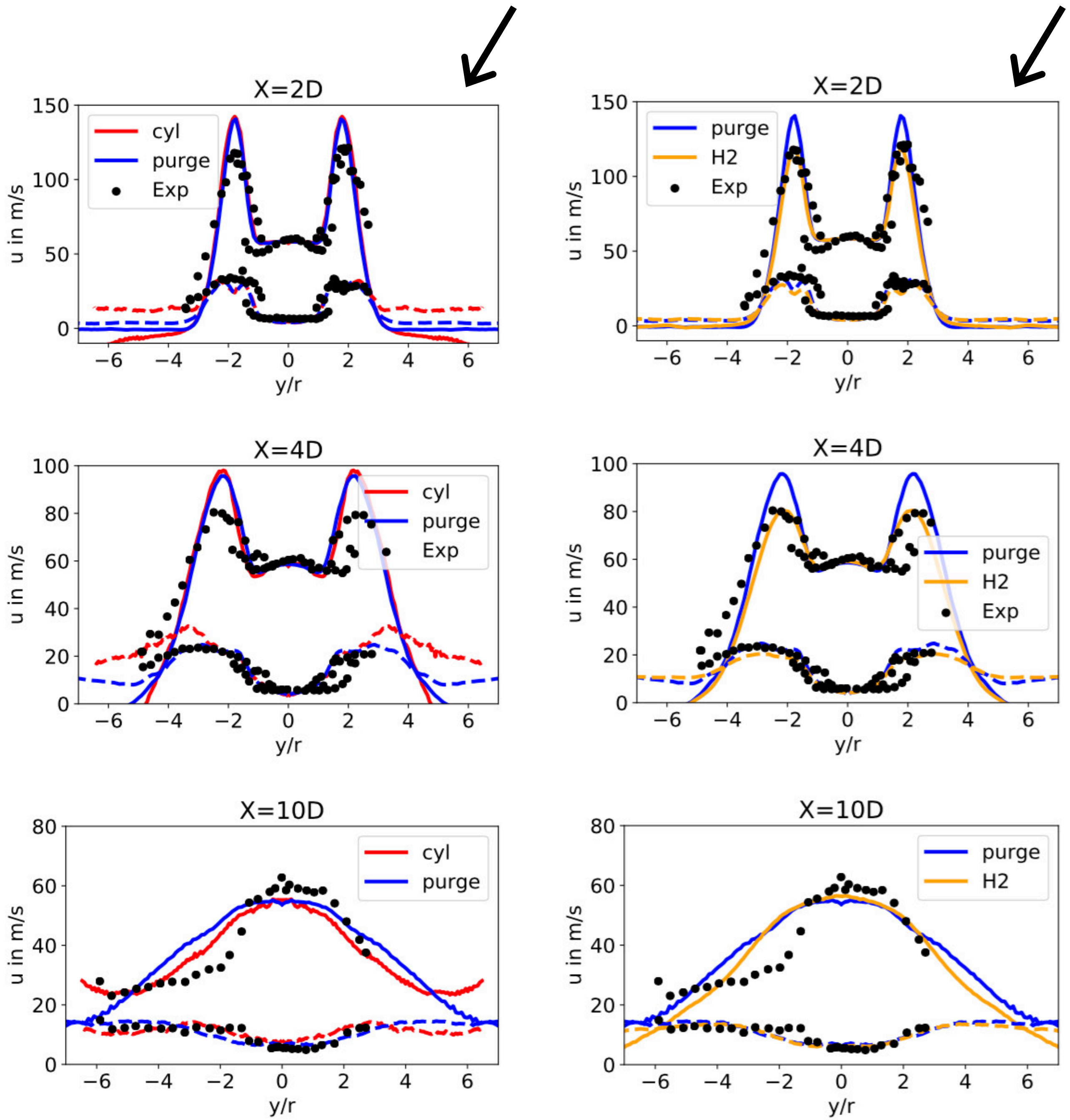
GH_2 Mass Flow Rate	1.03×10^{-2} kg/s
GO_2 Mass Flow Rate	4.2×10^{-2} kg/s
GO_2/GH_2 Mass Flow Ratio	4.0
GN_2 Mass Flow Rate (Purge)	0.01 kg/s
GH_2 Injector Velocity	177 m/s
GO_2 Injector Velocity	51 m/s
GO_2/GH_2 Velocity Ratio	0.29
Inlet Gas Temperature	297 K
Chamber Pressure	1.29 MPa
c^* Efficiency (with GN_2 purge) (without GN_2 purge)	 0.90 0.99

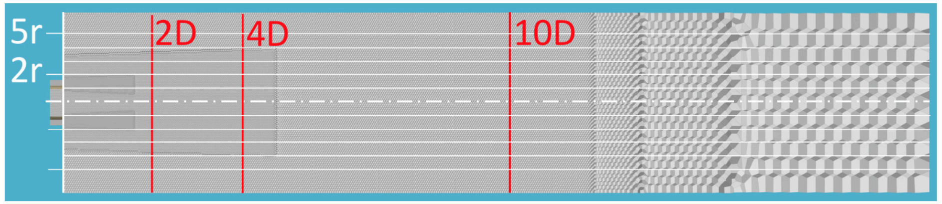
Table I. GO_2/GH_2 Hot-Fire Test Conditions

GH_2 Mass Flow Rate	0.011 kg/s (0.024 lbm/s)
GO_2 Mass Flow Rate	0.042 kg/s (0.093 lbm/s)
GO_2/GH_2 Mass Flow Ratio	3.8
GN_2 Mass Flow Rate (Purge)	0.014 kg/s (0.031 lbm/s)
GH_2 Injector Velocity	168 m/s (551 ft/s)
GO_2 Injector Velocity	49 m/s (161 ft/s)
GO_2/GH_2 Velocity Ratio	0.29
Post ID	7.75 mm (0.305 in.)
Annulus ID	9.53 mm (0.375 in.)
Annulus OD	12.7 mm (0.5 in.)
Nozzle Throat Diameter	11.35 mm (0.447 in.)
Chamber Pressure	1.37 MPa (198 psia)
GH_2 Reynolds Number	6.28×10^4
GO_2 Reynolds Number	3.18×10^5

	GO_2/GH_2
GH_2 mass flow kg/s (lb/s)	0.0103 (0.0226)
Oxidizer mass flow kg/s (lb/s)	0.0387 (0.0852)
O/F	3.8
GN_2 mass flow (purge) kg/s (lb/s)	0.0134 (0.0295)
GH_2 injection velocity m/s (ft/s)	184.6 (605.6)
Oxidizer injection vel m/s (ft/s)	52.8 (173.1)
Chamber pressure MPa (psia)	1.27 (186)

relatively insensitive to **chamber geometry**, more sensitive to **inlet BC**





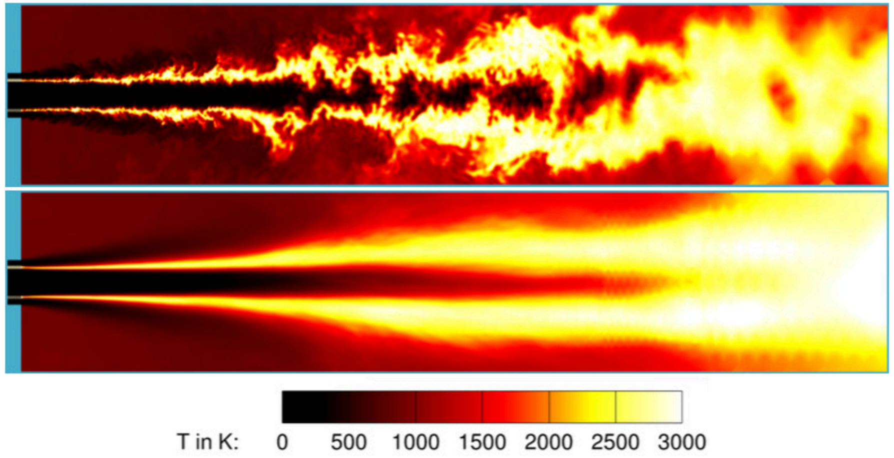


Figure 5: Instantaneous (top) and average (bottom) temperature.

