

Designing a high-efficiency, low-NOx hydrogen combustor for thermophotovoltaic power generation

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Power plants are dispatchable but emit CO₂



Clean

Solid state

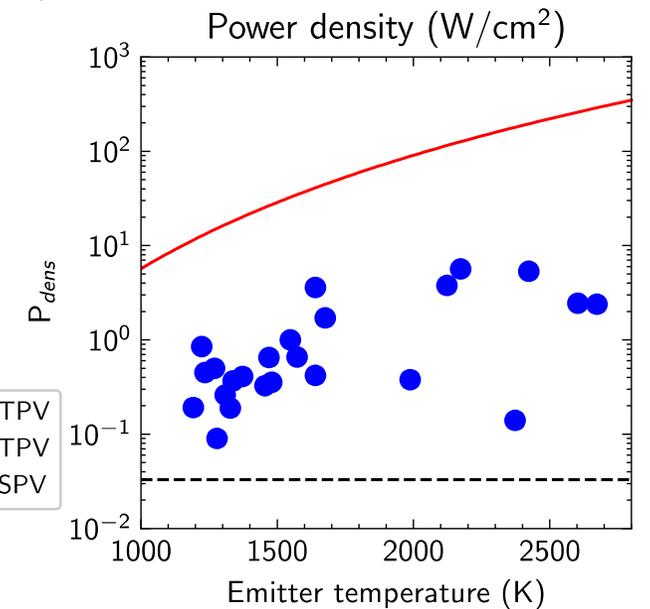
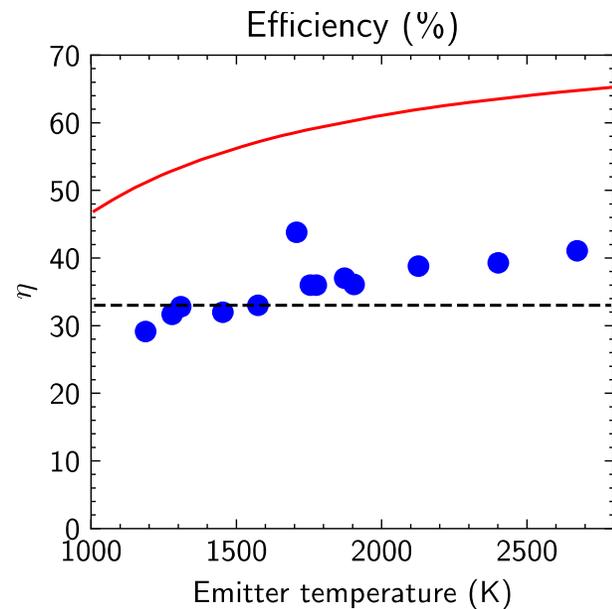
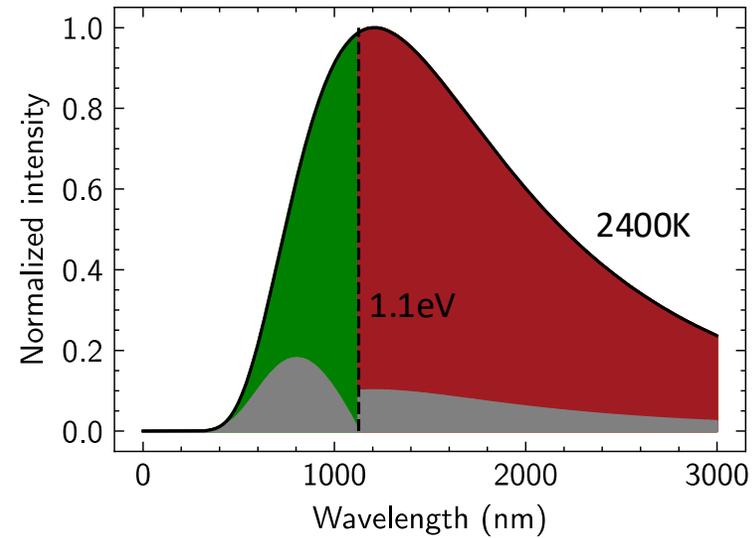
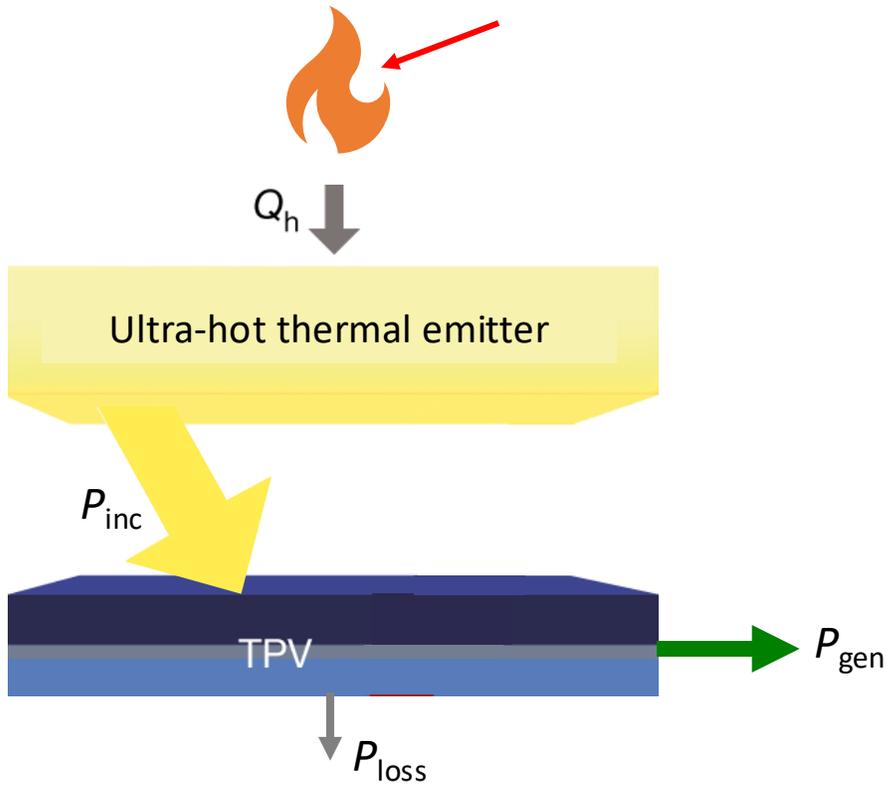
Intermittent

