LES of oxy-fuel combustion for sCO2 power cycles

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Award: DE-SC0017230

2018 UTSR Project Review Meeting

Project personnel

- Cascade Technologies
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- Consultants
  - Javier Urzay, Stanford CTR
  - Subith Vasu, UCF
- Acknowledgements
  - Jacob Delimont, SwRI
  - Mark Freeman, NETL

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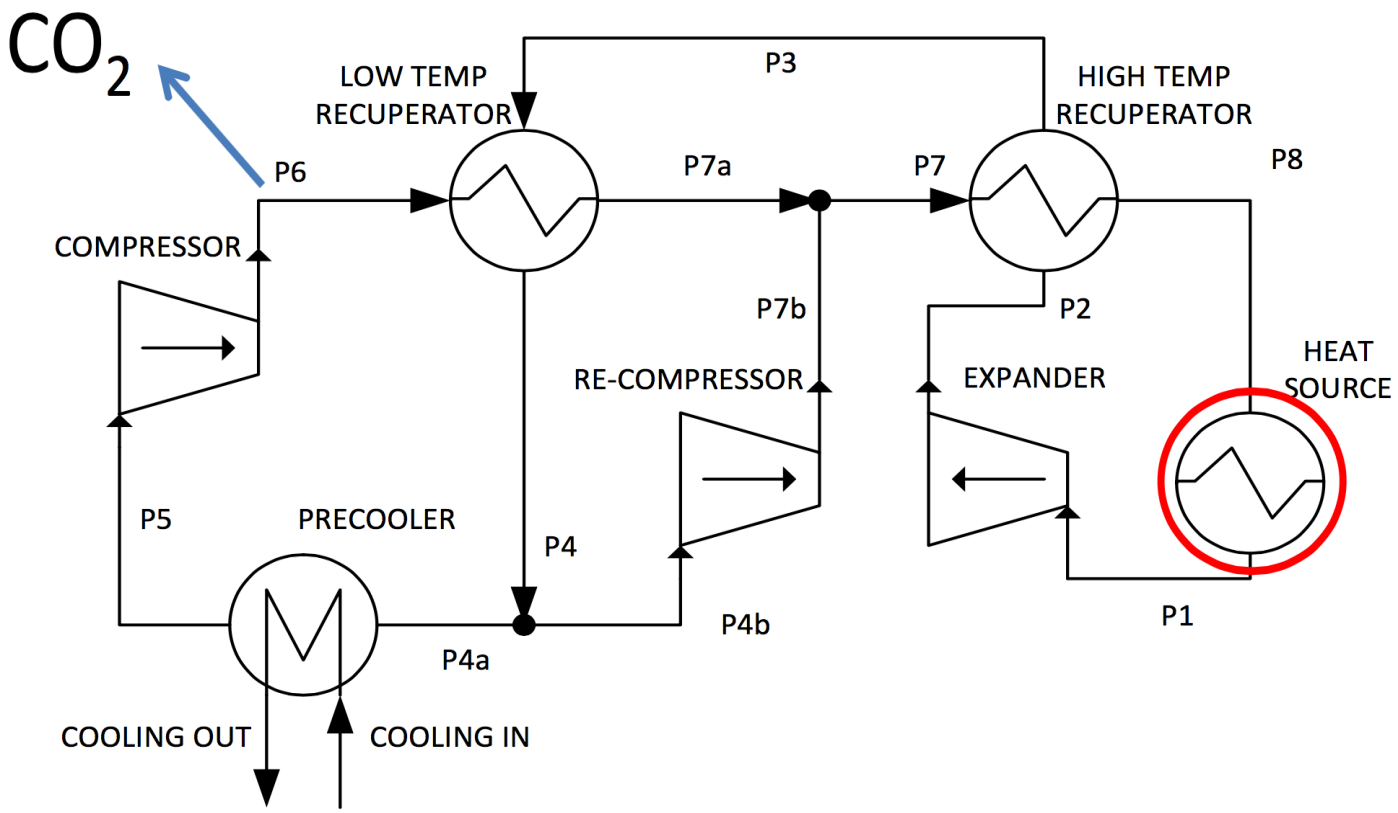
Project overview

- 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)
  - Put all the pieces together from phase-I
  - Demonstrate utility for scientific discovery and design exploration in practical sCO2 systems

Direct-fired sCO2 cycle - Allam cycle

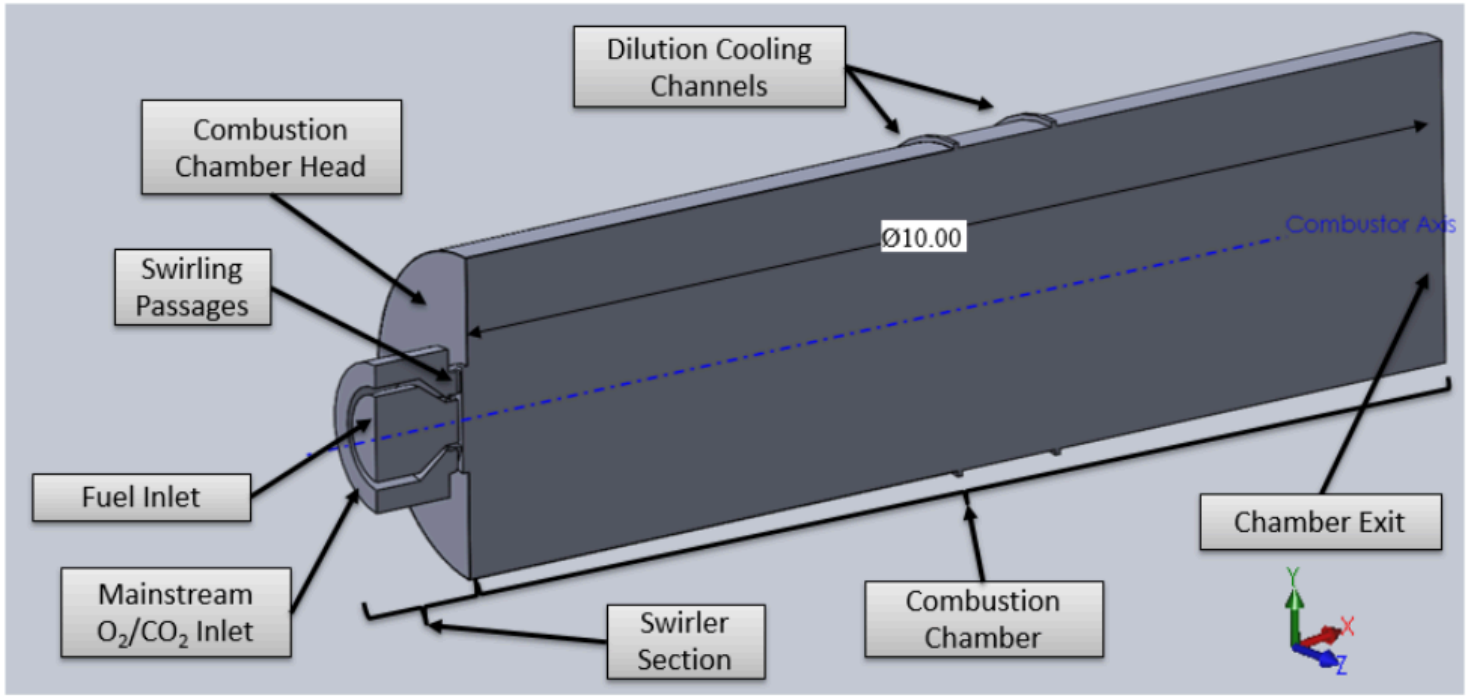


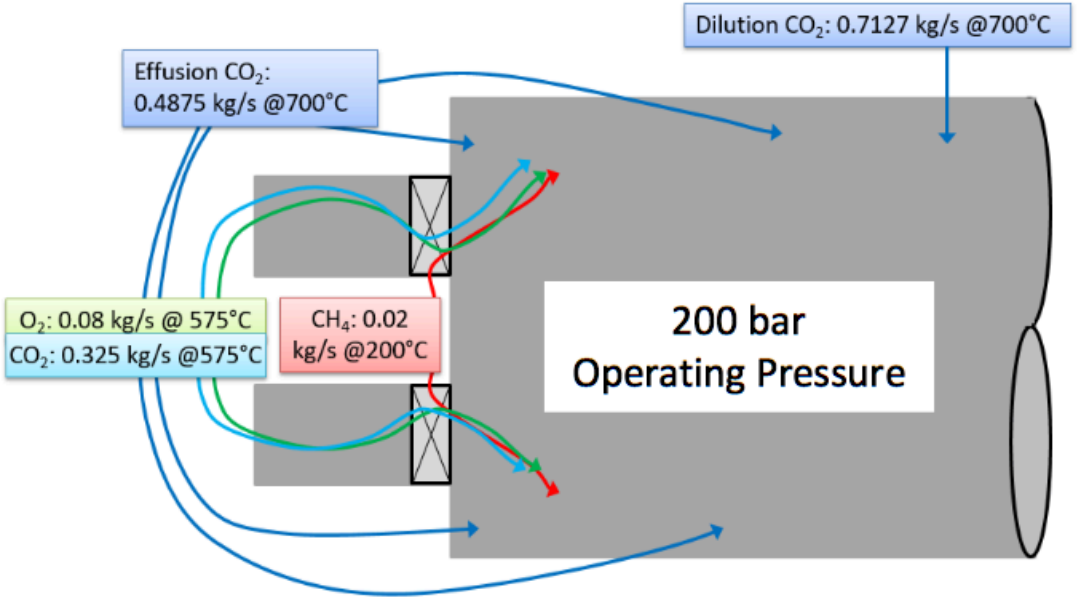
Delimont 2017

- 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

SwRI sCO2 concept combustor

OBJECTIVE: Examine sensitivity of LES results to various chemical mechanisms





from: Delimont et al 2018 sCO2 Symposium

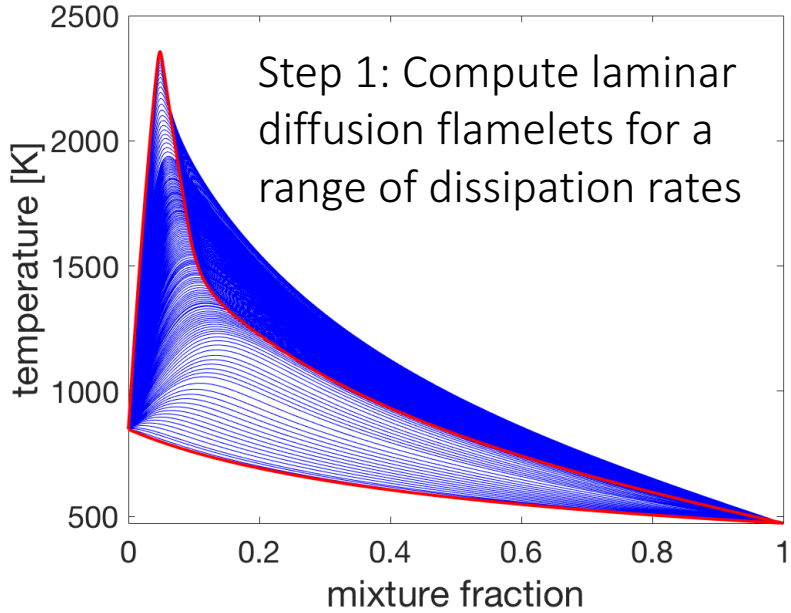
combustor stage	equivalence ratio	mixture fraction	pure CO_2 @T=973 K	80:20 CO_2:O_2 @T=962 K
post-injection	1.0	0.047059	2349.5 K	2349.5 K
post-effusion	0.45	0.021918	1671.8 K	1675.7 K
post-dilution	0.25	0.012306	1380.8 K	1380.7 K

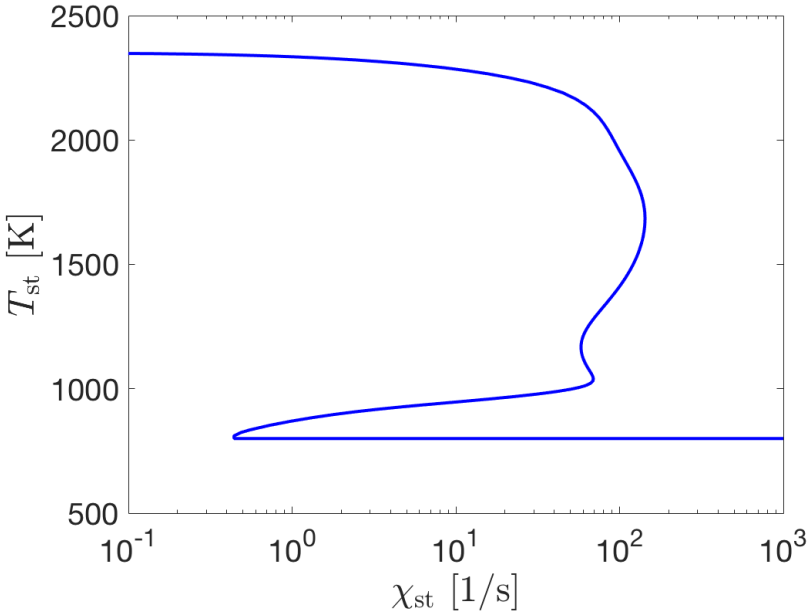
Chemical mechanisms

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

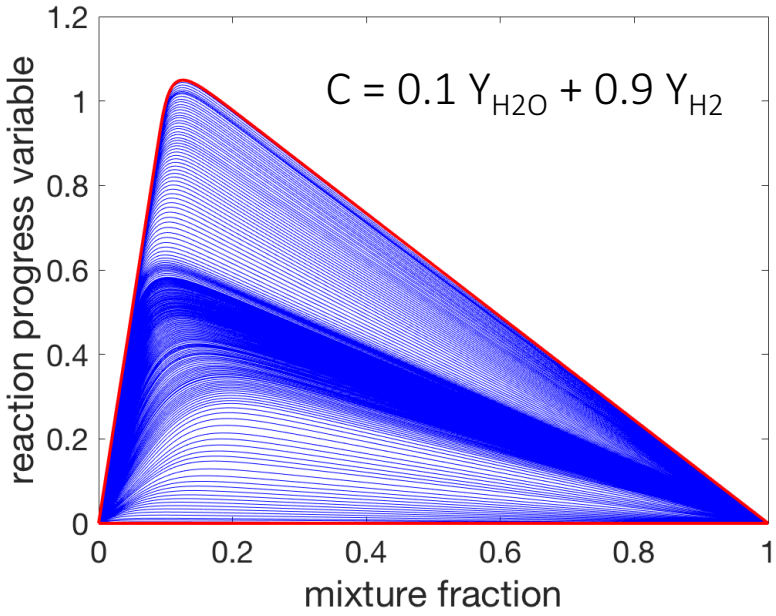
FPV combustion model

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



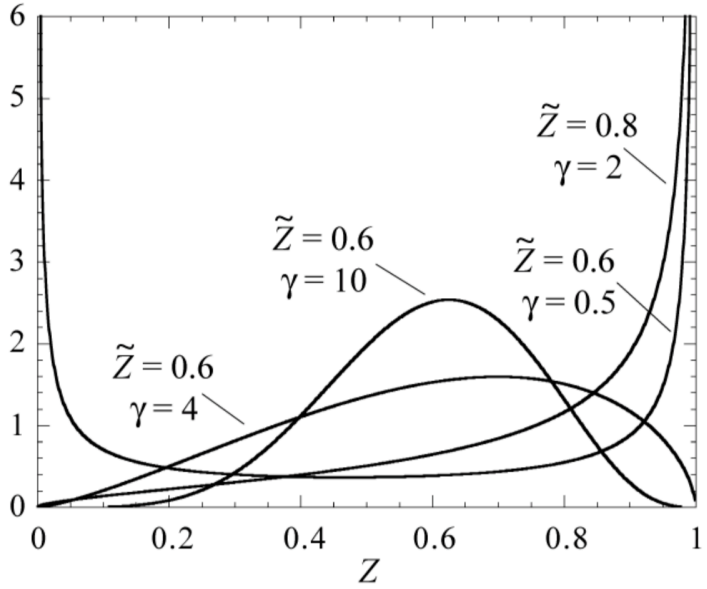


Step 2: Define a reaction progress variable and map flamelets to (Z, C)