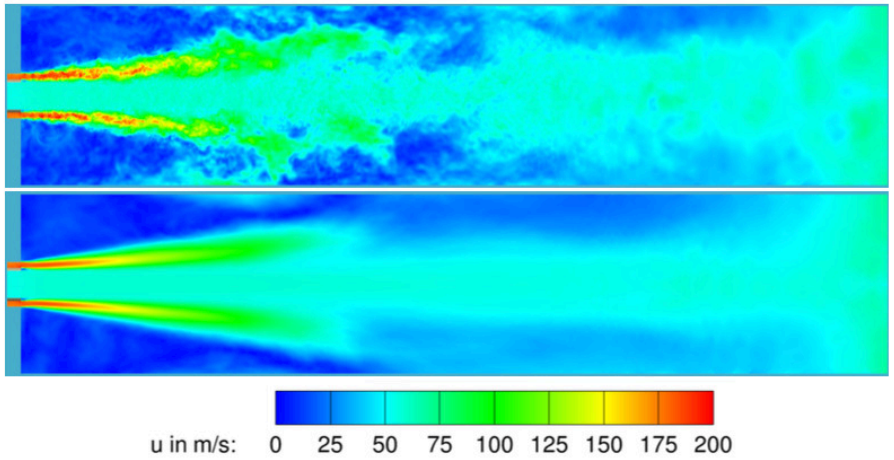
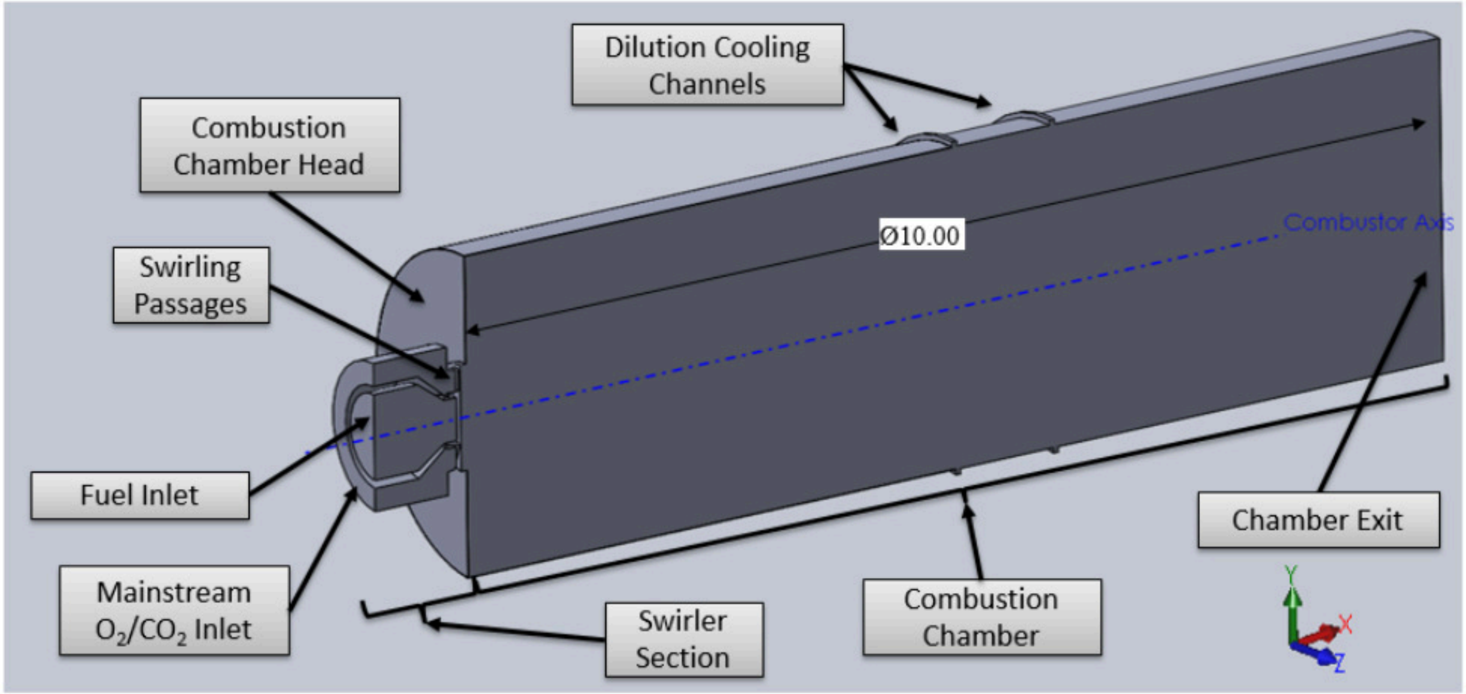


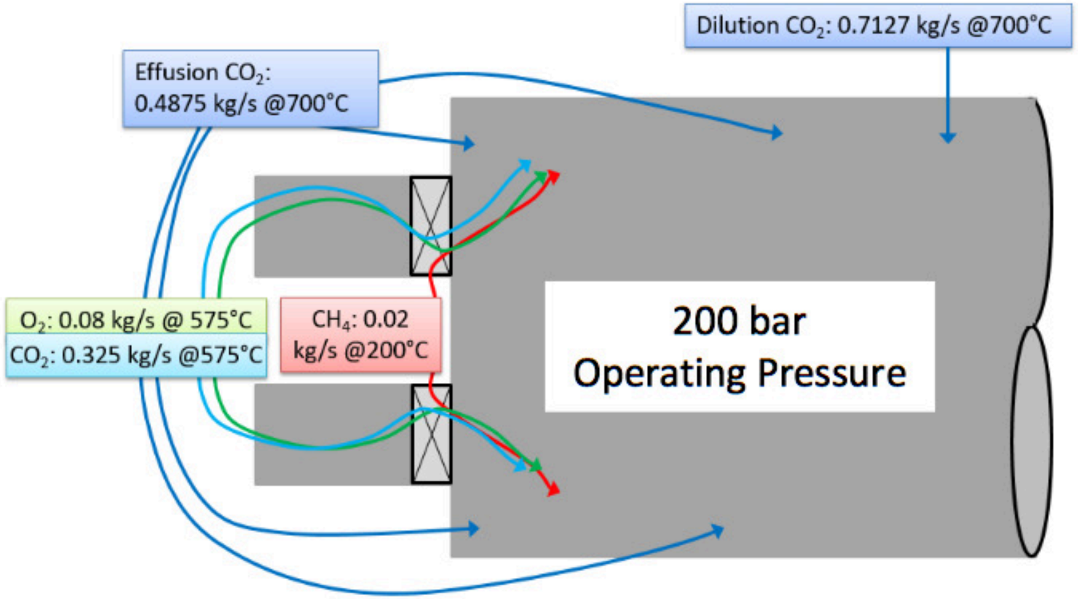
Figure 6: Instantaneous (top) and average (bottom) velocity.

SwRI sCO_2 concept combustor

SwRI sCO2 concept combustor

OBJECTIVE: Examine sensitivity of LES results to various chemical mechanisms





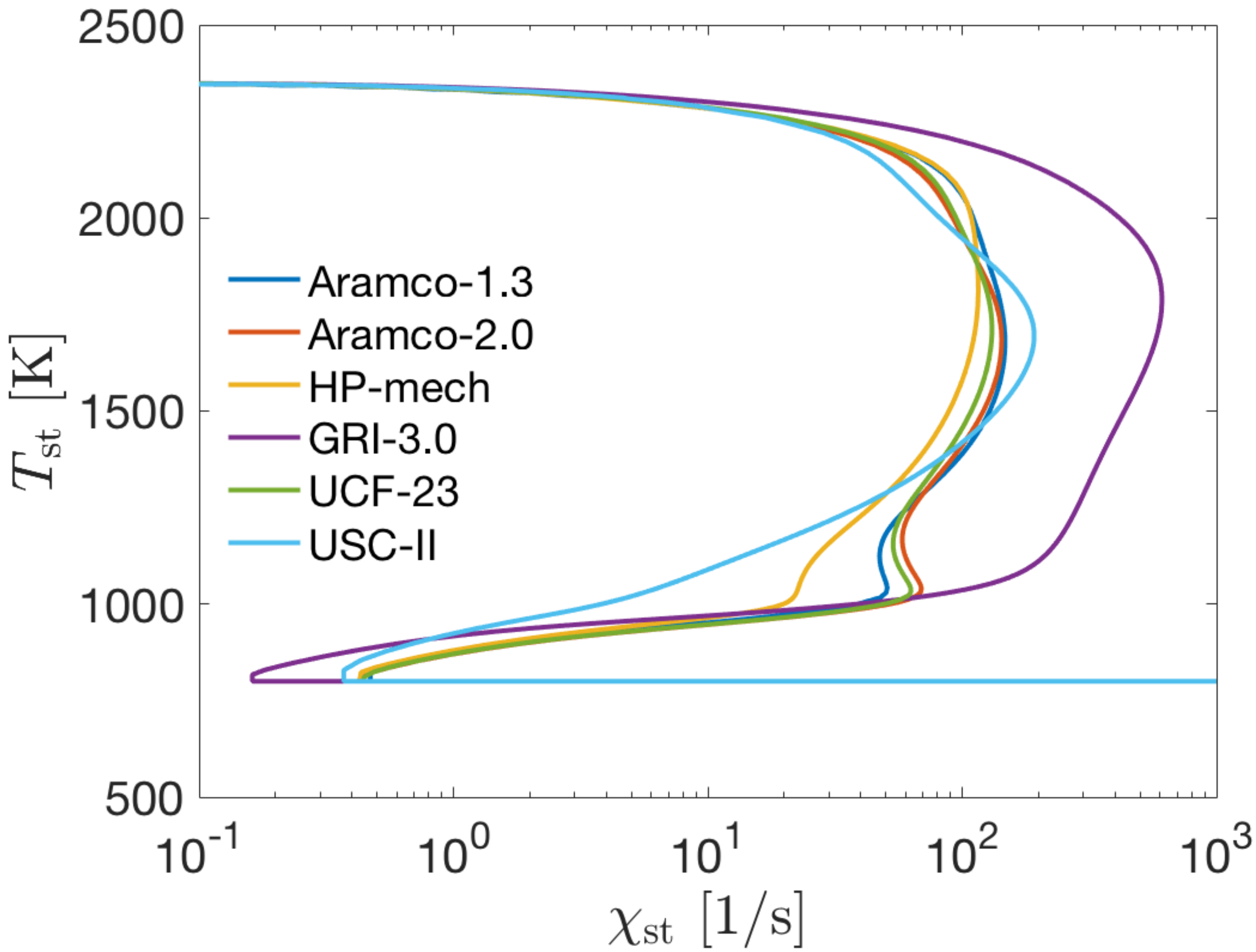
from: Delimont et al 2018 sCO2 Symposium

combustor stage	equivalence ratio	mixture fraction	pure CO_2 @T=973 K	80:20 CO_2:O_2 @T=962 K
post-injection	1.0	0.047059	2349.5 K	2349.5 K
post-effusion	0.45	0.021918	1671.8 K	1675.7 K
post-dilution	0.25	0.012306	1380.8 K	1380.7 K