Emits CO₂

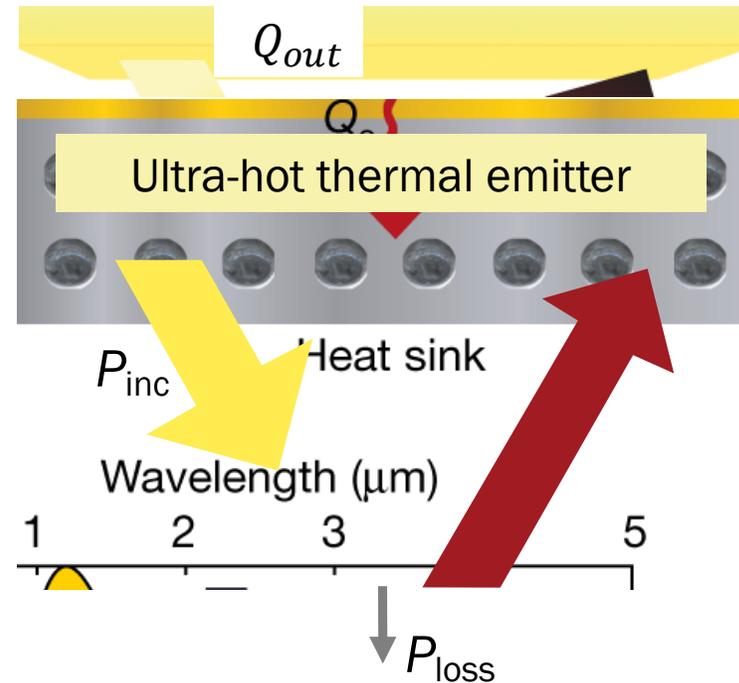
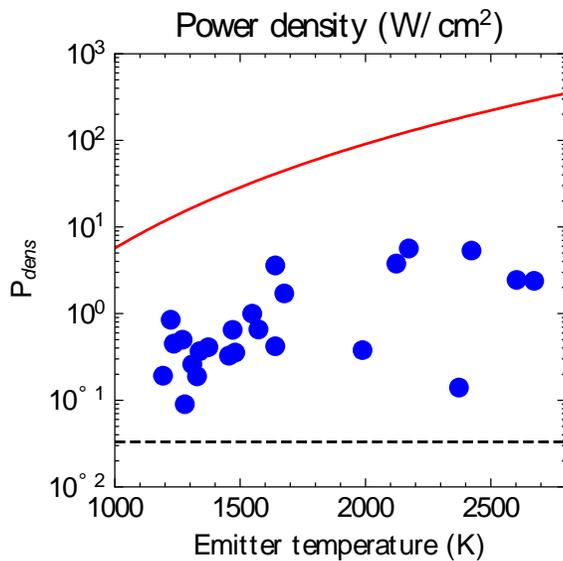
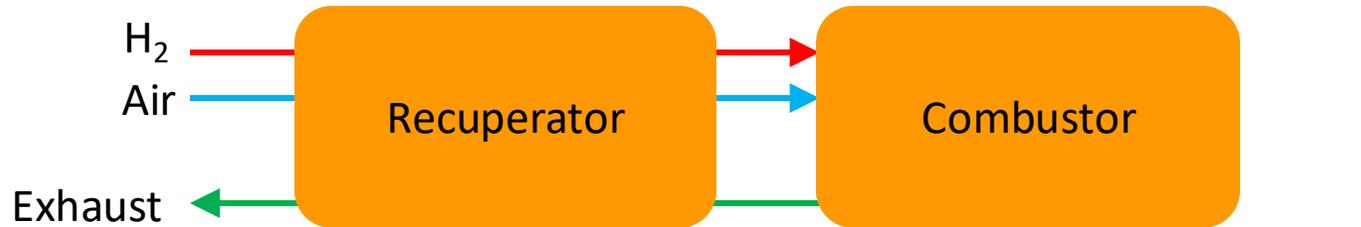
Rotating machinery