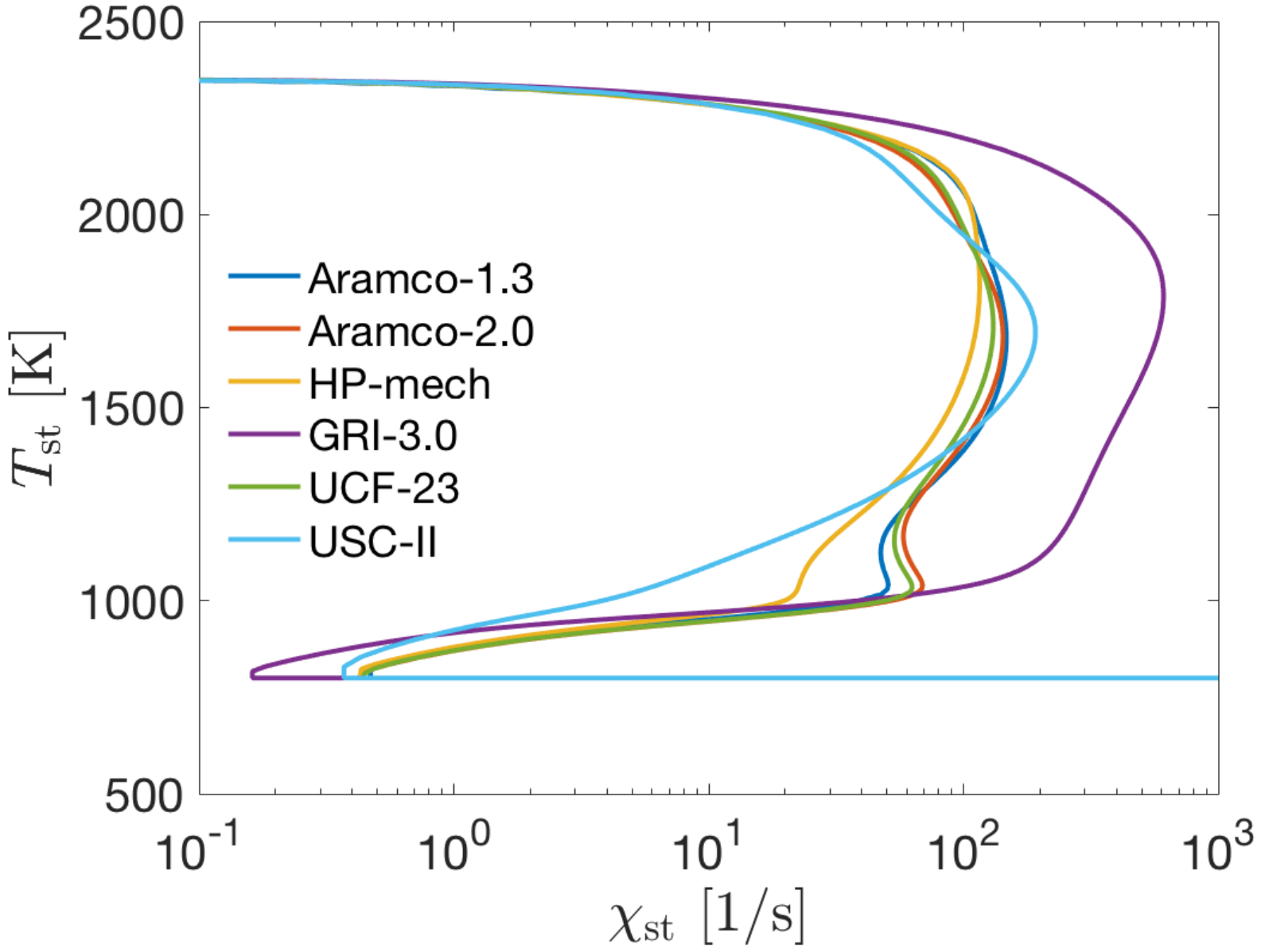


Step 3: Assume PDF closure for SGS turbulence-chemistry interactions

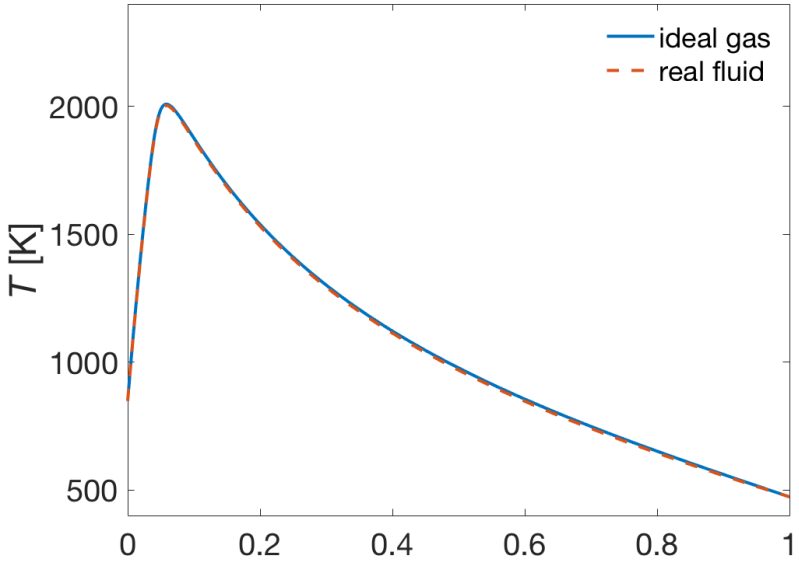
$$\widetilde{\psi} = \int\int \psi(z,\Lambda)\widetilde{P}(z)\widetilde{P}(\Lambda)\mathrm{d}z\mathrm{d}\Lambda$$

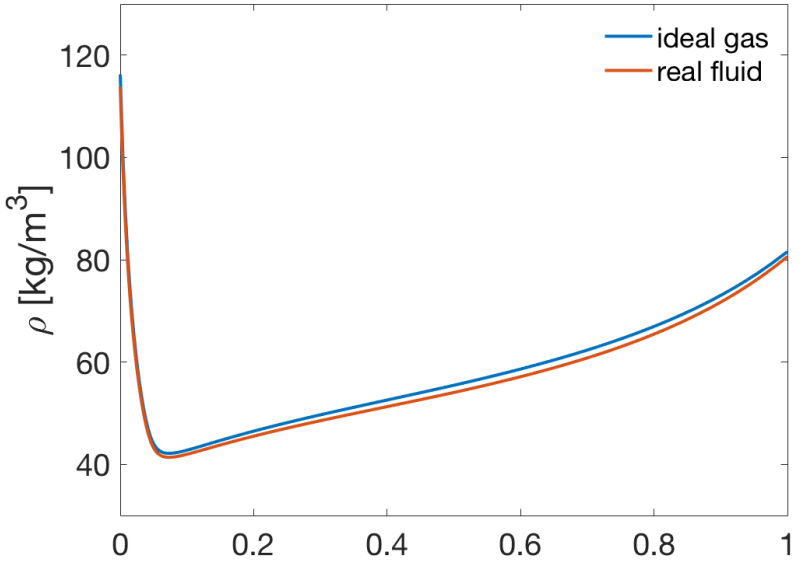


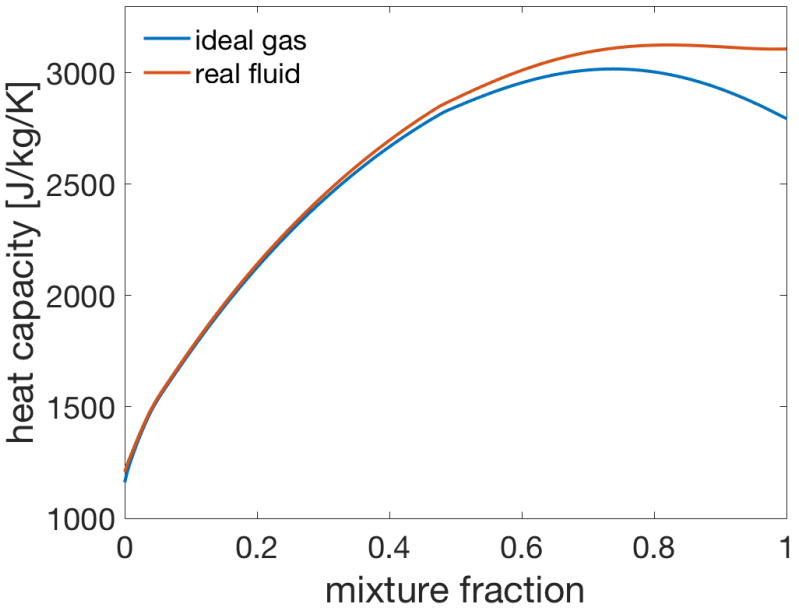
Flamelet s-curve (IG EOS)

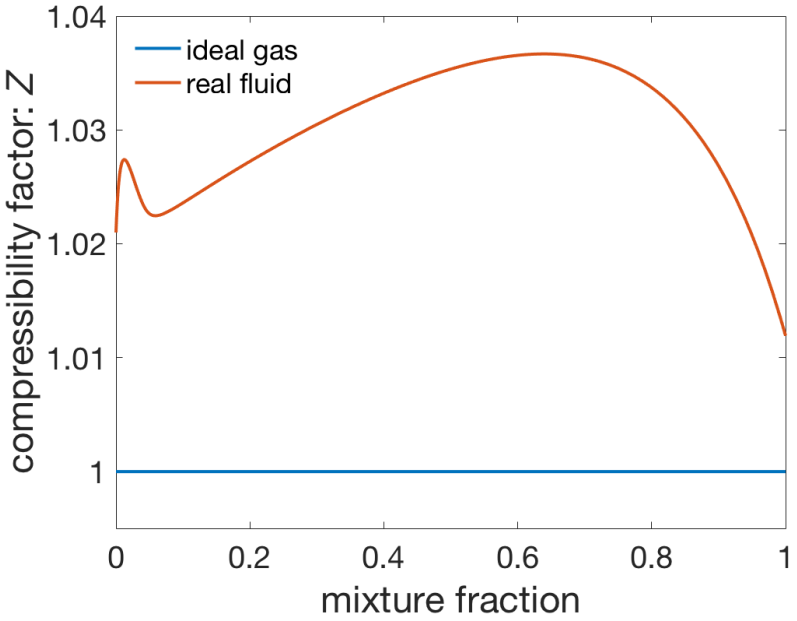


Real-gas effects









χ_{st} = 100 s^{-1}

chem: UCF-23

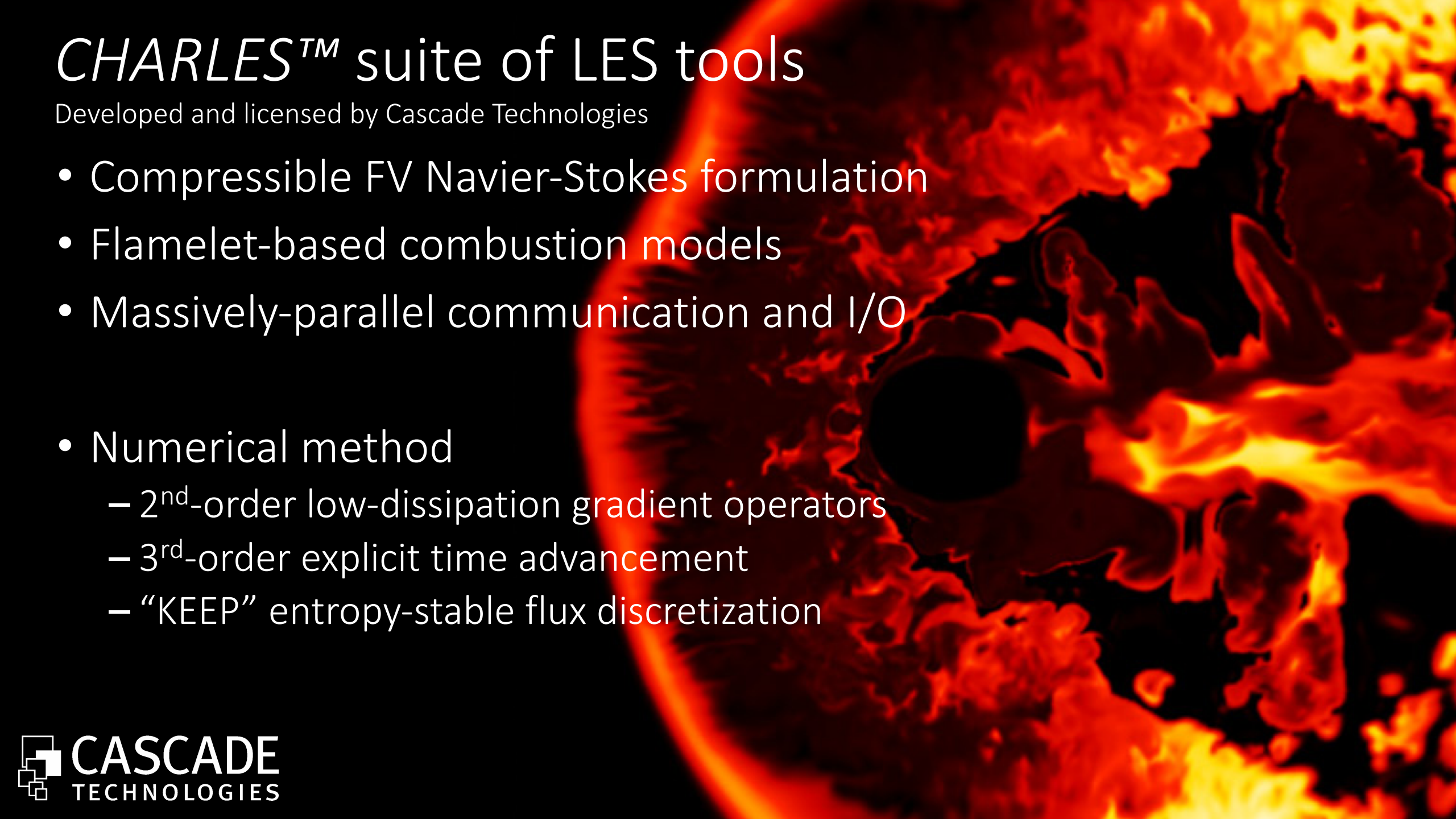
Given the mild real-gas effects in this problem, we will continue with IG EOS for this analysis

CHARLES™ suite of LES tools

Developed and licensed by Cascade Technologies

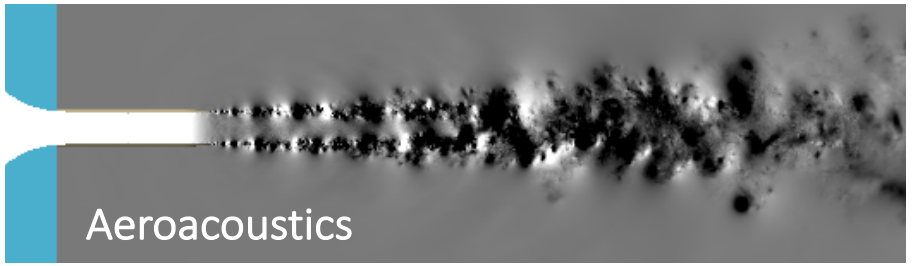
- Compressible FV Navier-Stokes formulation
- Flamelet-based combustion models
- Massively-parallel communication and I/O

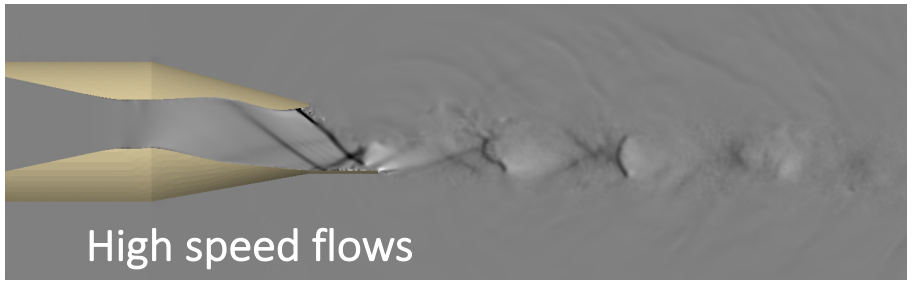
- Numerical method
  - 2^{nd}-order low-dissipation gradient operators
  - 3^{rd}-order explicit time advancement
  - “KEEP” entropy-stable flux discretization

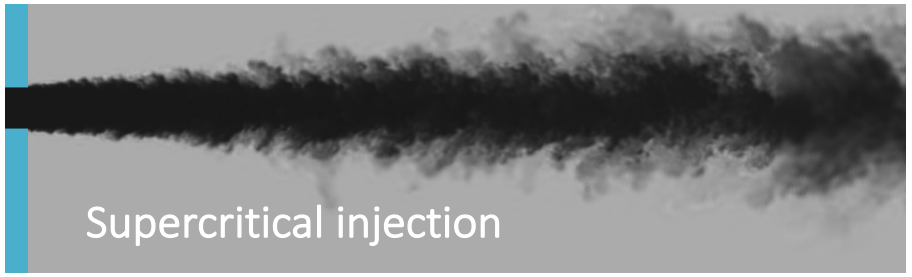


CASCADE TECHNOLOGIES

Stability using physics, not dissipation!







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

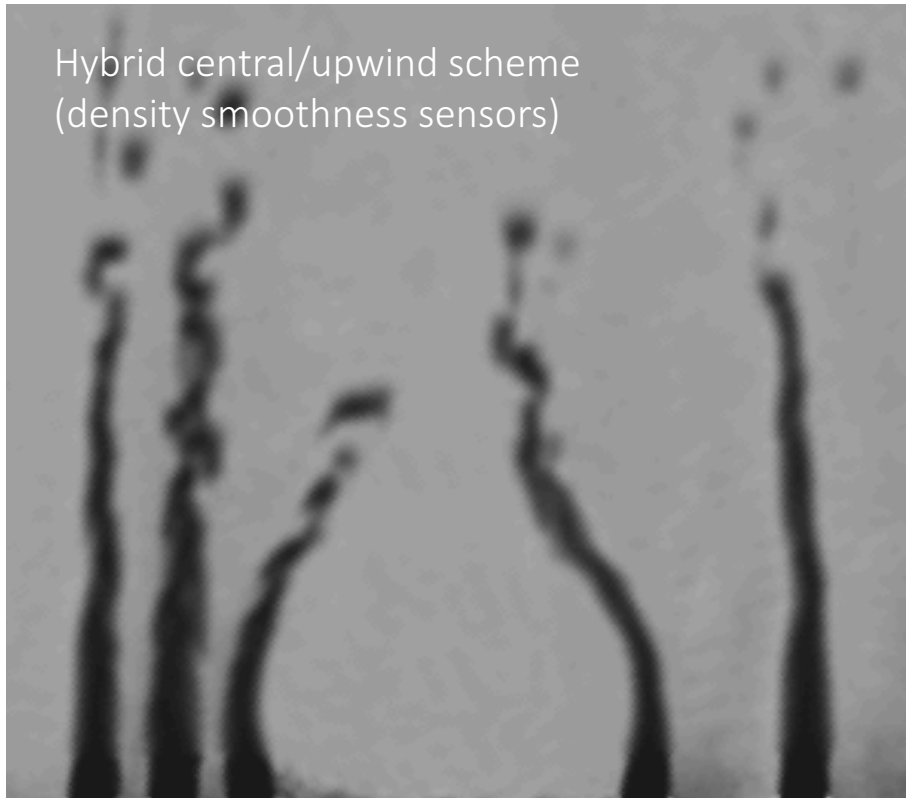
Stability conditions based on discrete satisfaction of Gibbs-Duhem condition (2nd law of thermodynamics)