Chemical mechanisms

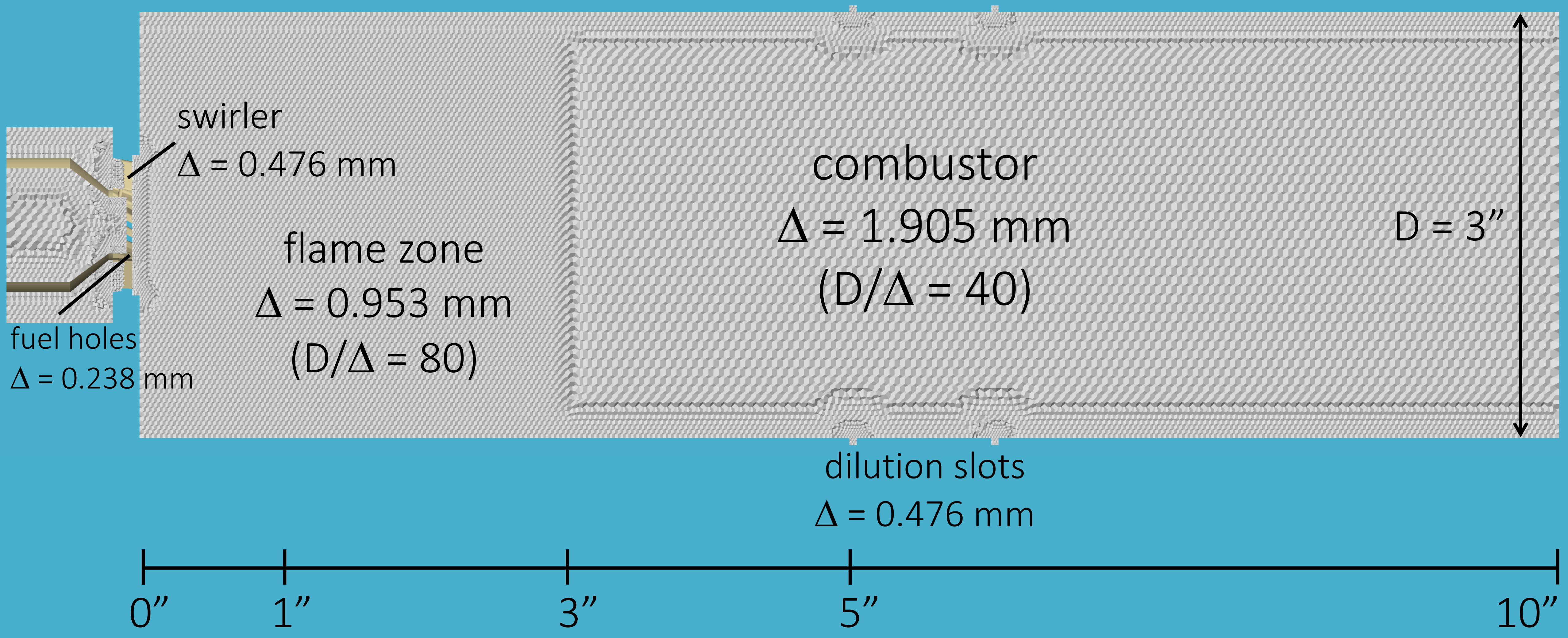
mechanism	# species	# rxns	max PLOG	comments
Aramco-1.3	253	1542	100 atm	(C1-C4) Curran et al. 2013
Aramco-2.0	73	426	1000 atm	(C1-C2) Curran et al. 2017
HP-mech	92	615	1e+5 atm	Ju et al. 2017
GRI-3.0	53	325	none	Gas Research Institute
UCF-23	23	142	none	Reduced from Aramco-2.0
USC-II	111	784	none	Wang et al. 2007

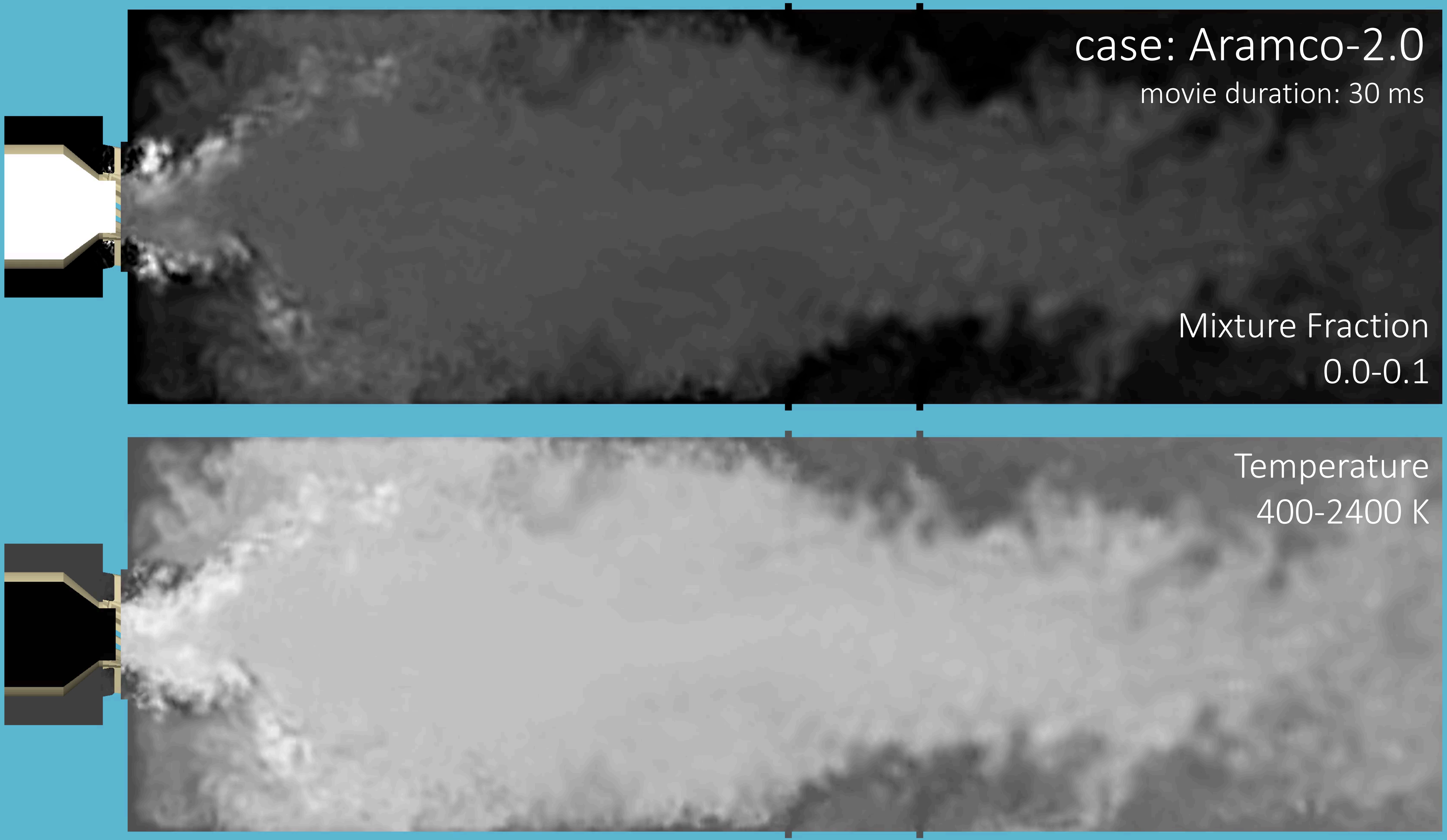
Flamelet s-curve (IG EOS)



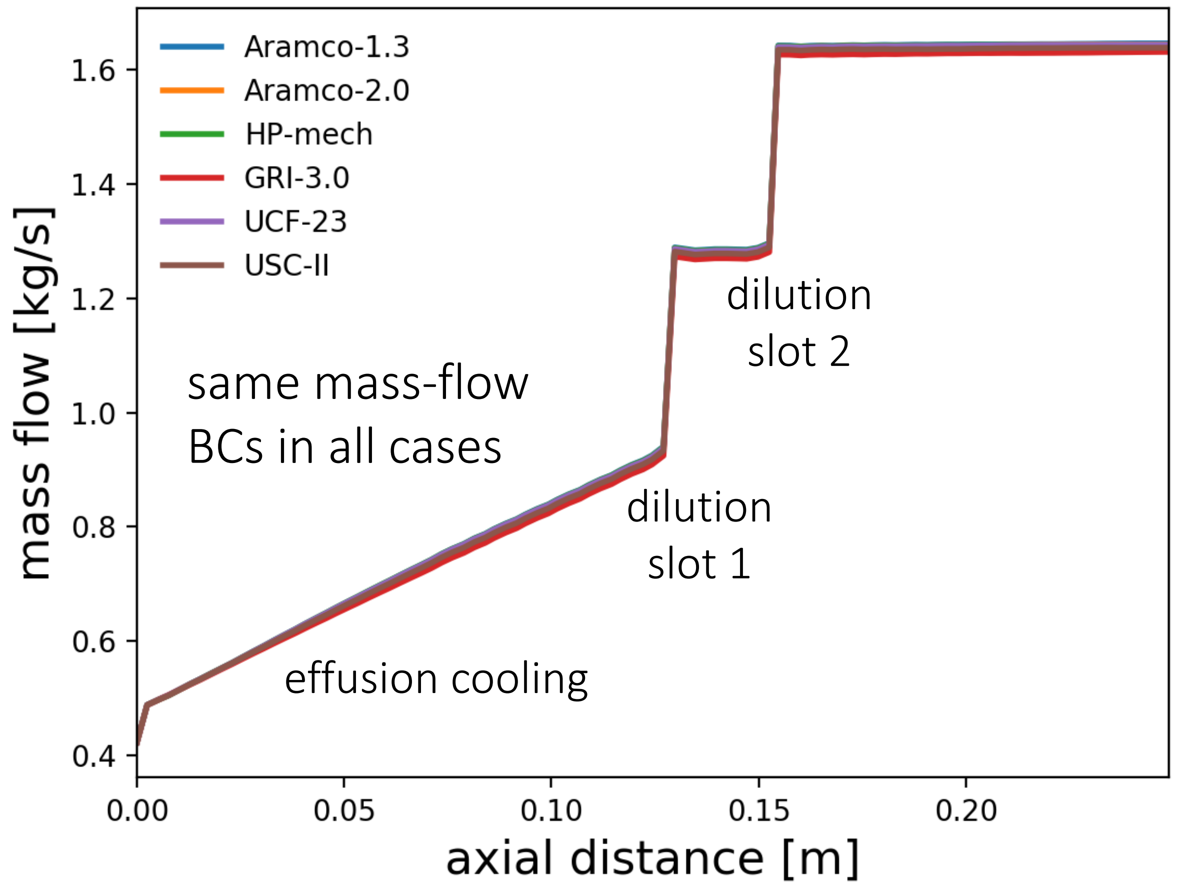
"Coarse" LES mesh

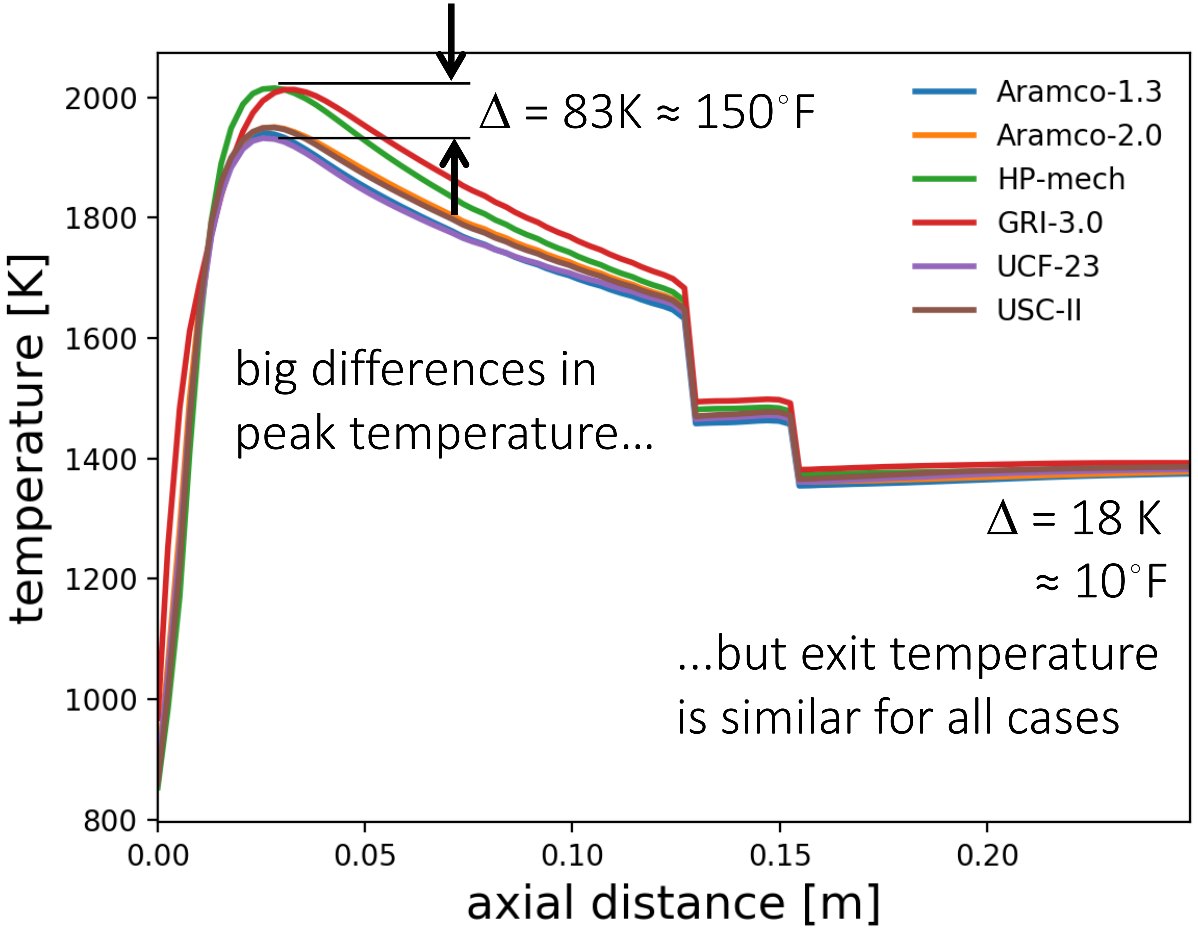
1.1M Voronoi CVs



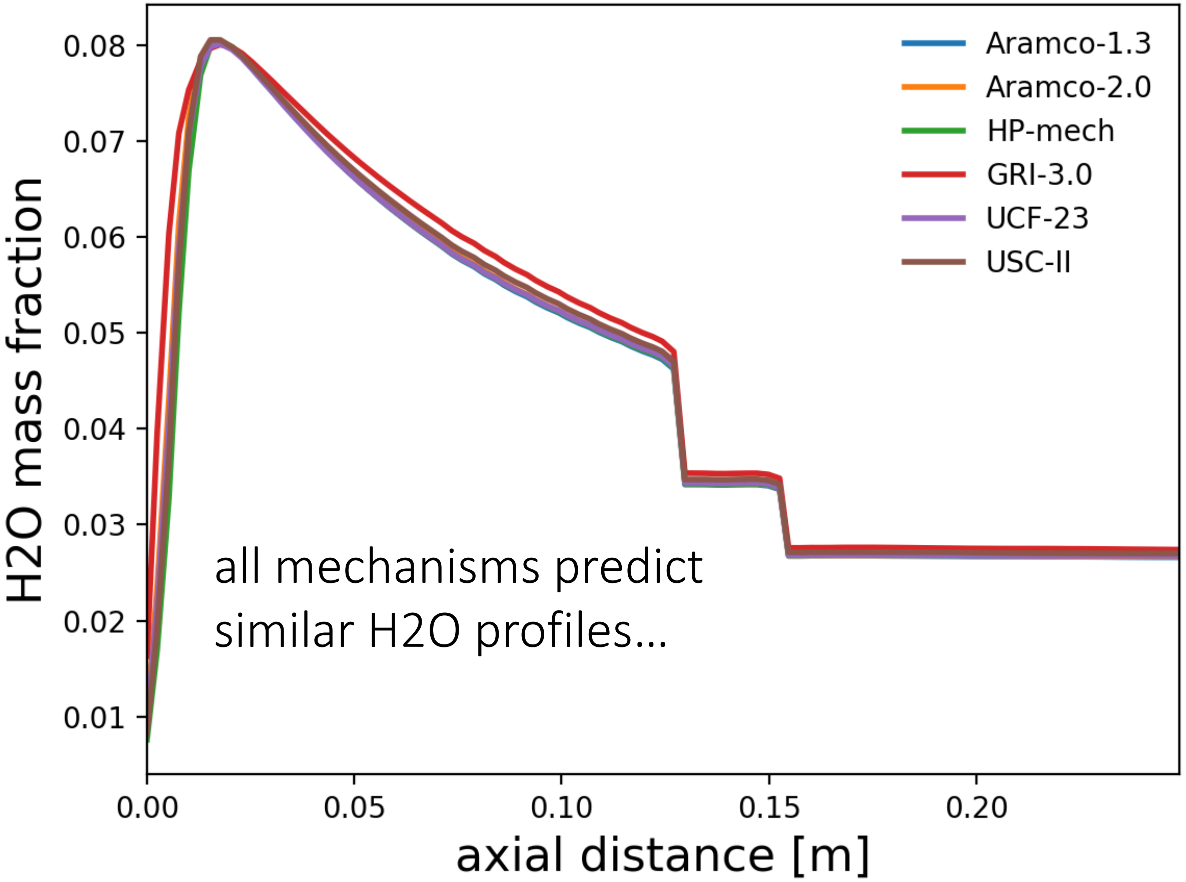

case: Aramco-2.0
movie duration: 30 ms
Mixture Fraction
0.0-0.1
Temperature
400-2400 K