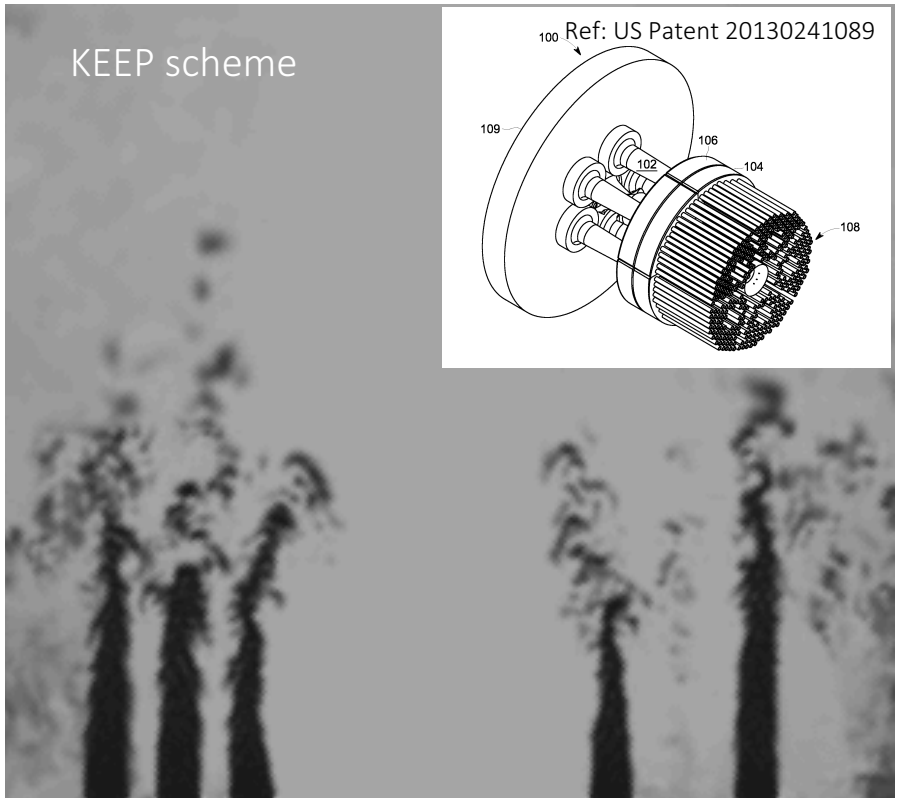
$$d(\rho s) = \frac{1}{T} d(\rho E) - \frac{u}{T} d(\rho u) + \left(s + \frac{u^2}{2T} - \frac{h}{T} \right) d\rho$$

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

KEEP schemes drastically improve solution quality and numerical stability

Example: Premixed combustion in industrial multi-element combustor



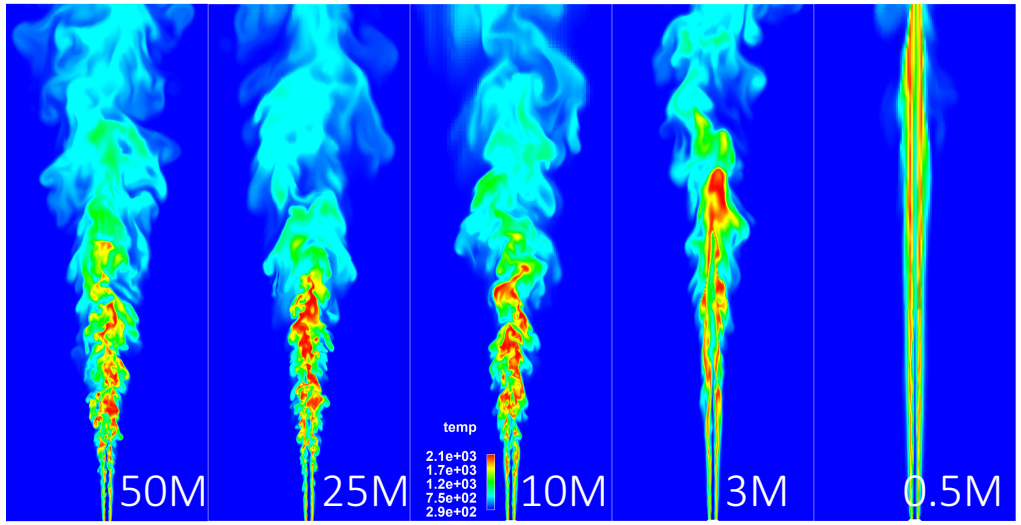


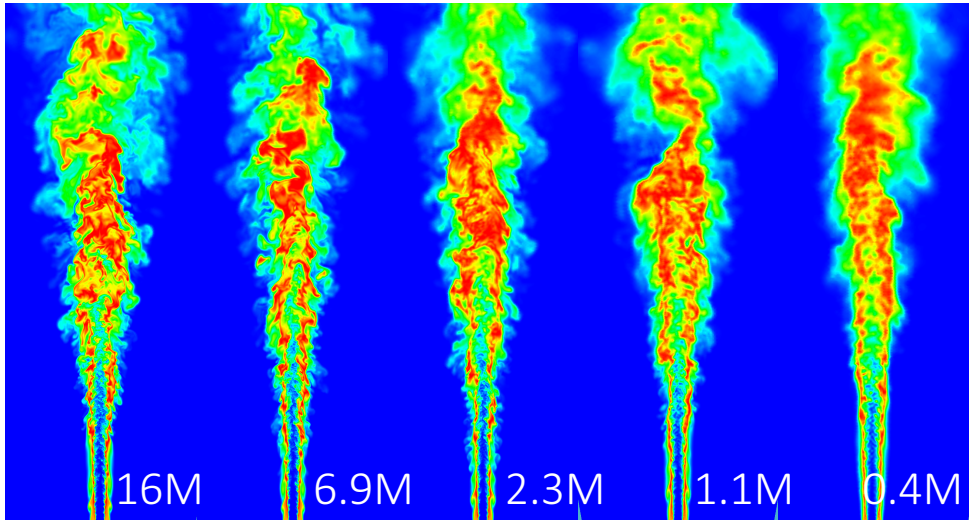
System level LES calculations necessarily result in coarsely resolved structures

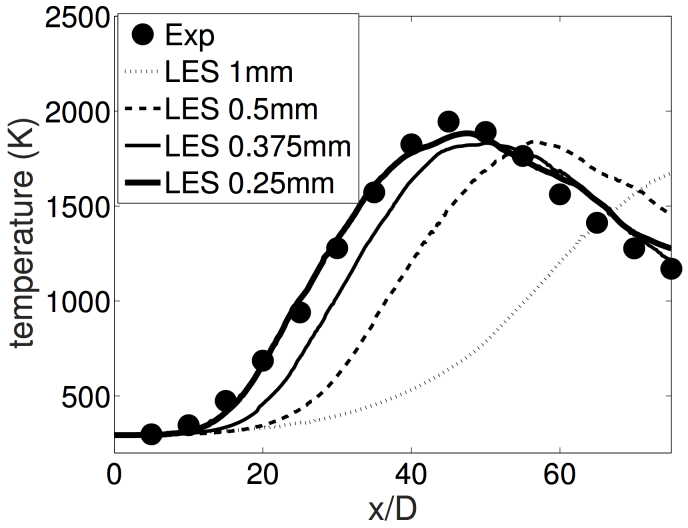
- KEEP schemes improve accuracy (e.g., flame length consistent with experiments)
- Simulations are more robust and less sensitive to mesh resolution and transitions

Not all LES are equal!

Sandia D LES flame comparison: >10X cost reductions from better numerics and modeling

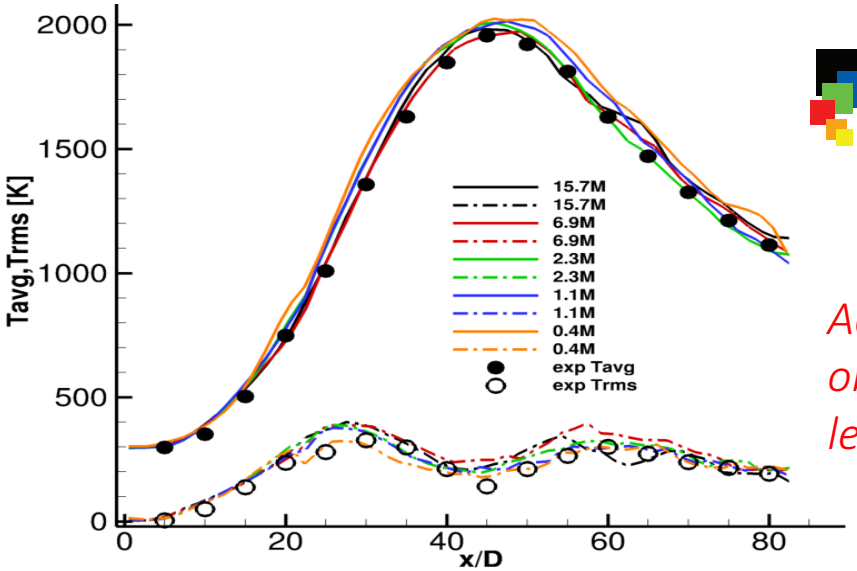






CONVERGE CFD SOFTWARE

Liu et al, 2018, AIAA

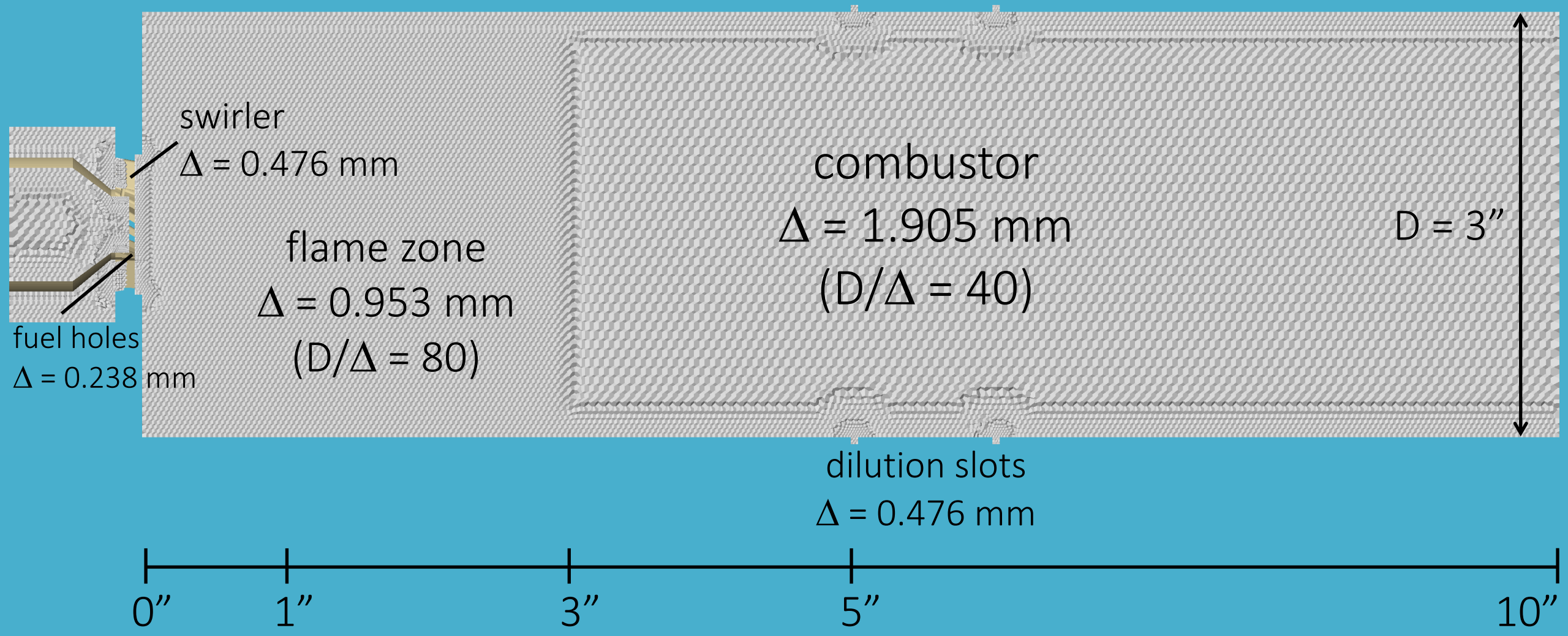


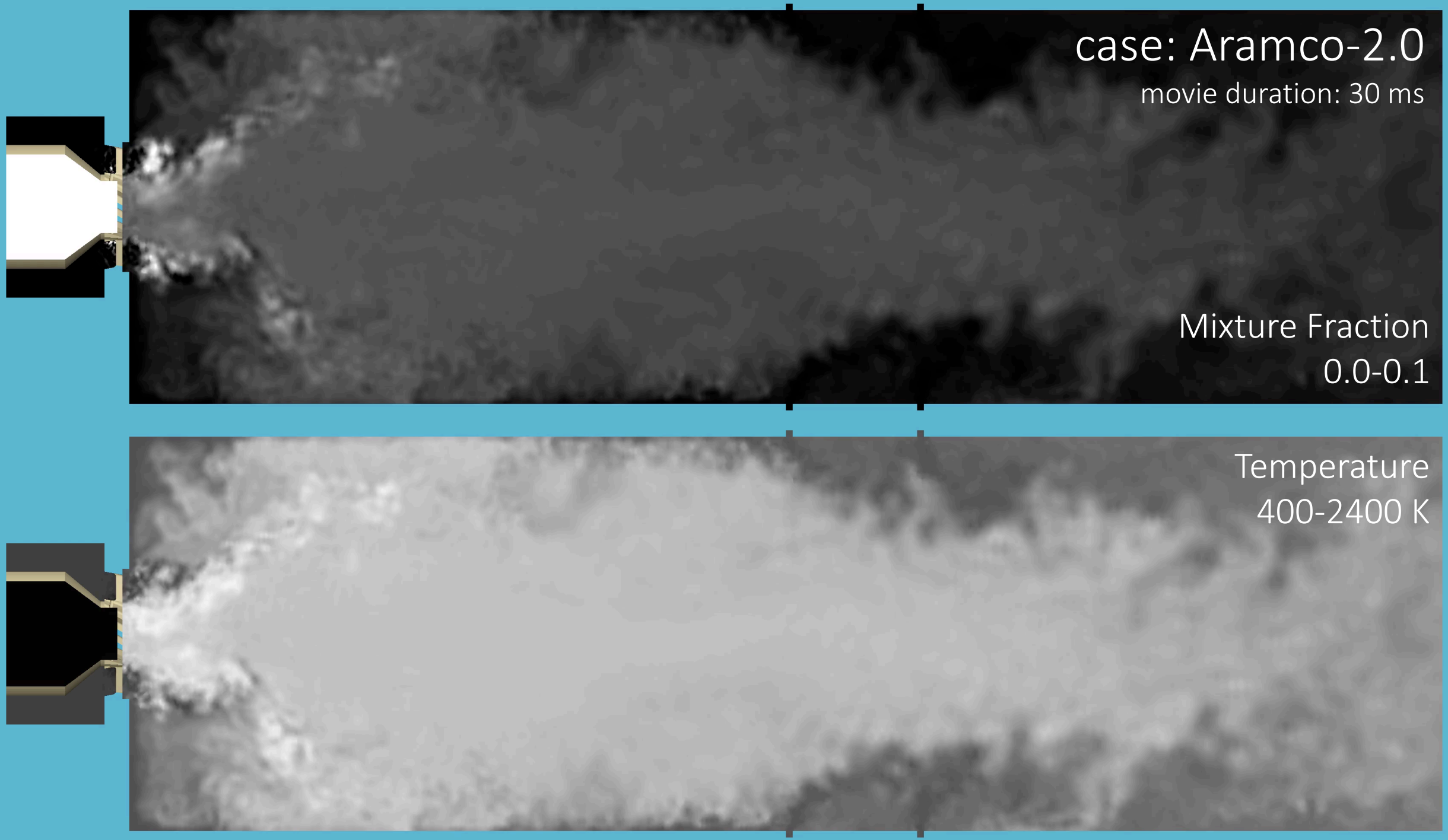
CASCADE TECHNOLOGIES

Acceptable accuracy obtained for >50X less cost

“Coarse” LES mesh

1.1M Voronoi CVs

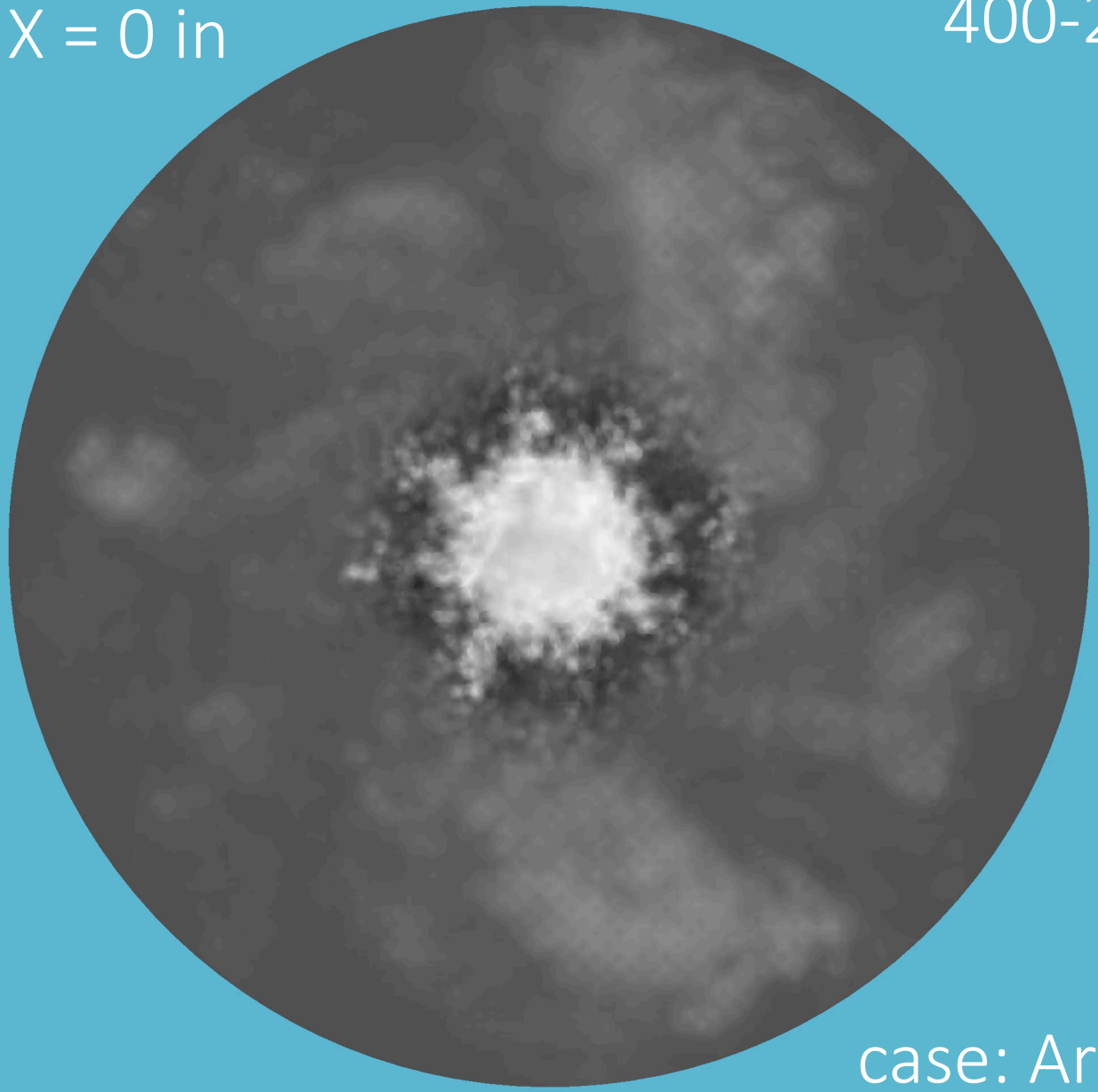



case: Aramco-2.0
movie duration: 30 ms
Mixture Fraction
0.0-0.1
Temperature
400-2400 K

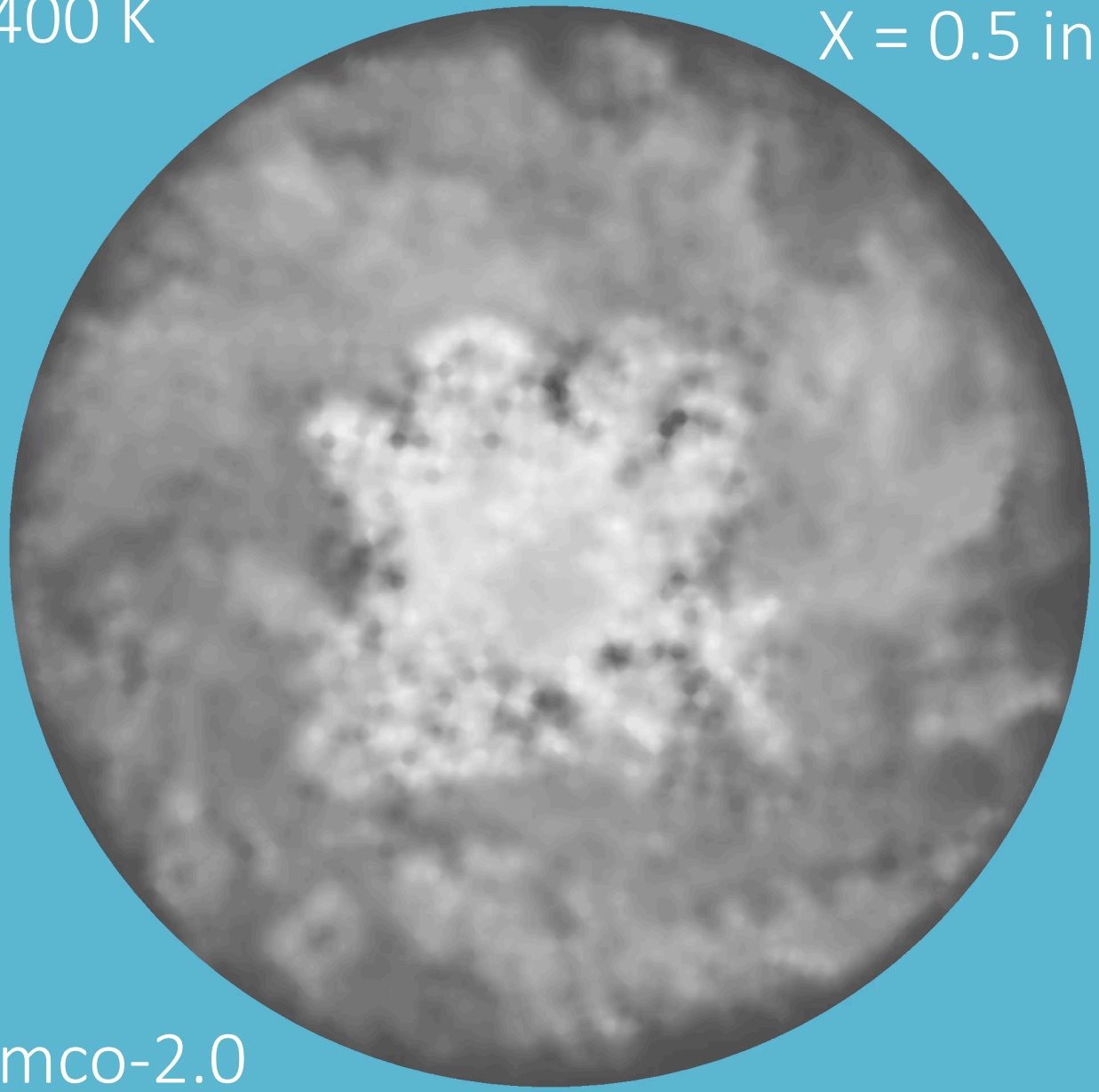
Temperature

400-2400 K

X = 0 in



X = 0.5 in

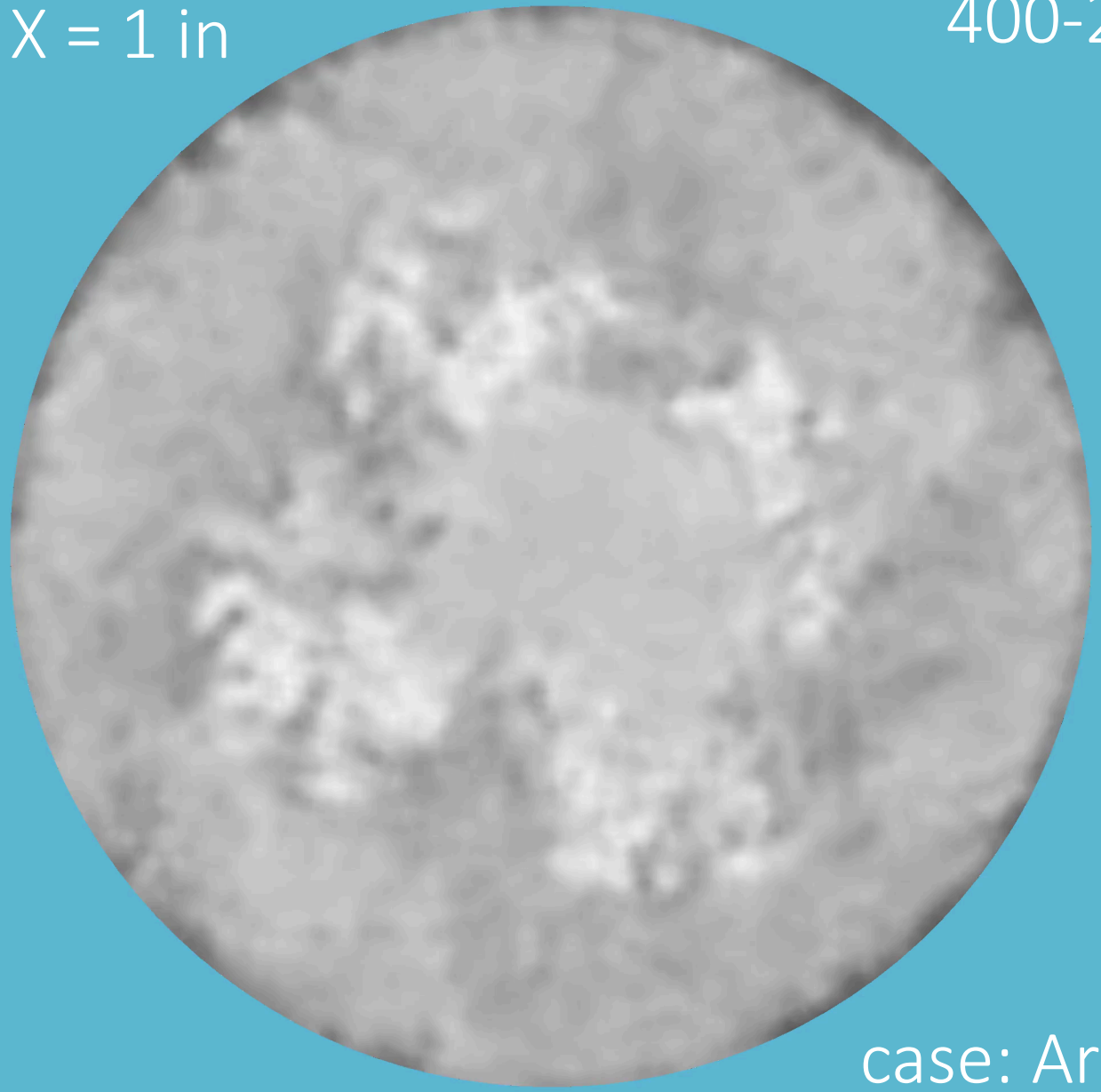


case: Aramco-2.0

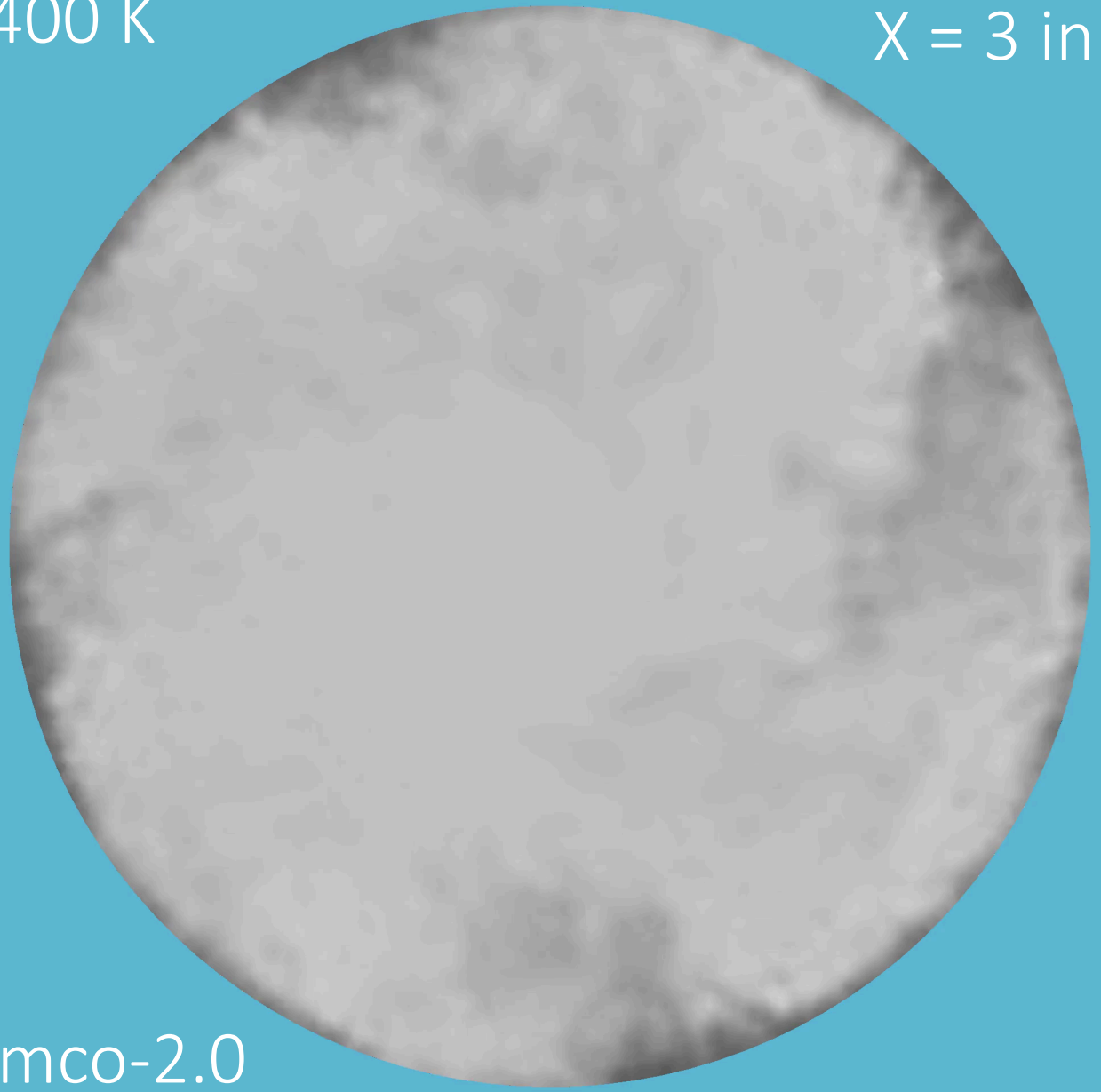
Temperature

400-2400 K

X = 1 in



X = 3 in

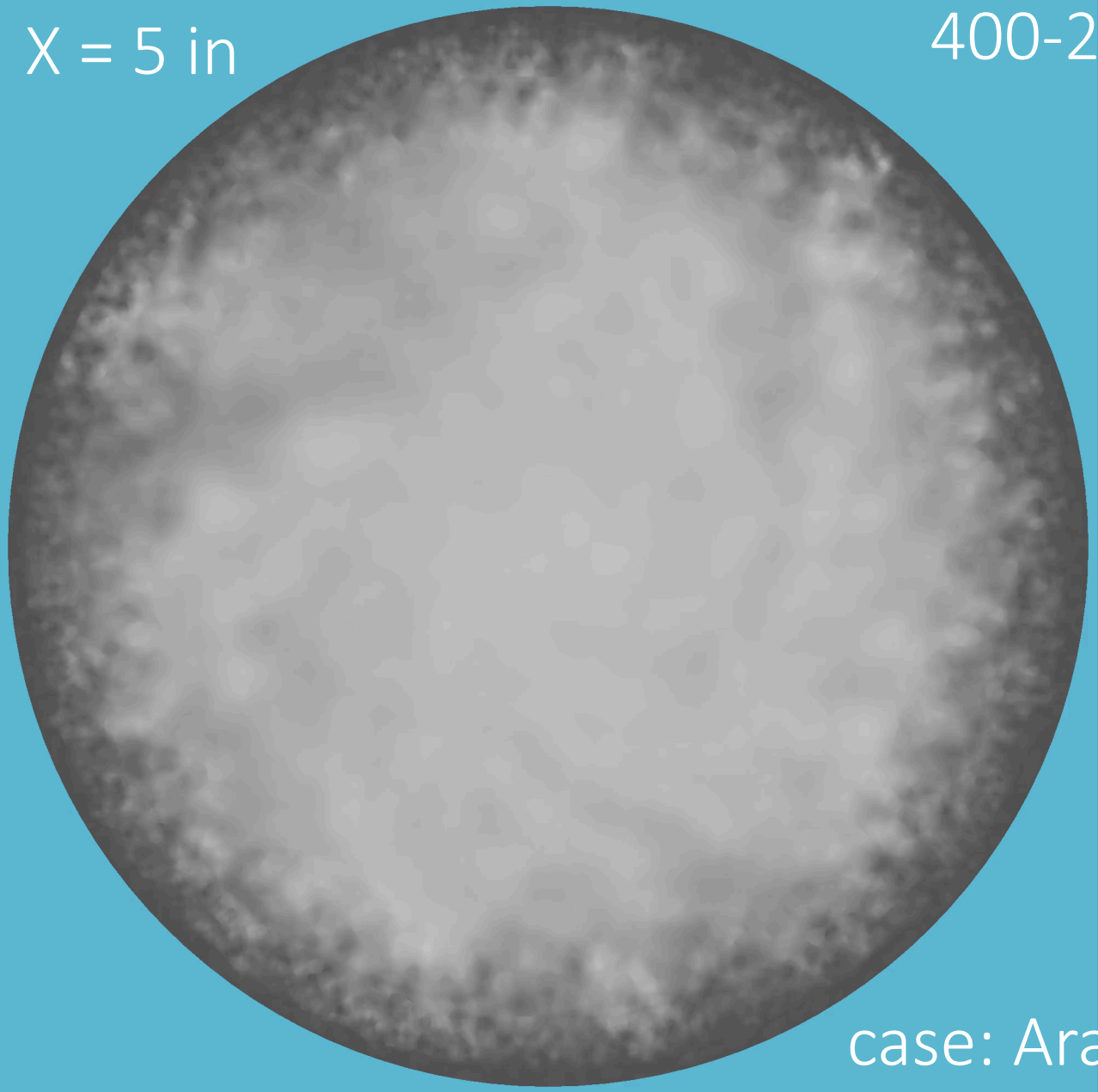


case: Aramco-2.0

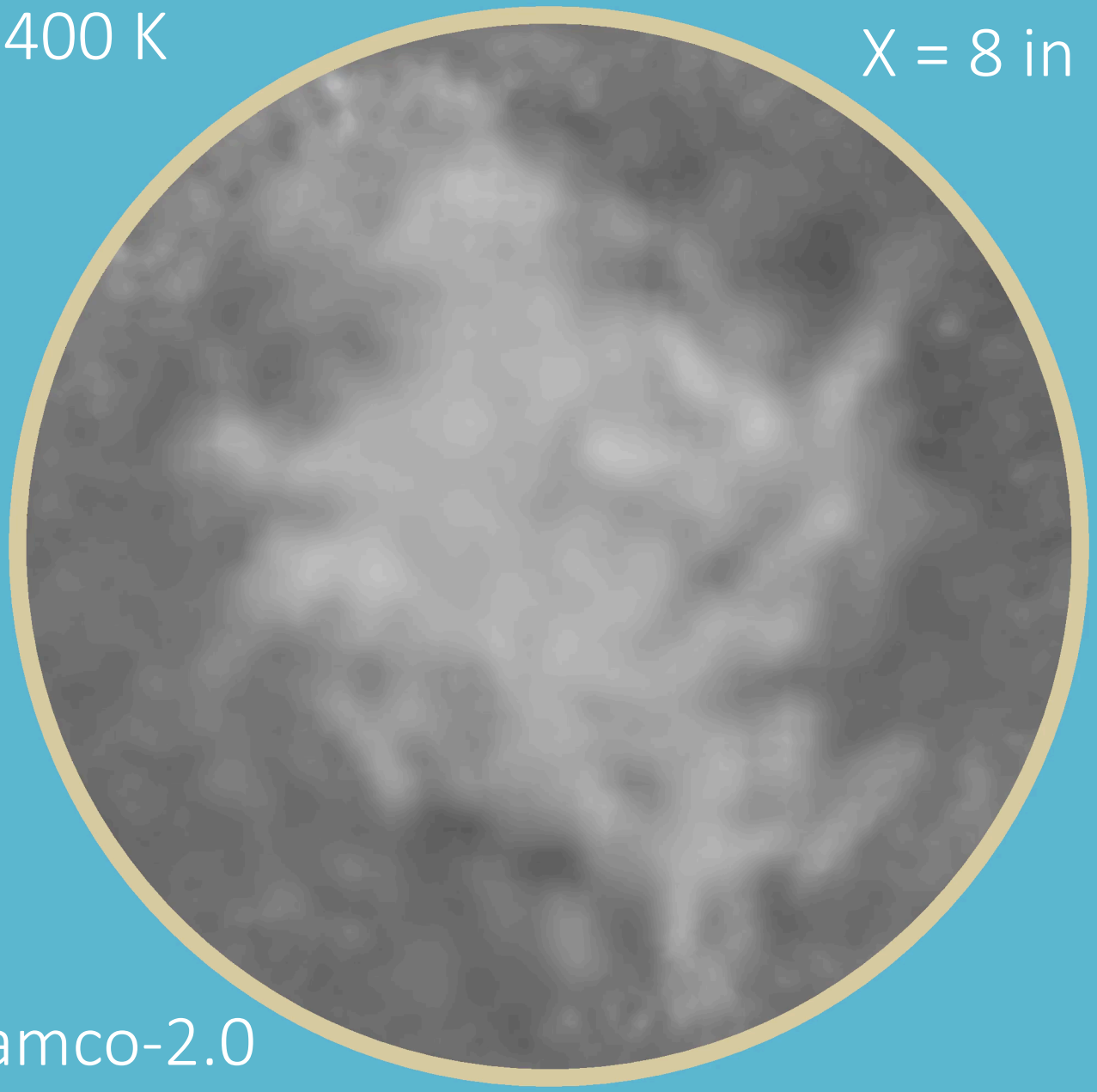
Temperature