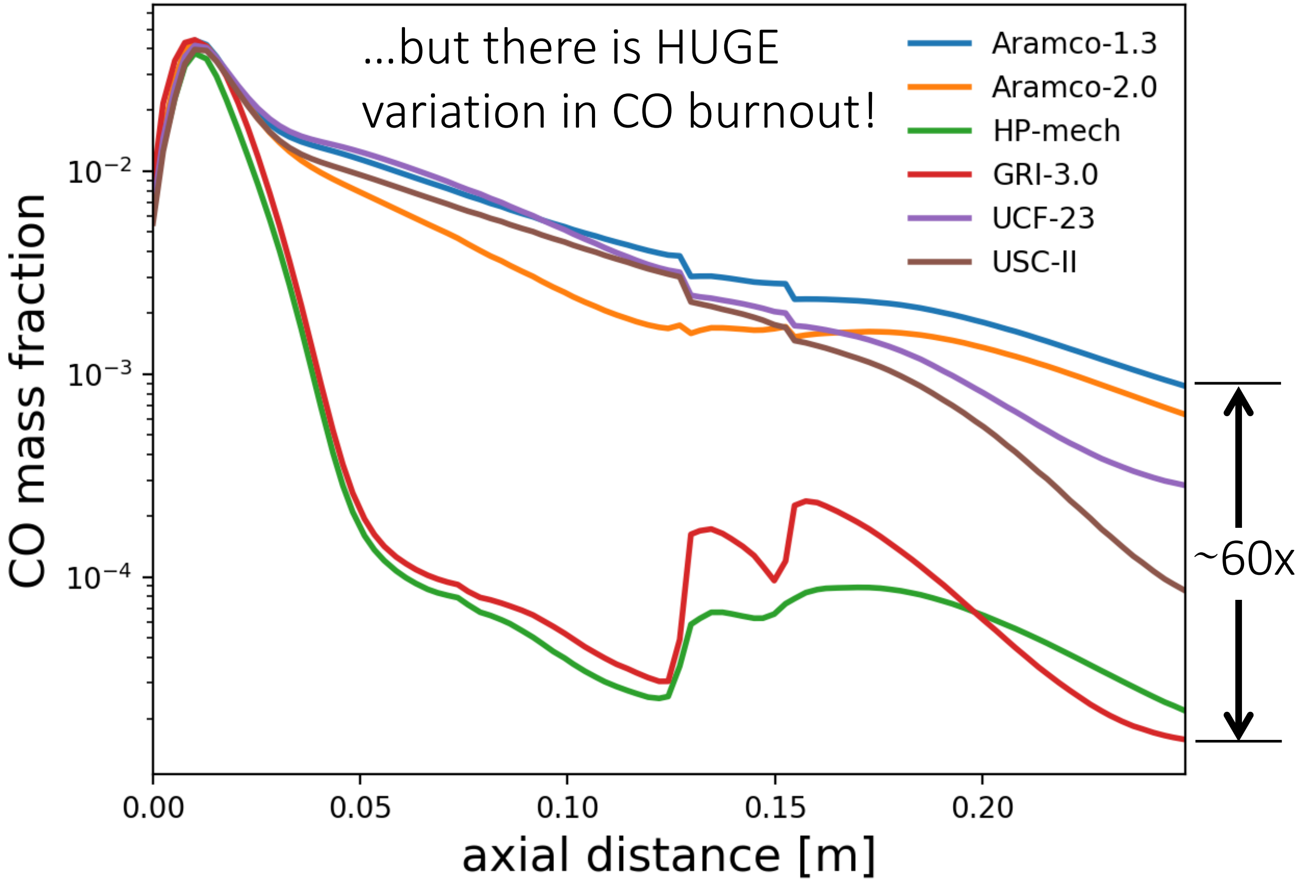
Axial profiles
(cross-section mass-avg)





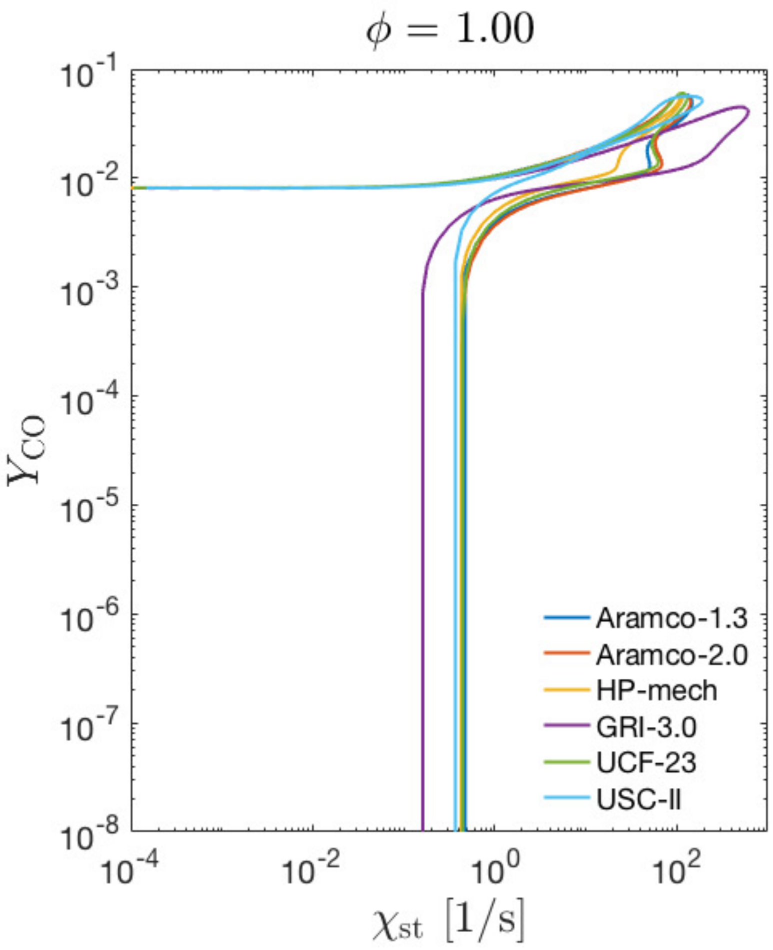
Combustion products and emissions
(cross-section mass-avg)



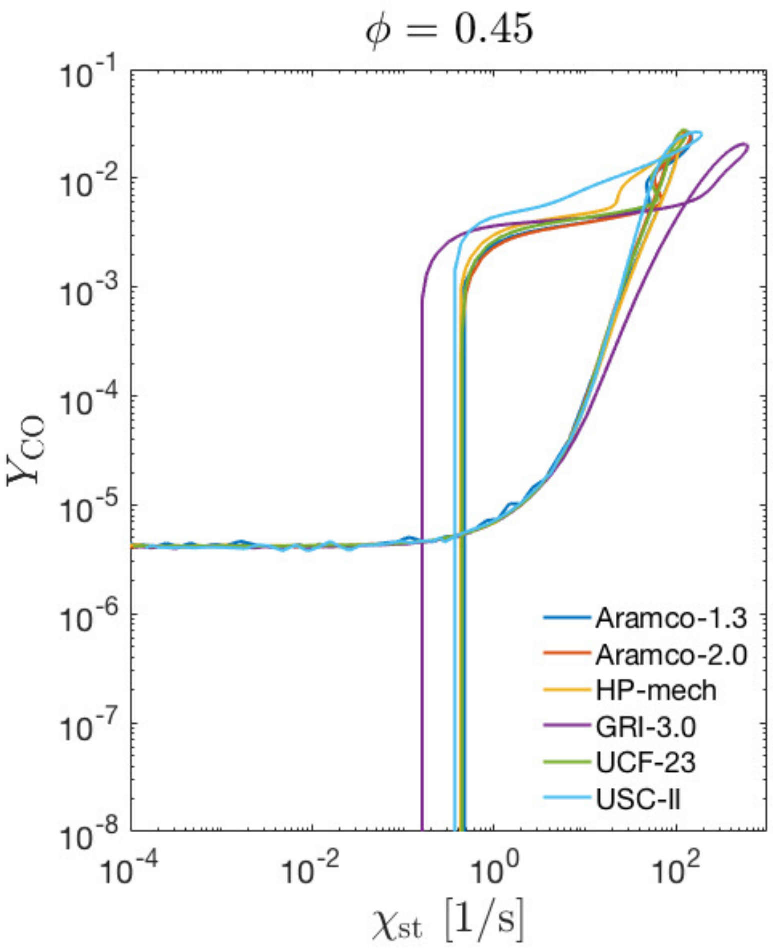


Flamelet s-curve (revisited for CO)

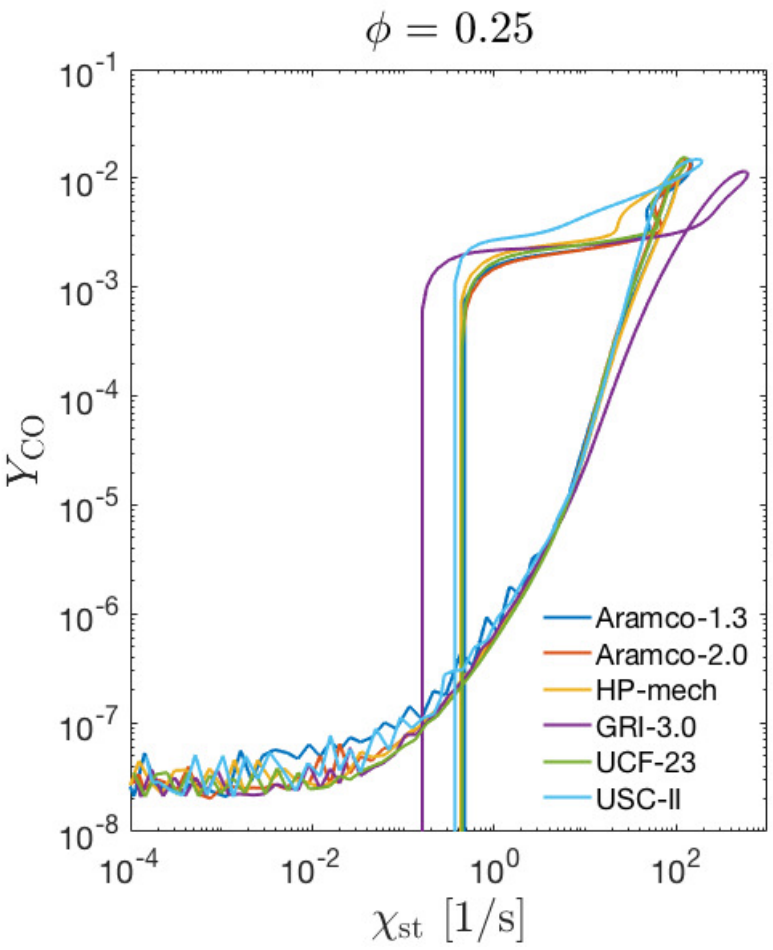
injection



post-effusion



post-dilution



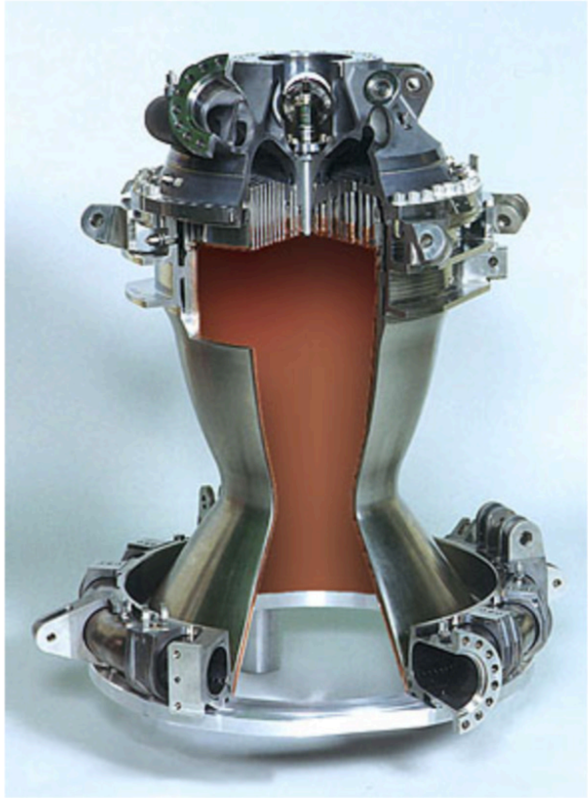
All mechanisms predict the same equilibrium CO (as $\chi_{st} \rightarrow 0$), yet notable differences manifest in the simulations

Conclusions

- Simulation results are affected by the underlying chemical mechanism
- This is particularly true to sensitive species (e.g. CO)
- Interactions between kinetics and flow scales can be subtle
- Chemical uncertainties are much larger than assumptions about ideal gas vs real fluid behavior (for these conditions)

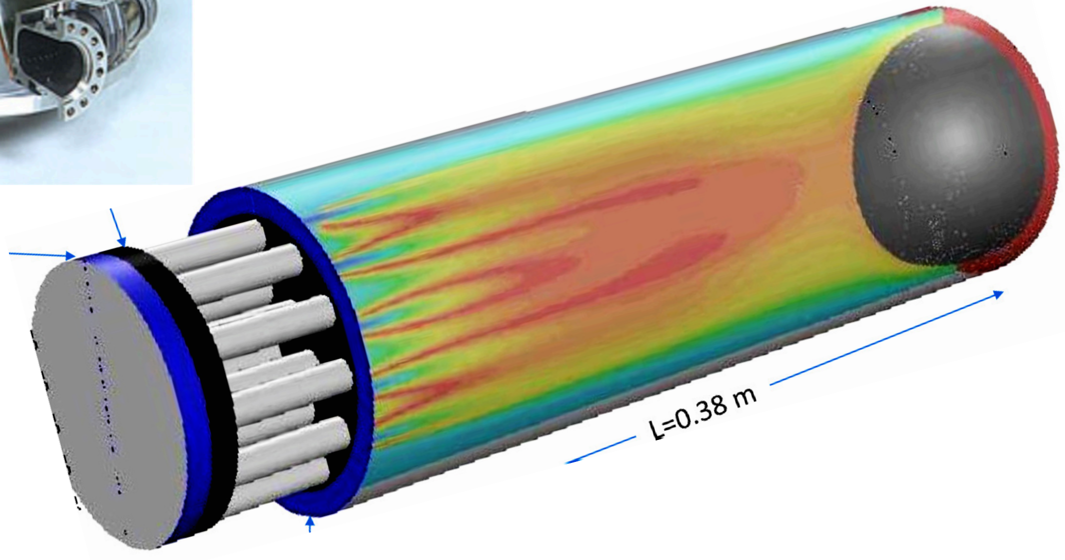
bi-periodic sCO_2 injector

motivation: multi-element rocket injectors



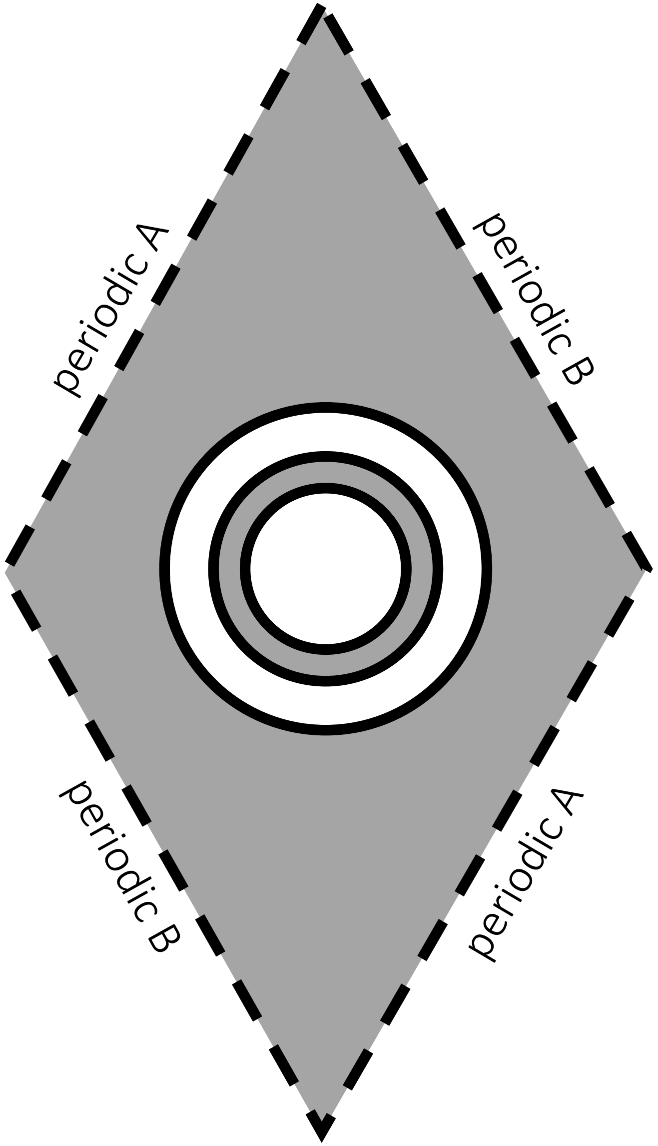
Vulcain2 injector plate (source: Astrium GmbH)

Application to sCO2 combustors
(Strakey, 6th sCO2 symposium 2018)