400-2400 K

X = 5 in

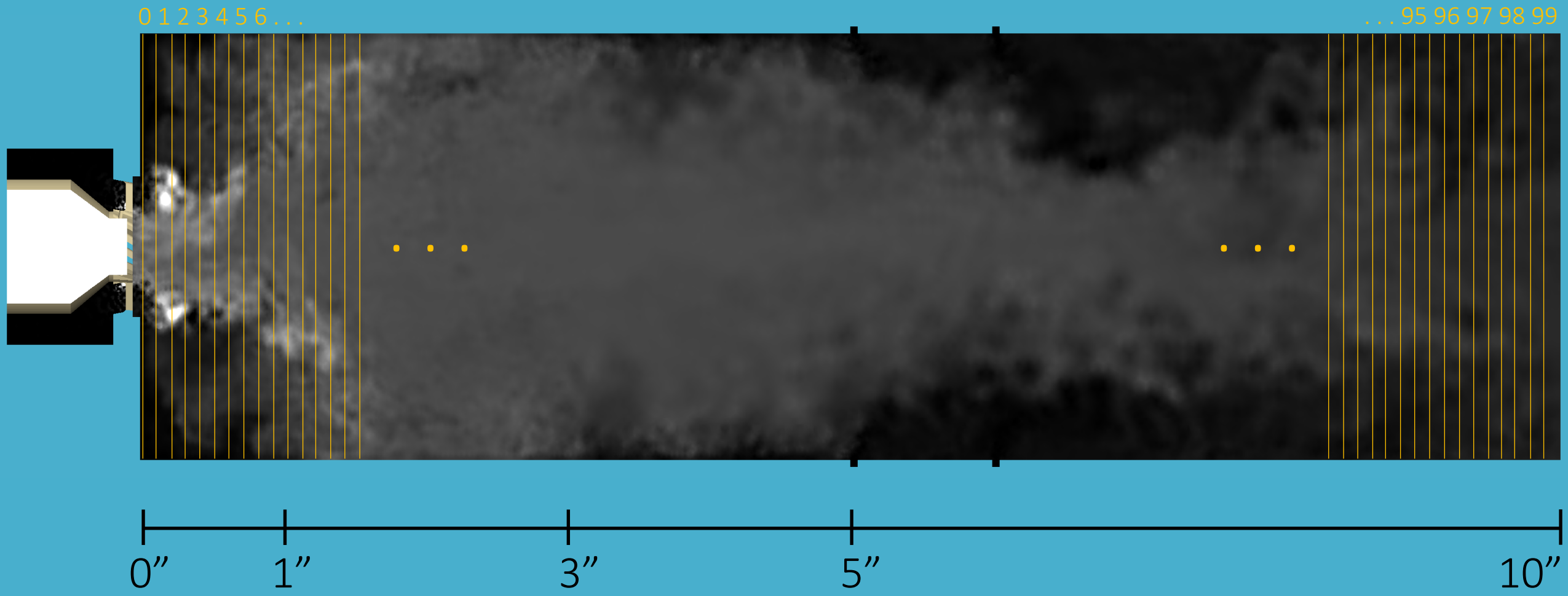


X = 8 in



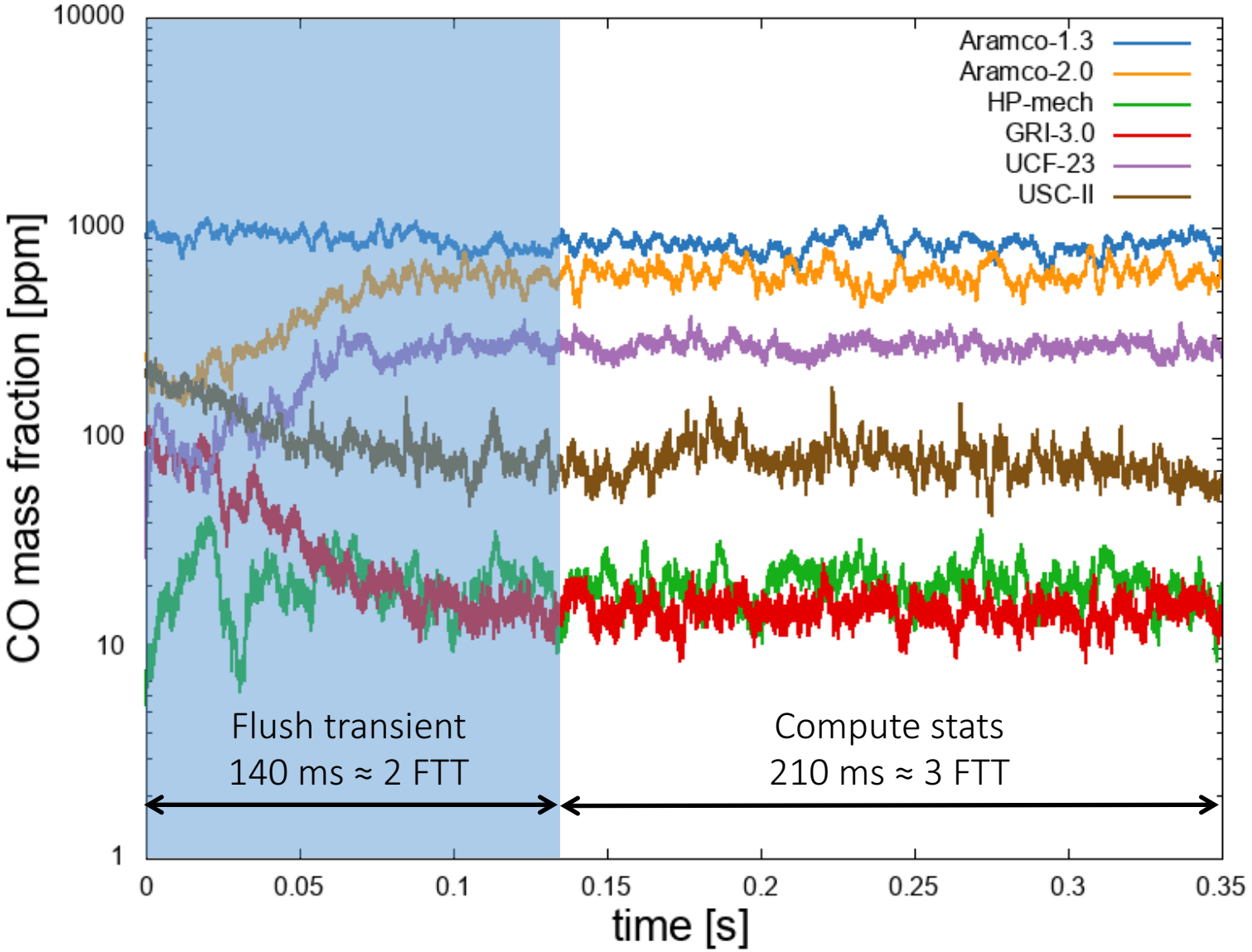
case: Aramco-2.0

“Flux probe” setup
(massflow-weighted variables @ 100 axial cross-sections)

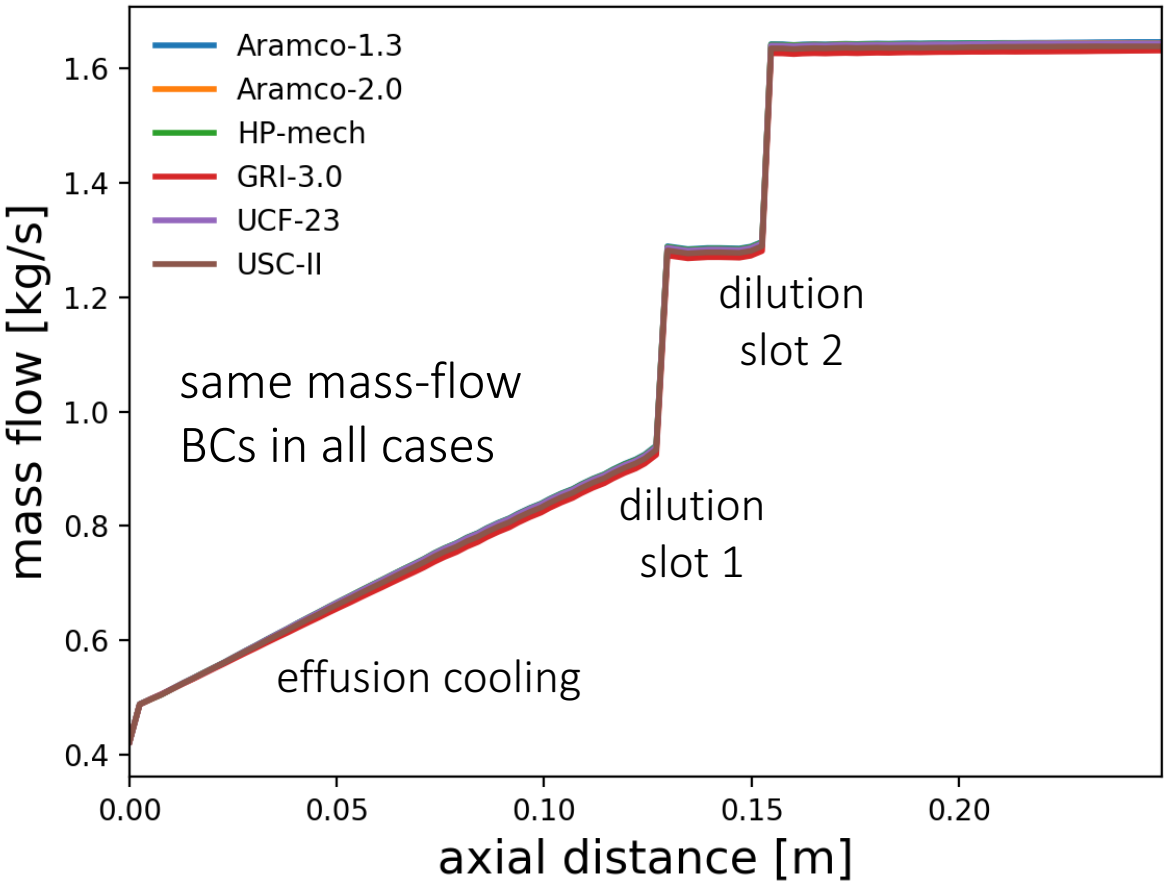


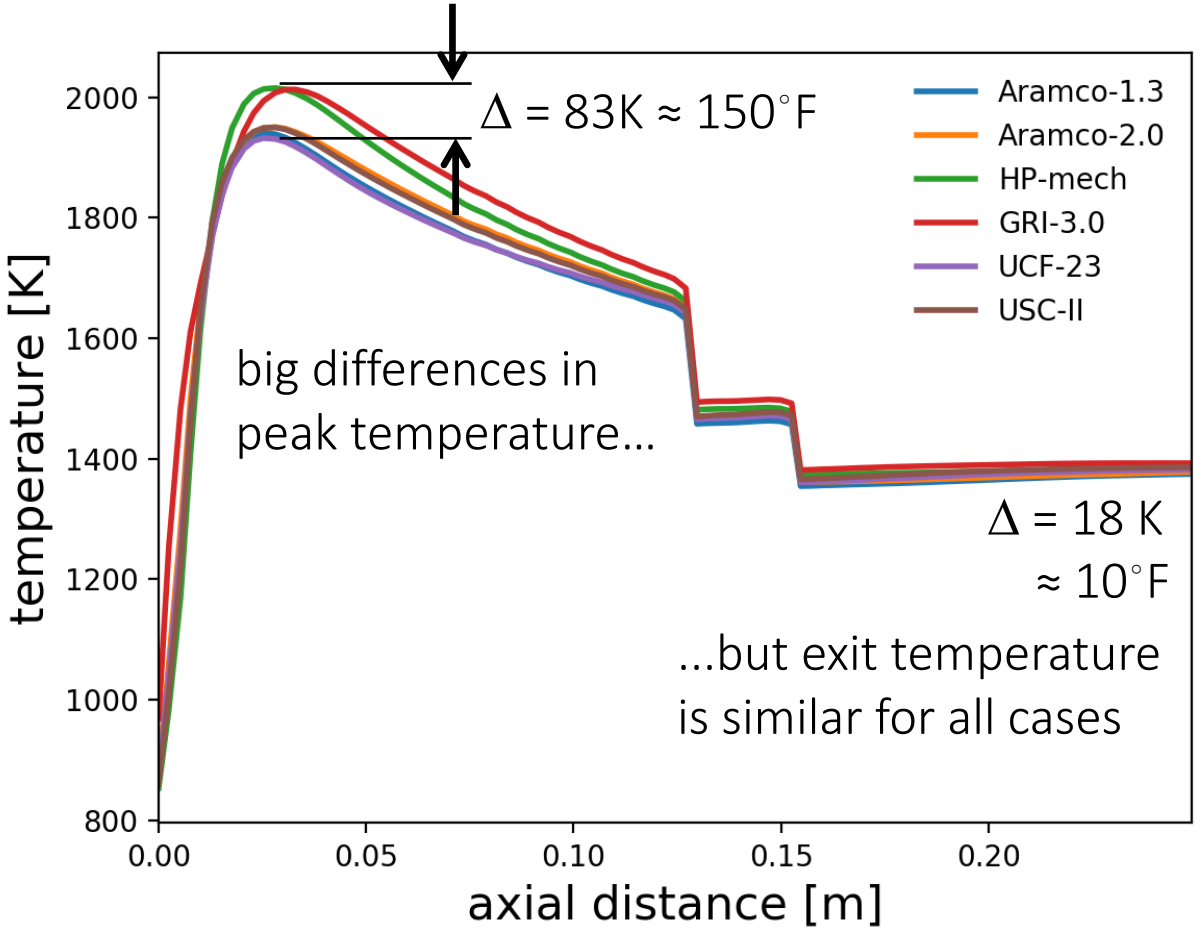
“Flux probe” example

(CO flux-probe at combustor exit: x = 10”)