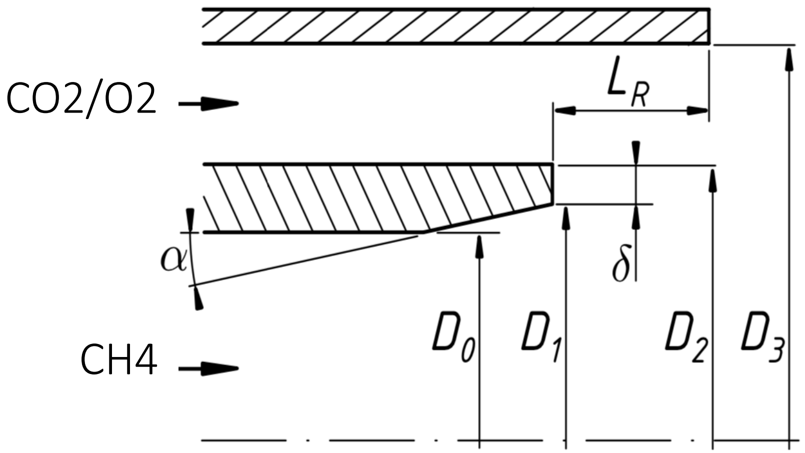


computational setup

TOP VIEW



SIDE VIEW



$D_0 = D_1 = 0.005$ m

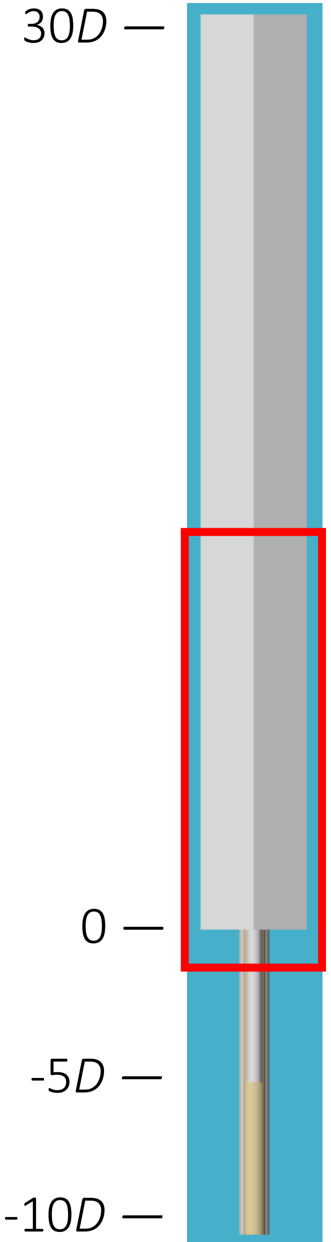
$D_2 = 0.007$ m

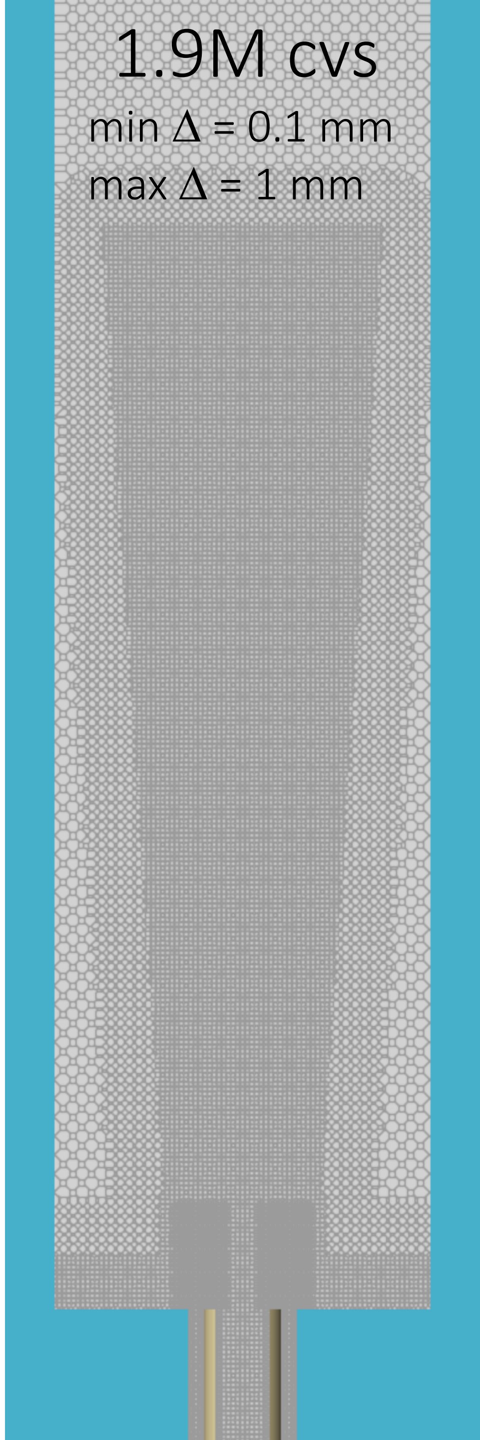
$D_3 = 0.01$ m

$\delta = 0.001$ m

$\alpha = 0$ deg

$L_R = 0$





operating conditions

pressure: p = 30 MPa

fuel: CH4, T_f = 300, 400, 500 K; Φ = 1.0

oxid: 80% CO2, 20% O2 (mass), T_o = 900, 1000, 1100 K

annulus (oxid)

T [K]	ρ [kg/m³]	U [m/s]	Re
900	164.1	169.1	2.11e+06
1000	147.7	187.9	1.96e+06
1100	134.3	206.6	1.84e+06

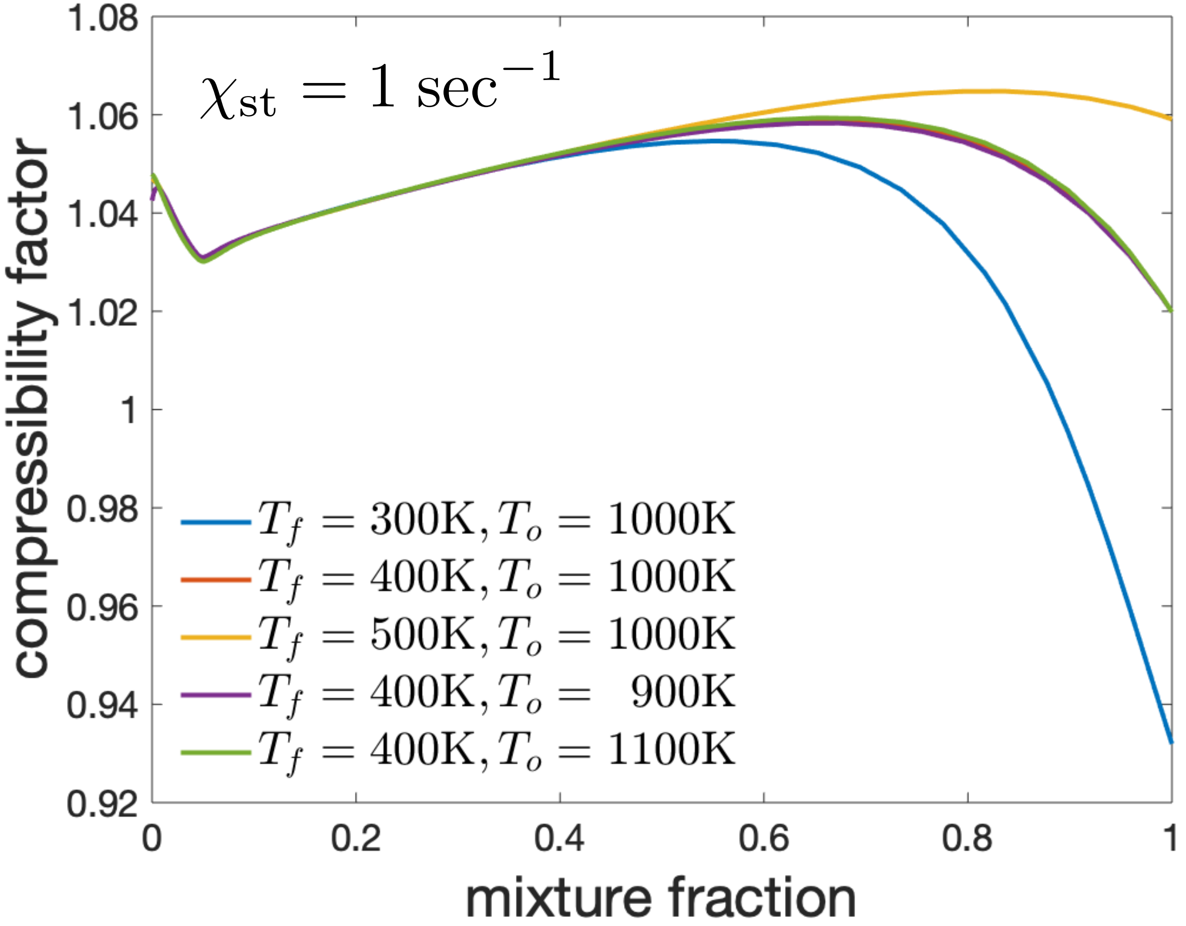
pipe (fuel)

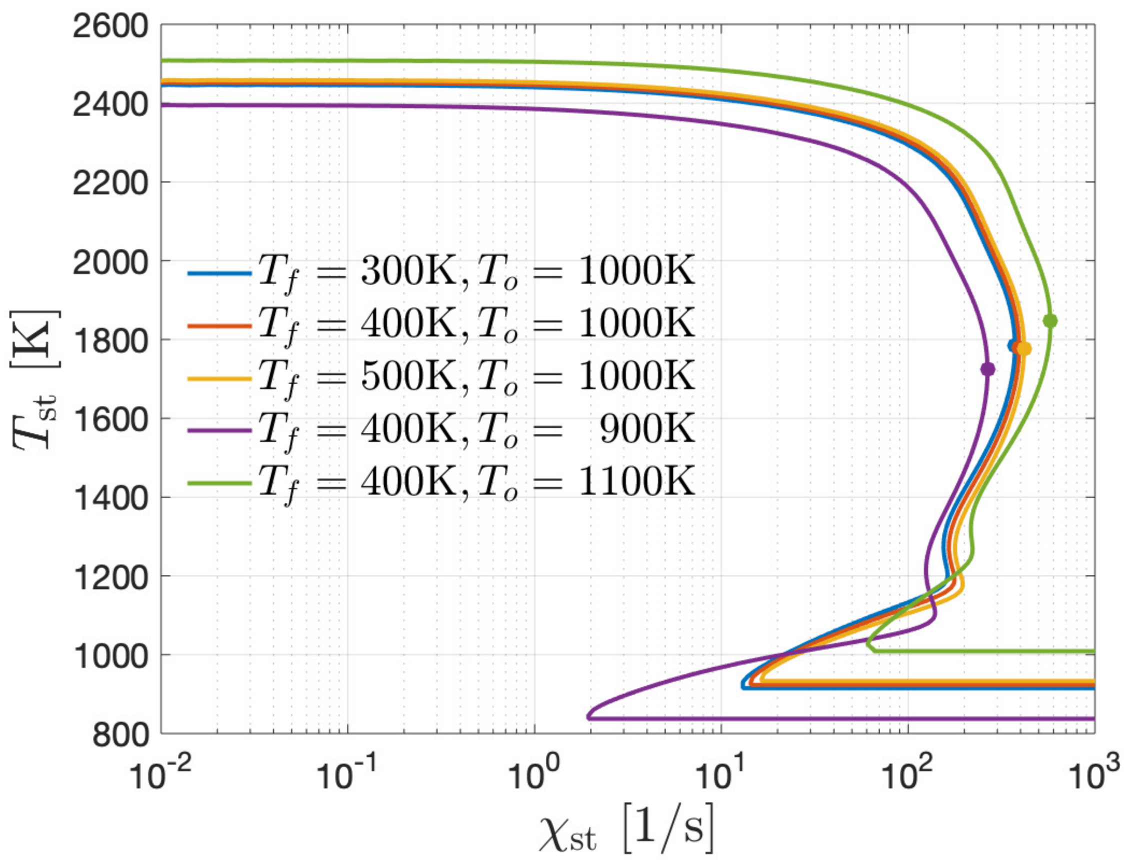
T [K]	ρ [kg/m³]	U [m/s]	Re
300	192.9	14.71	1.24e+06
400	144.7	19.61	9.83e+05
500	115.8	24.51	8.30e+05

$$J = \frac{\rho_2 U_2^2}{\rho_1 U_1^2}$$

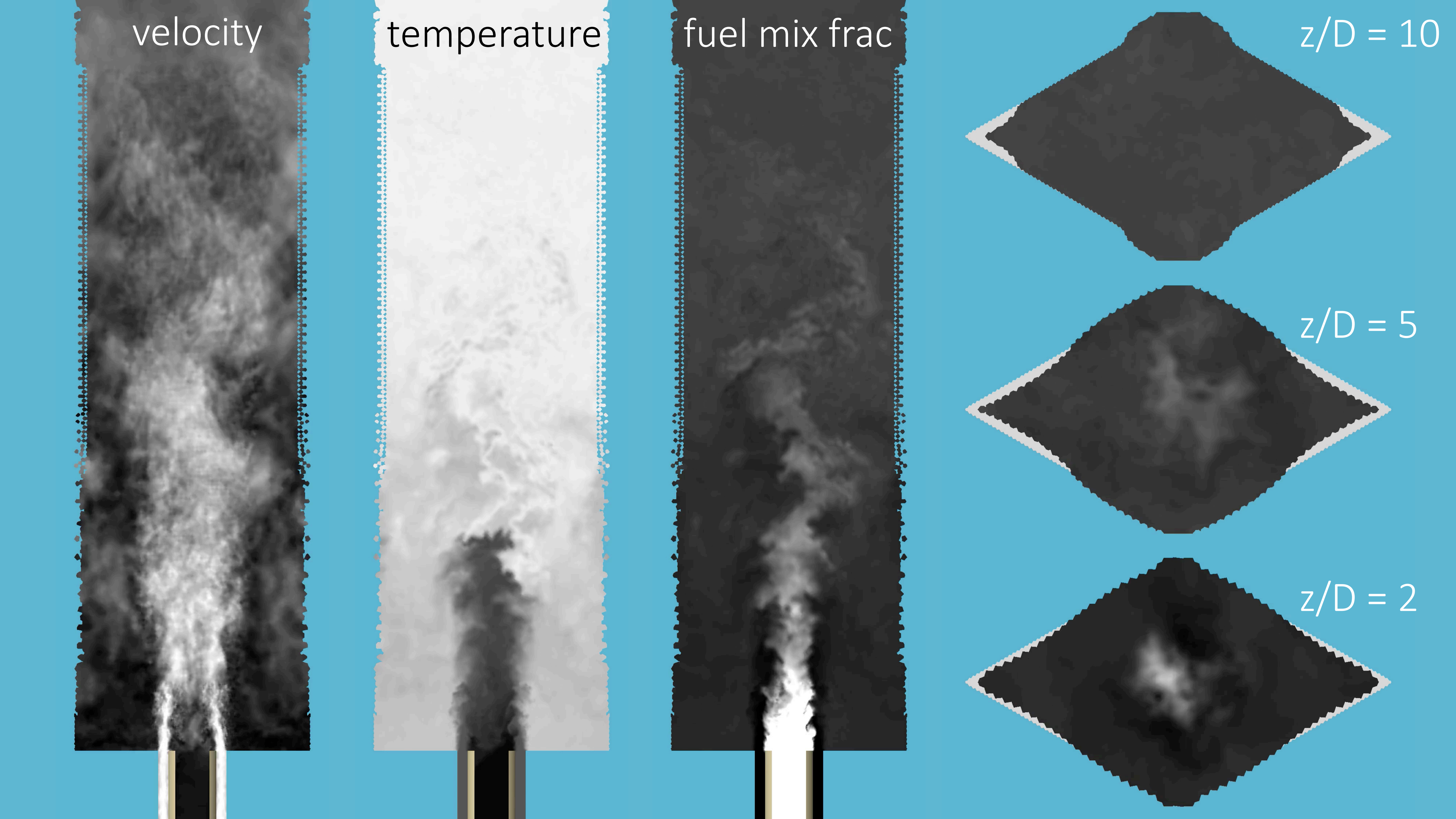
T_f [K]	T_o [K]	J (mom flux ratio)
300	1000	125.
400	1000	93.7
500	1000	74.9
400	900	84.3
400	1000	93.7
400	1100	103.

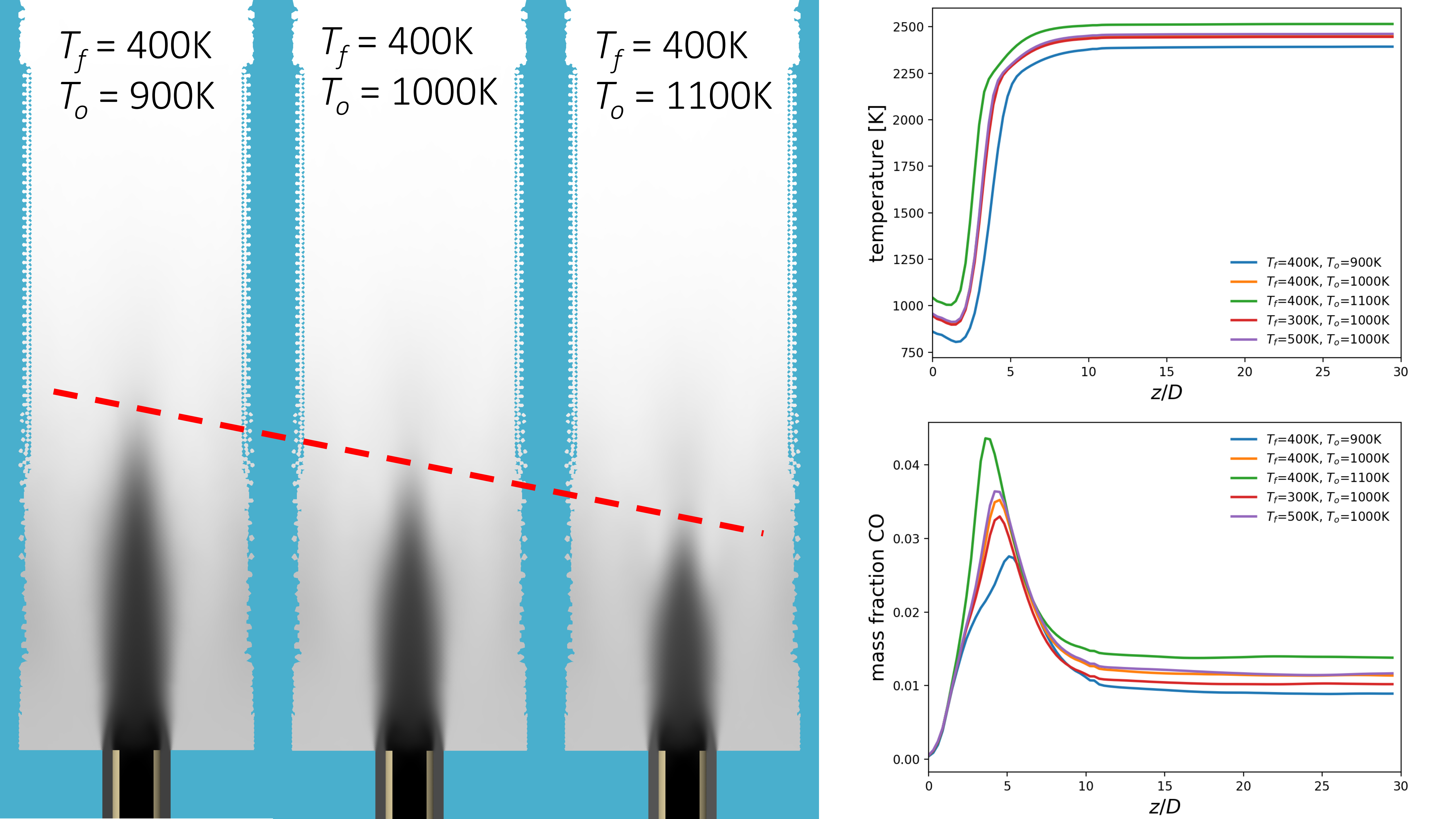
real-fluid effects





T_f , T_o [K]	χ_{crit} [1/s] (ideal gas)	χ_{crit} [1/s] (real fluid)	Δ (IG vs RF)
300, 1000	372.6	393.1	5.2 %
400, 1000	392.6	421.8	6.9 %
500, 1000	416.8	452.1	7.8 %
400, 900	266.0	282.2	5.7 %
400, 1100	577.1	625.7	7.8 %


velocity
temperature
fuel mix frac
z/D = 10
z/D = 5
z/D = 2



T_f = 400K
T_o = 900K
T_f = 400K
T_o = 1000K
T_f = 400K
T_o = 1100K
temperature [K]
z/D
mass fraction CO
z/D
T_f=400K, T_o=900K
T_f=400K, T_o=1000K
T_f=400K, T_o=1100K
T_f=300K, T_o=1000K
T_f=500K, T_o=1000K

Ongoing work

- Bi-periodic sCO2 injector
  - Expand flow/chemistry/thermo sensitivity studies
  - Injector-injector interactions using 4-jet configuration
- Continue to build-out thermochemical/physics models for LES
  - Ongoing validation for real-fluid tabulated combustion models
  - Transported species (finite-rate chemistry) implementation
  - Multicomponent + multiphase applications w/ cubic EOS
  - Subgrid-scale models for high-pressure turbulent flows

CASCADE TECHNOLOGIES

Discovery through simulation