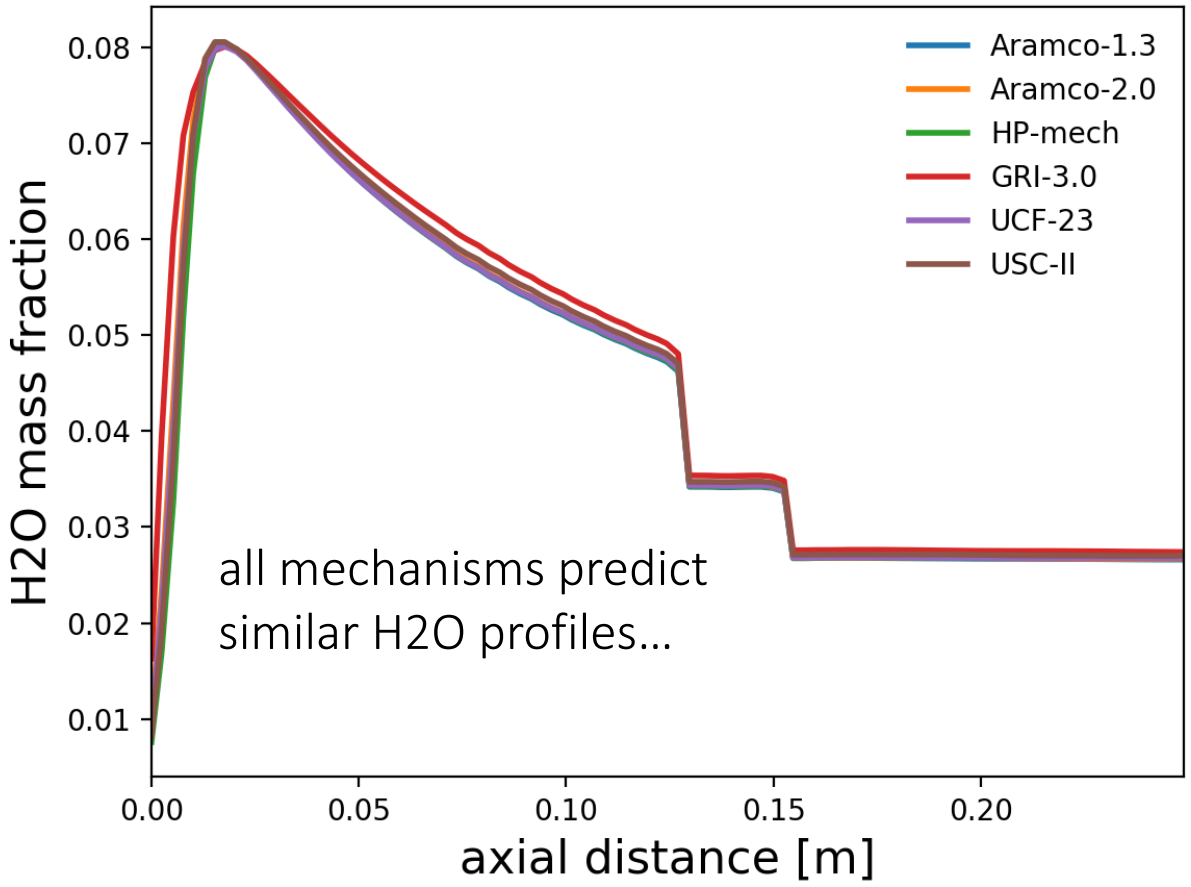
Axial profiles
(cross-section mass-avg)

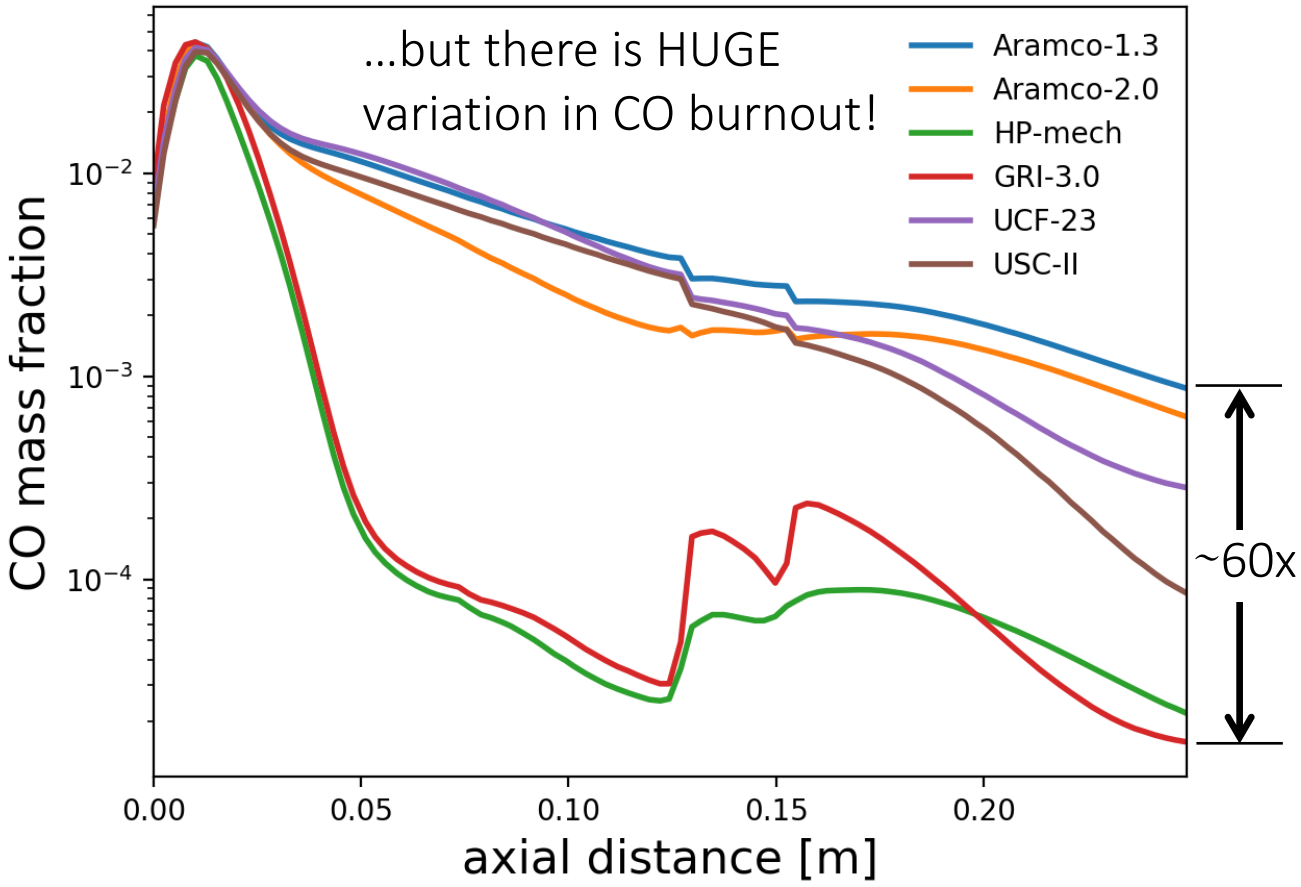




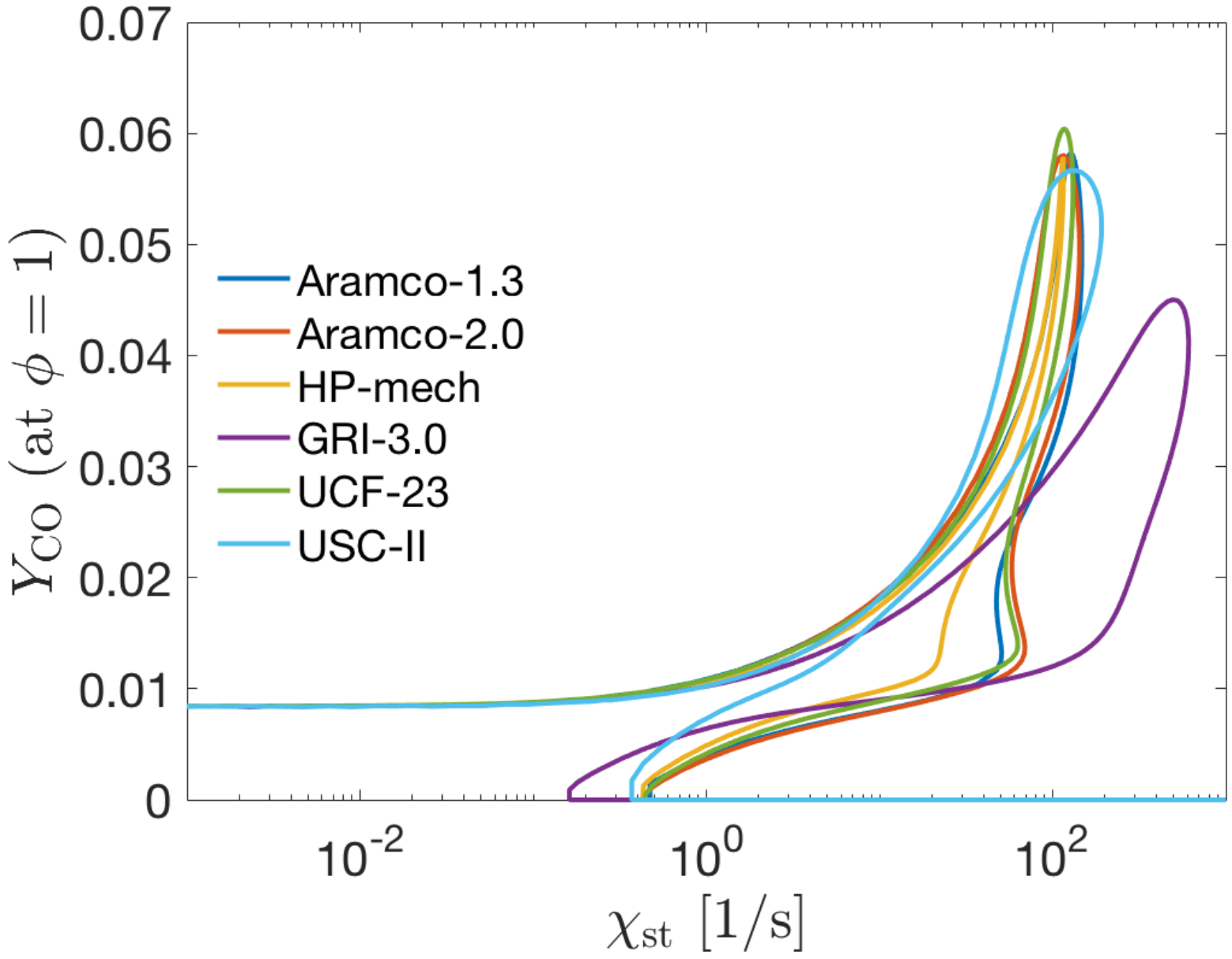
Combustion products and emissions

(cross-section mass-avg)



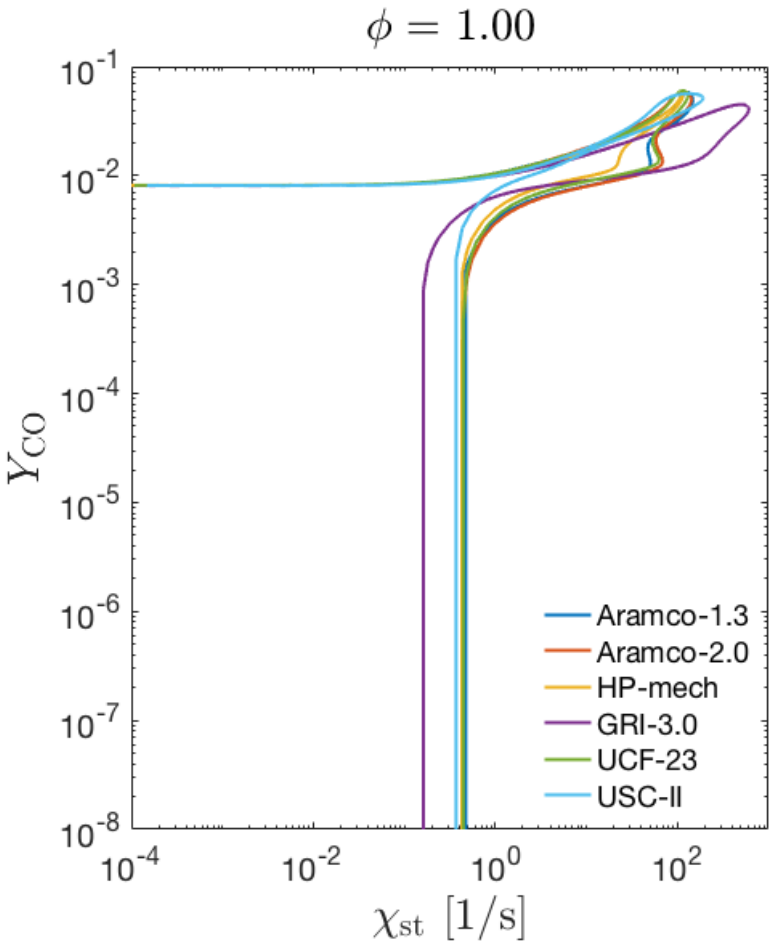


Flamelet s-curve (revisited for CO)

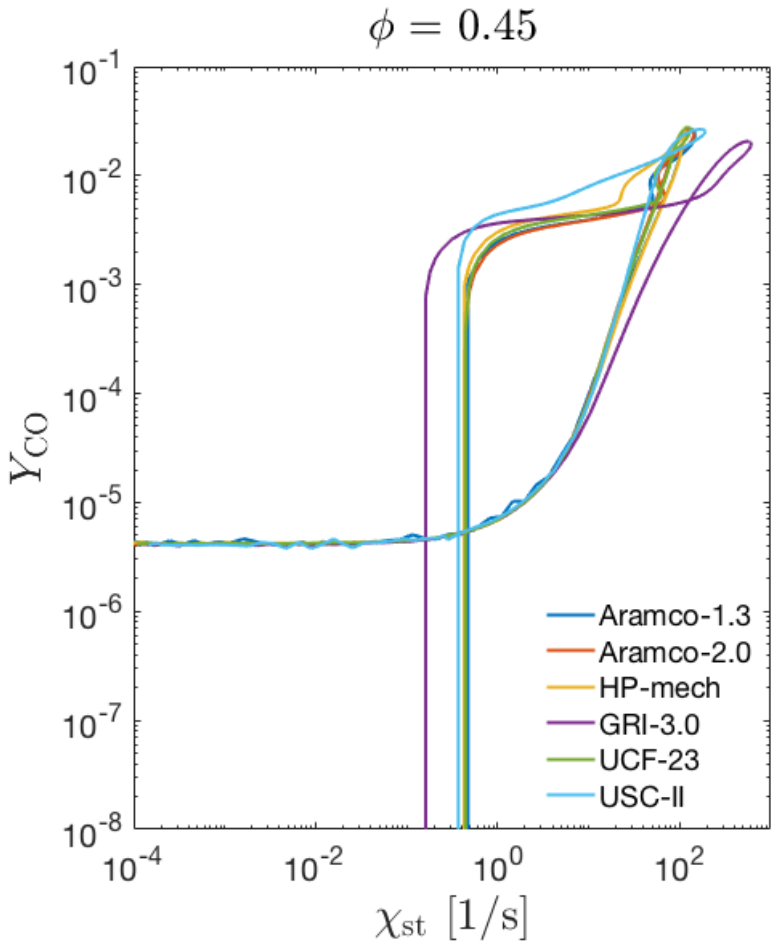


Flamelet s-curve (revisited for CO)

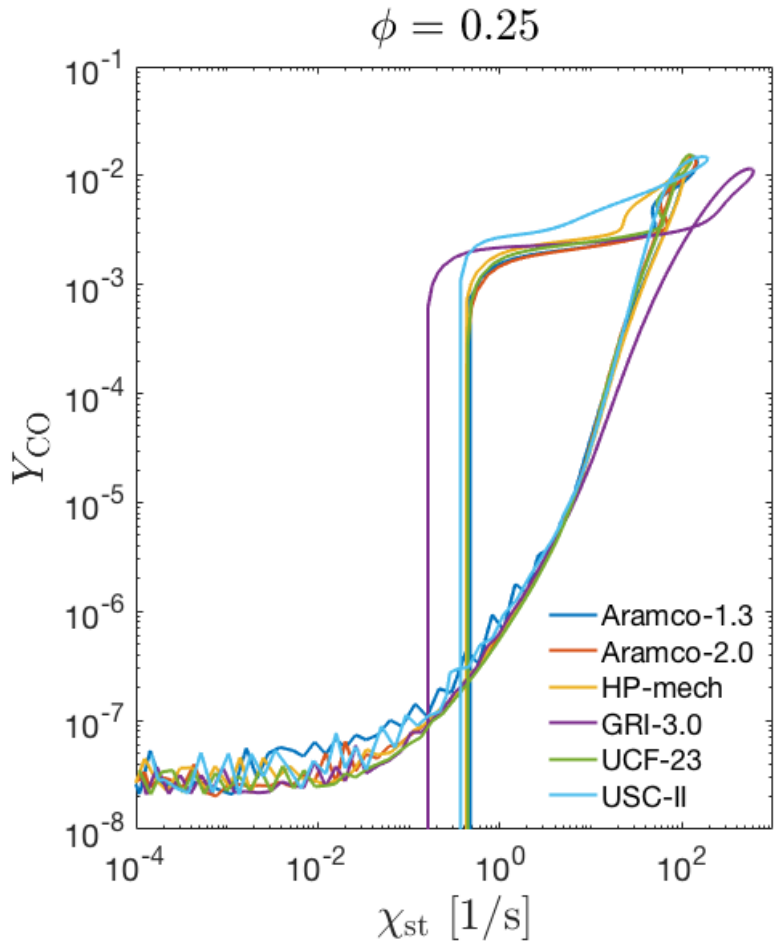
injection

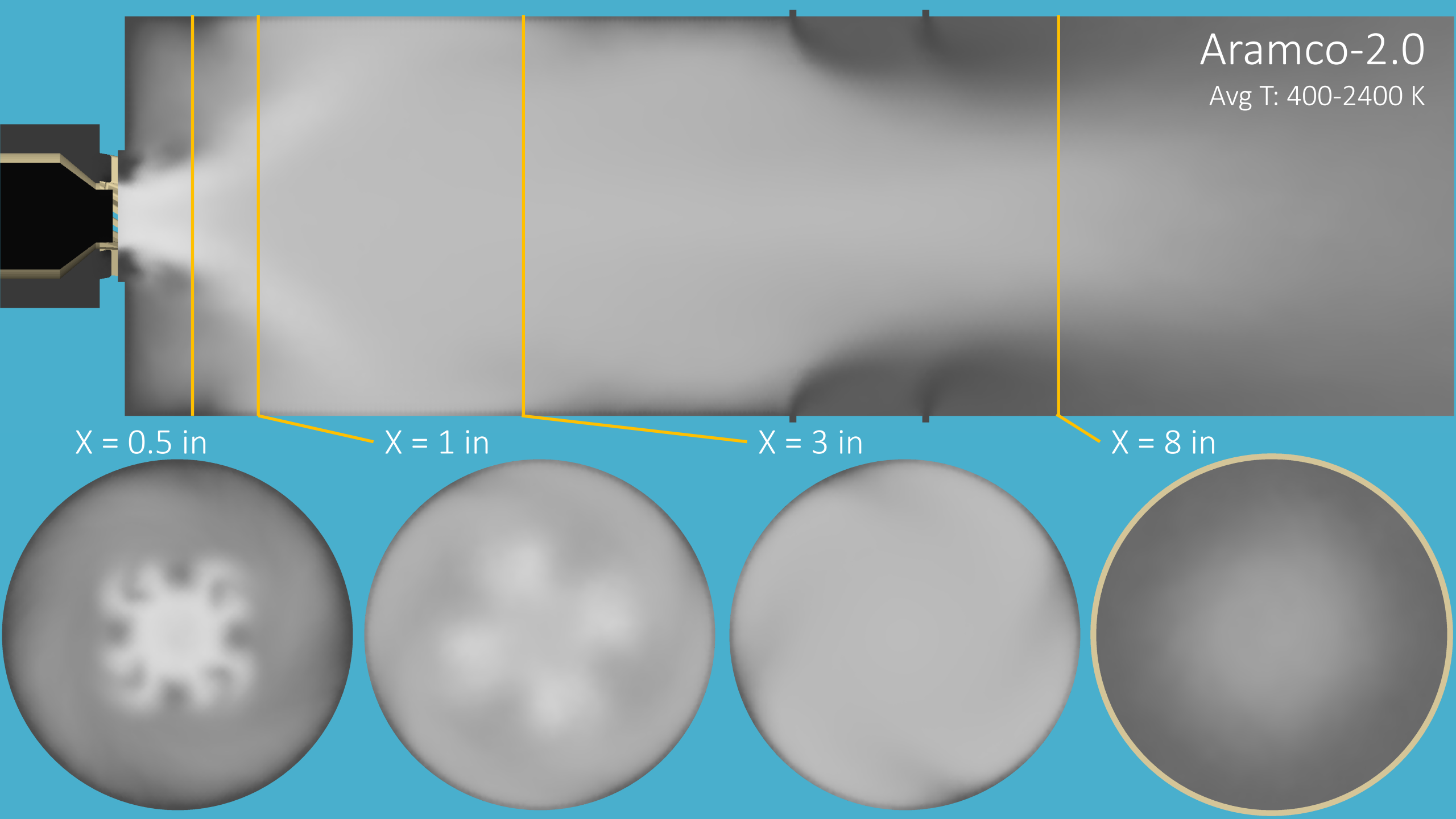


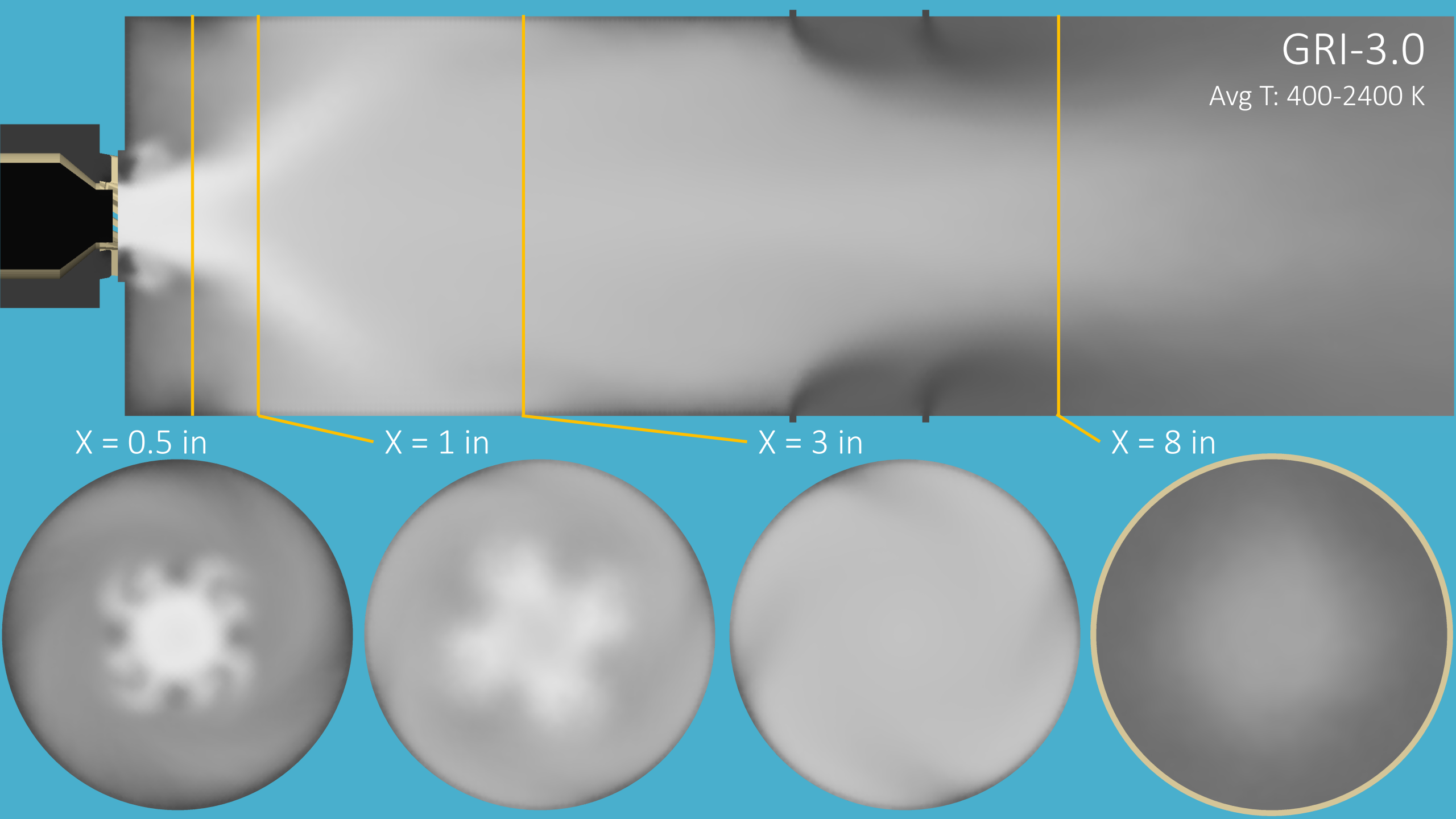
post-effusion



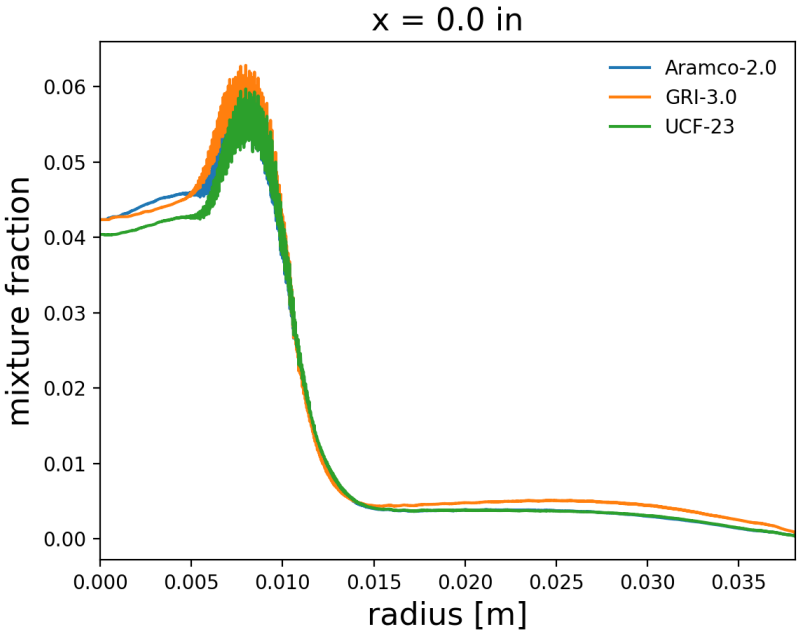
post-dilution

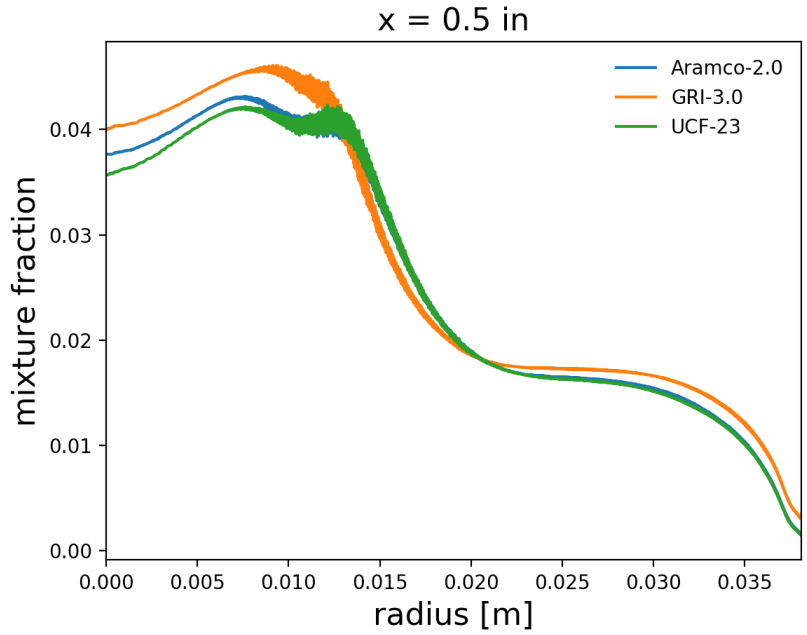


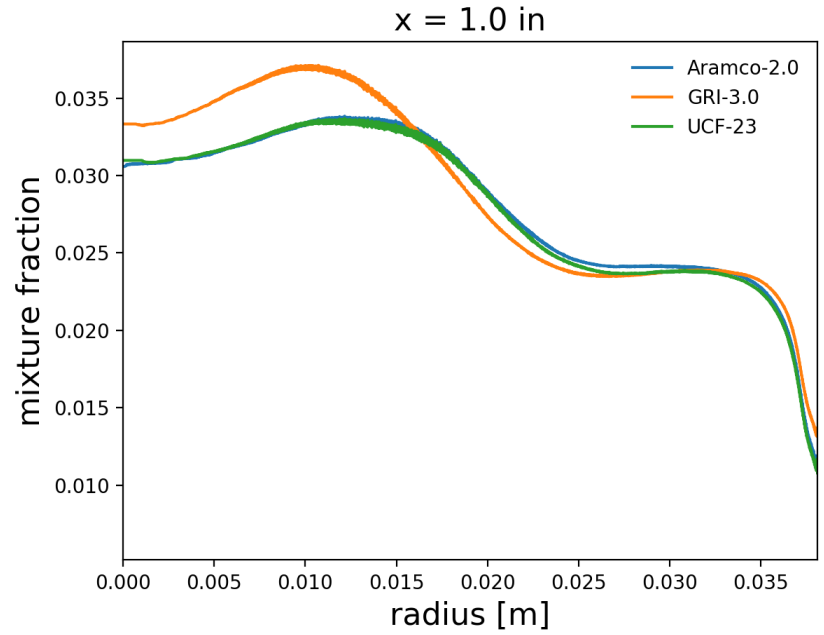

Aramco-2.0
Avg T: 400-2400 K
X = 0.5 in
X = 1 in
X = 3 in
X = 8 in

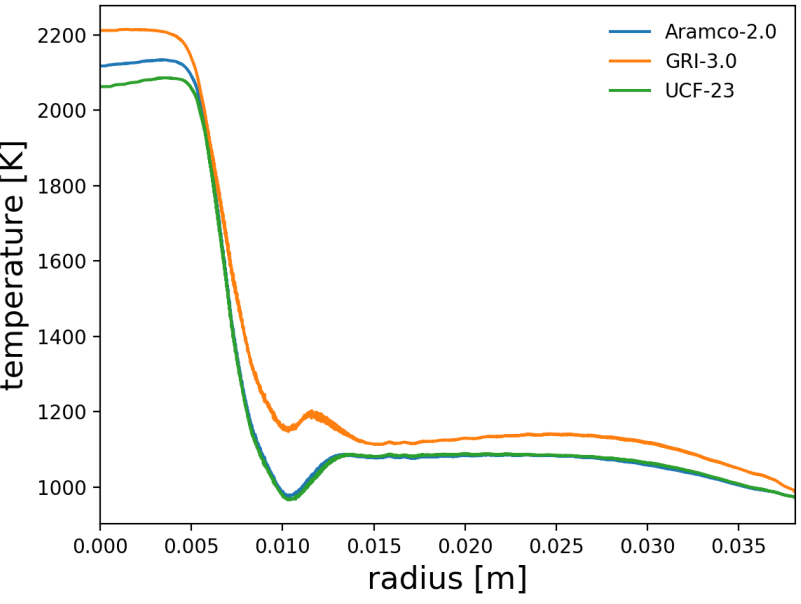

GRI-3.0
Avg T: 400-2400 K
X = 0.5 in
X = 1 in
X = 3 in
X = 8 in

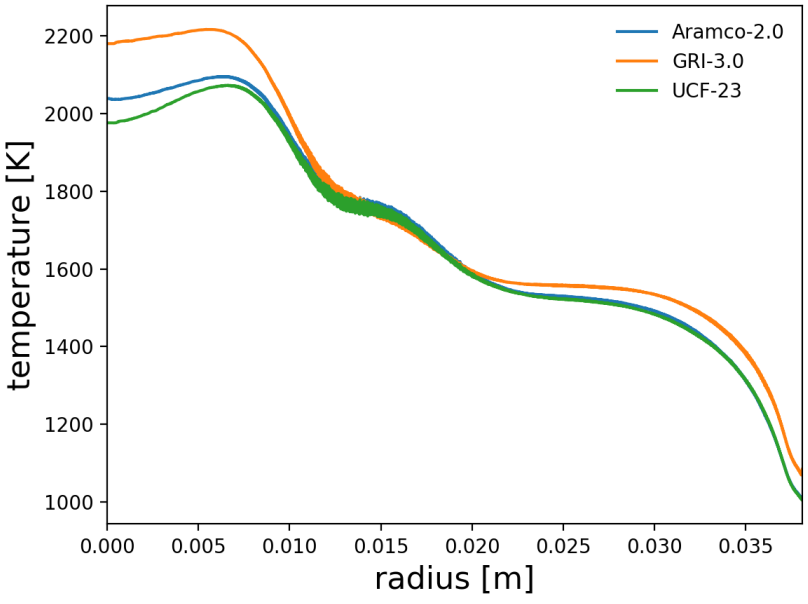
Radial profiles (near injector)

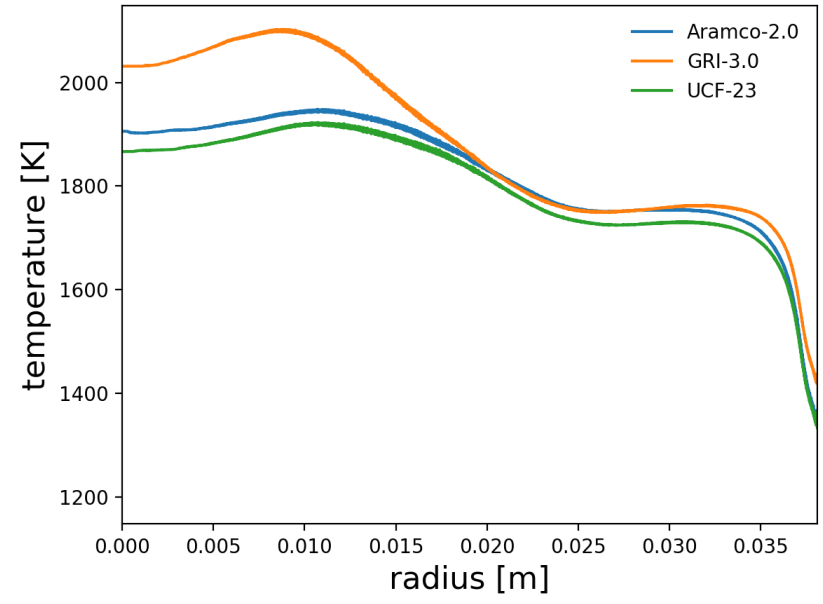




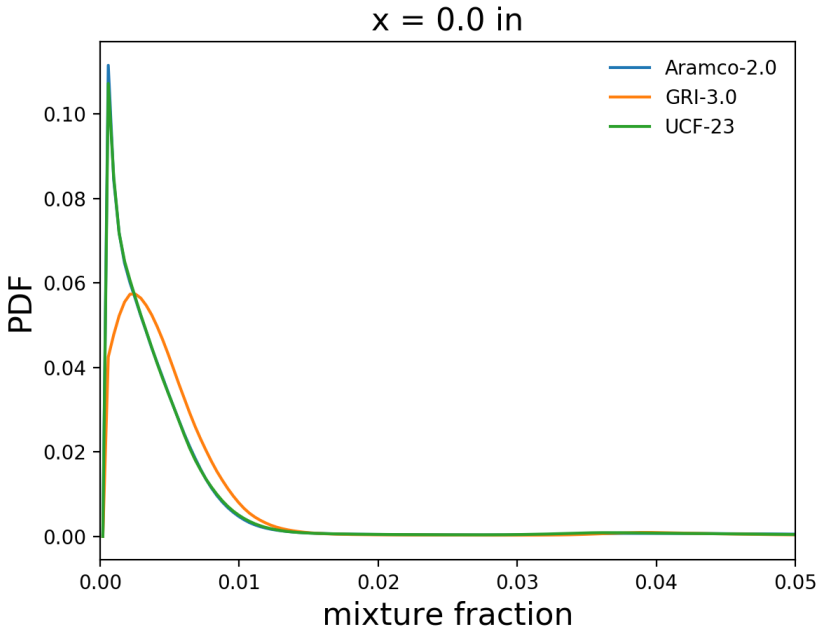


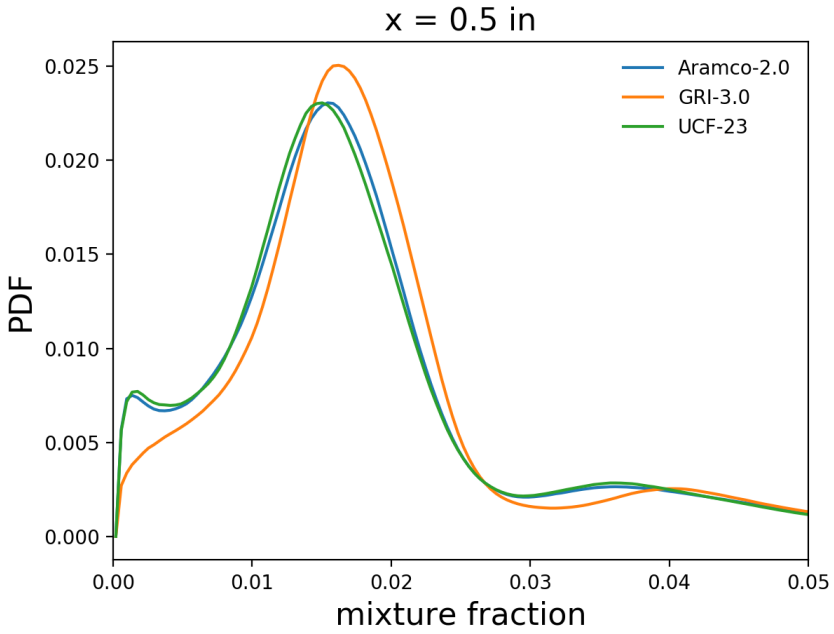


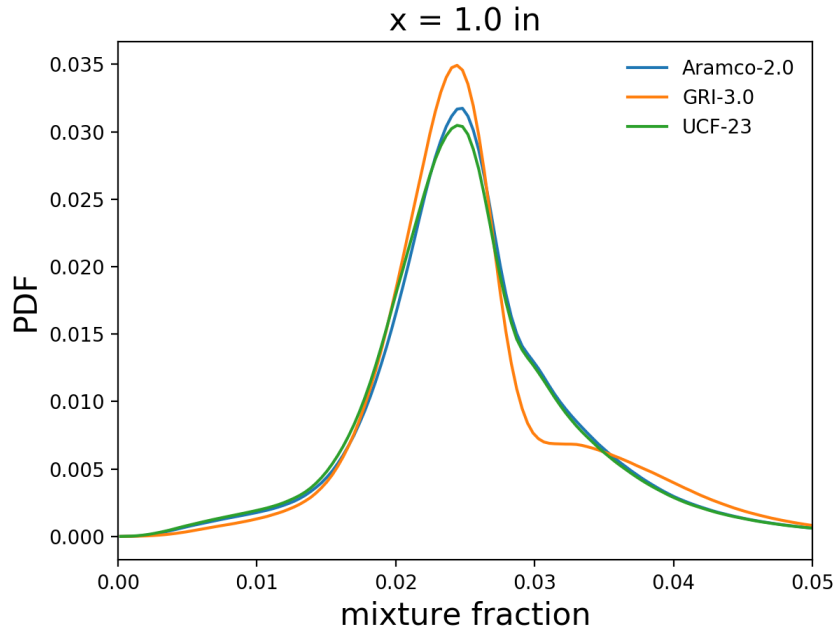


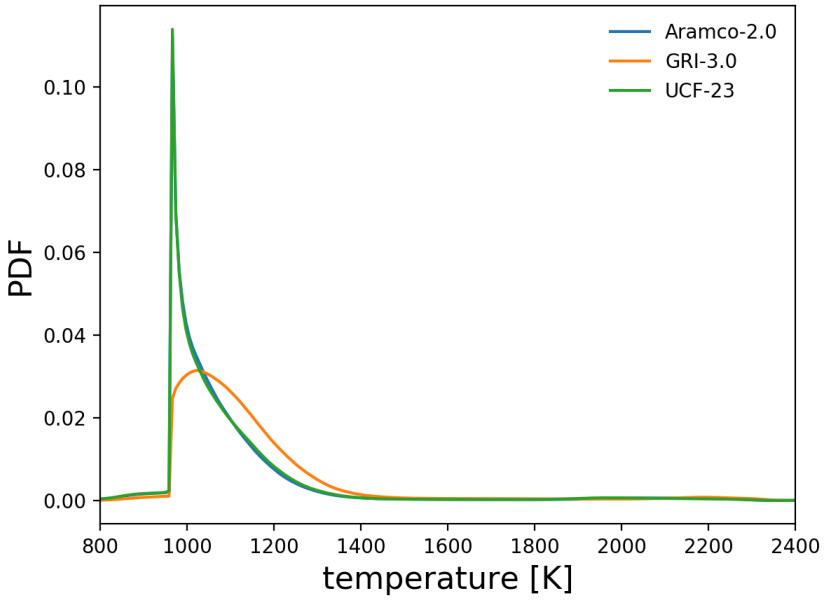


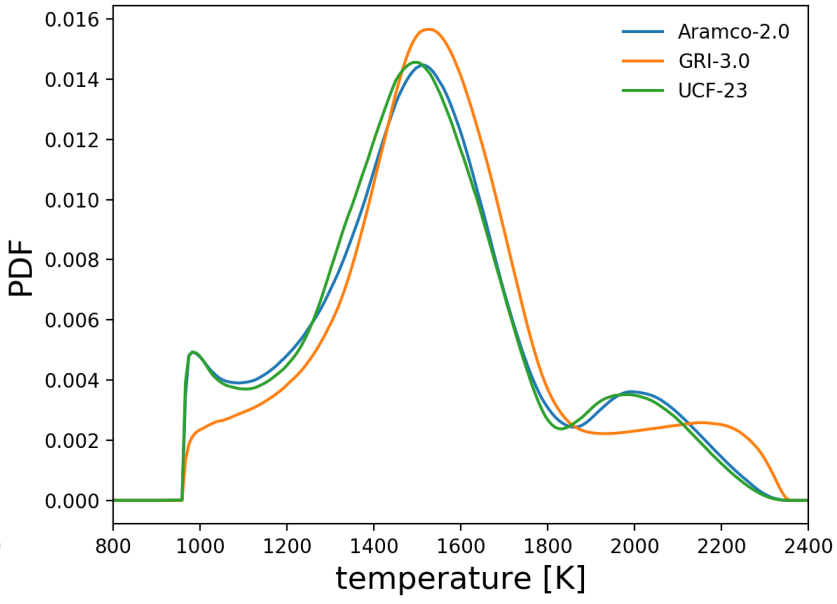
PDF evolution (near injector)

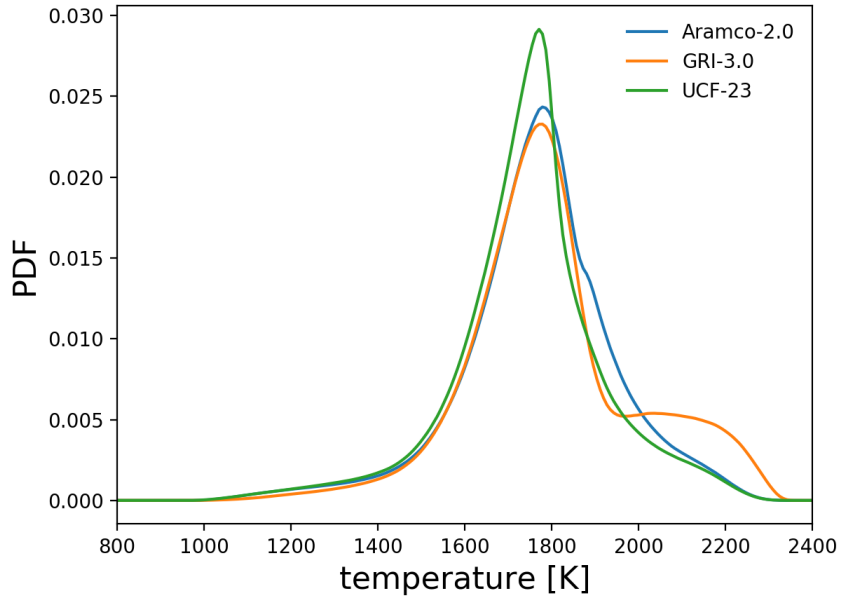




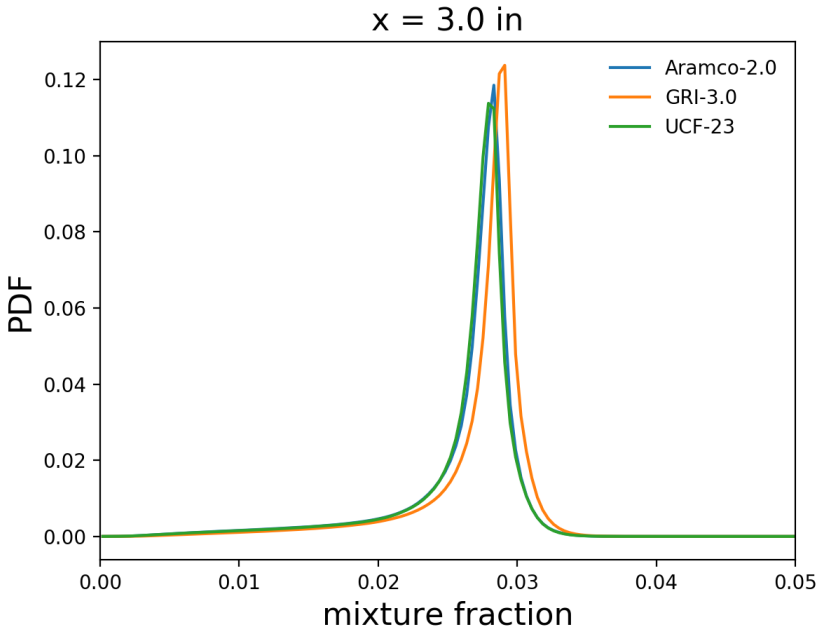


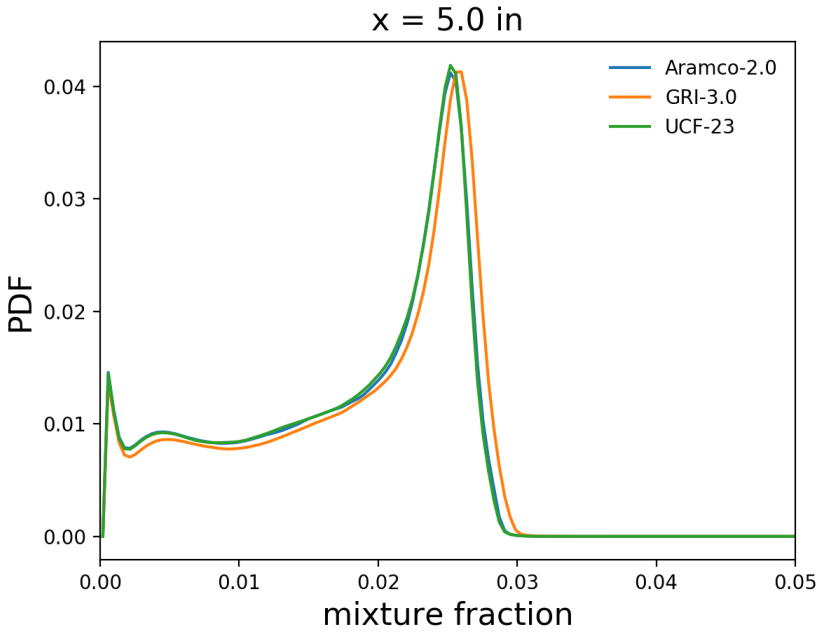


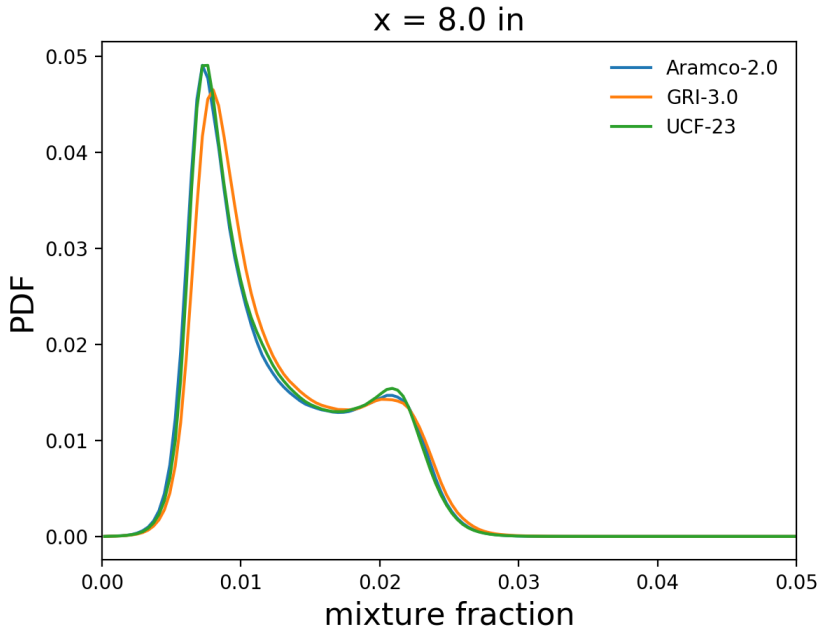


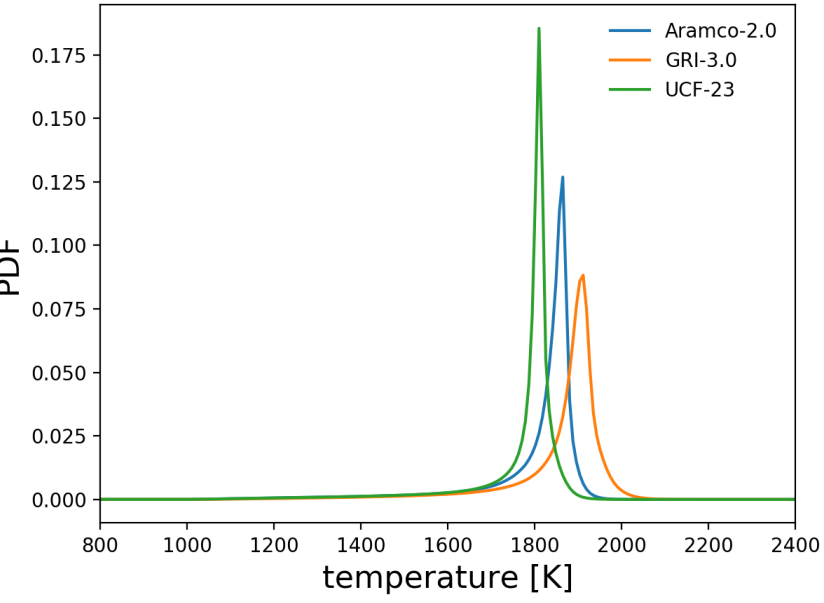


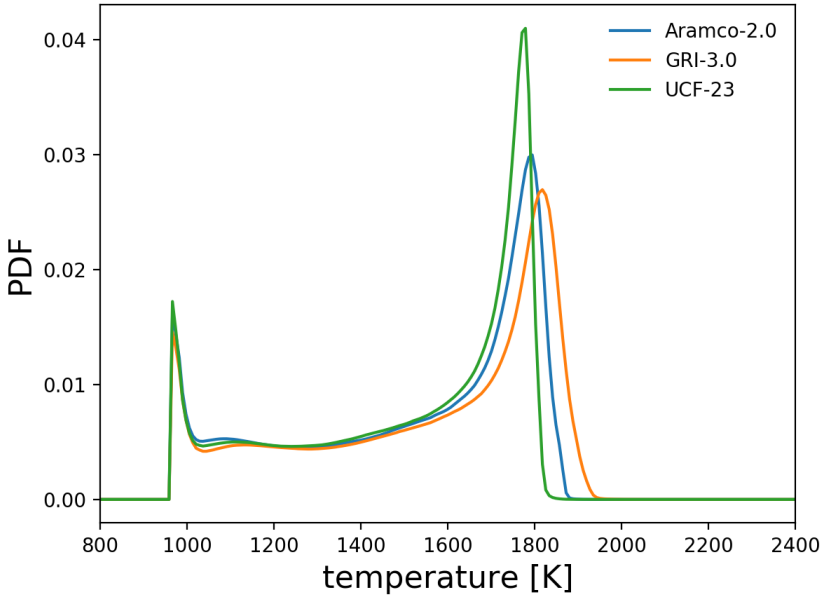
PDF evolution (downstream)

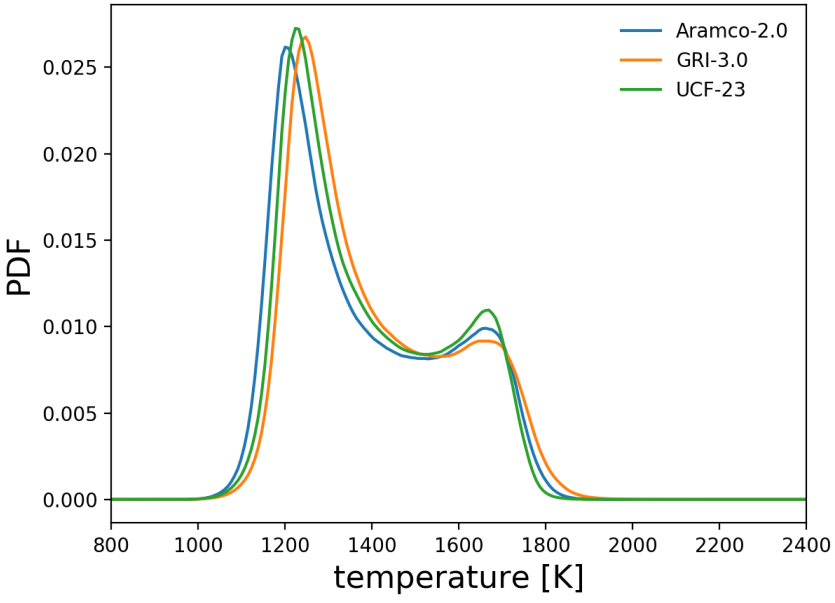






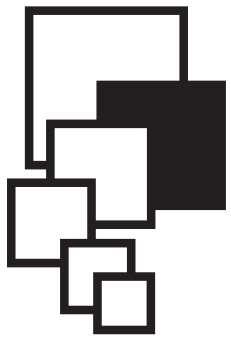






Conclusions

- Computational results are affected to the underlying chemical mechanism
- This is particularly true to sensitive species (e.g. CO)
- Interactions between kinetics and flow scales can be subtle
- These chemical uncertainties seem to be much larger than assumptions about ideal gas vs real fluid behavior (at least for these conditions)
- Use reduced mechanisms with caution



CASCADE TECHNOLOGIES

Discovery through simulation