Dispatchable

Thermophotovoltaics (TPV) has the best of both worlds



Using hydrogen combustion with TPV provides clean and dispatchable power



Combustion efficiency:

$$\eta_{comb} = \frac{Q_{out}}{Q_{fuel}} = \frac{P_{inc} - P_{ref}}{\dot{m}HV_{fuel}}$$

TPV efficiency:

$$\eta_{TPV} = \frac{P_{elec}}{P_{net}} = \frac{P_{elec}}{P_{inc} - P_{ref}}$$

System efficiency:

$$\eta_{system} = \eta_{comb}\eta_{TPV}$$

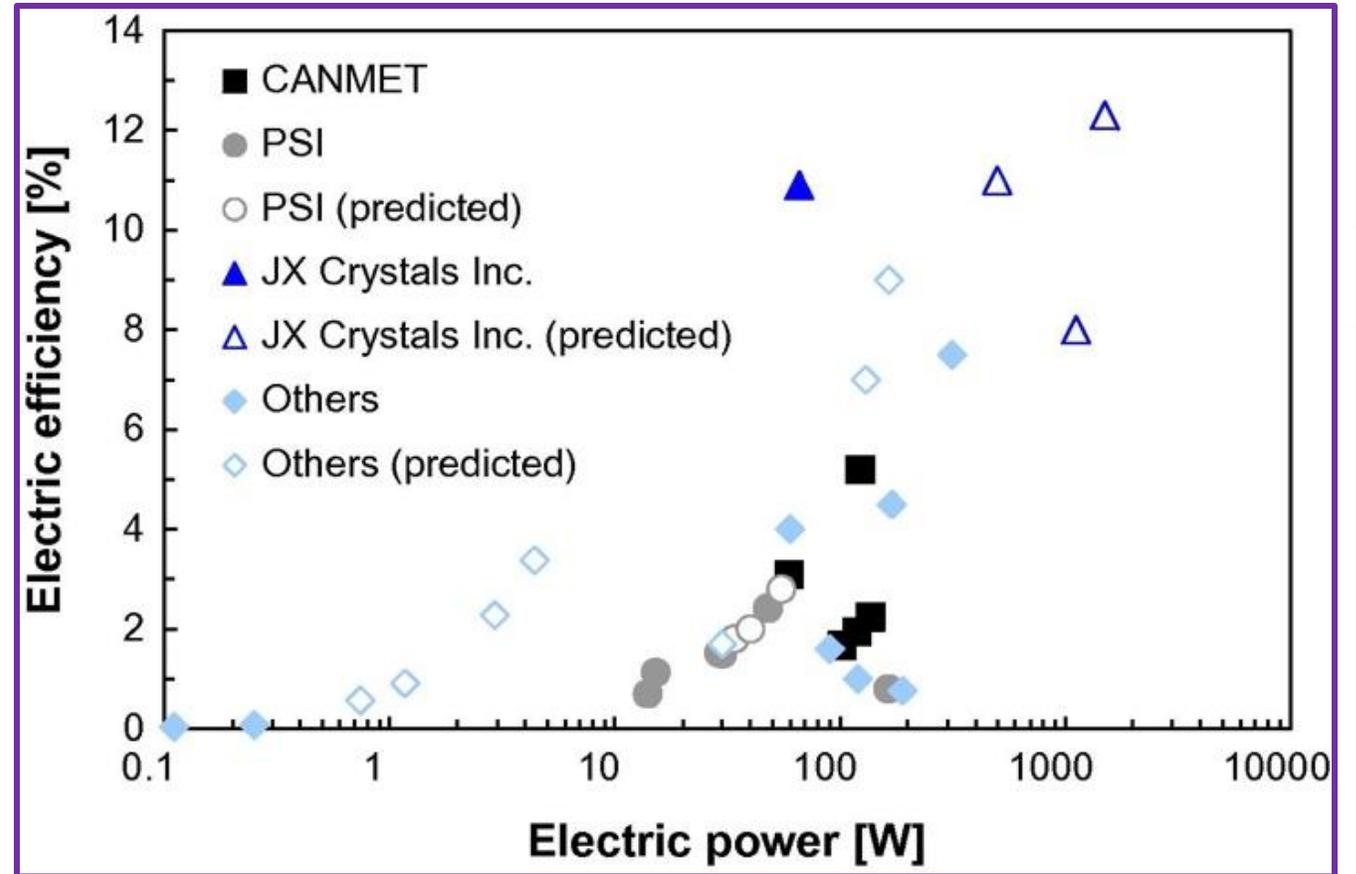
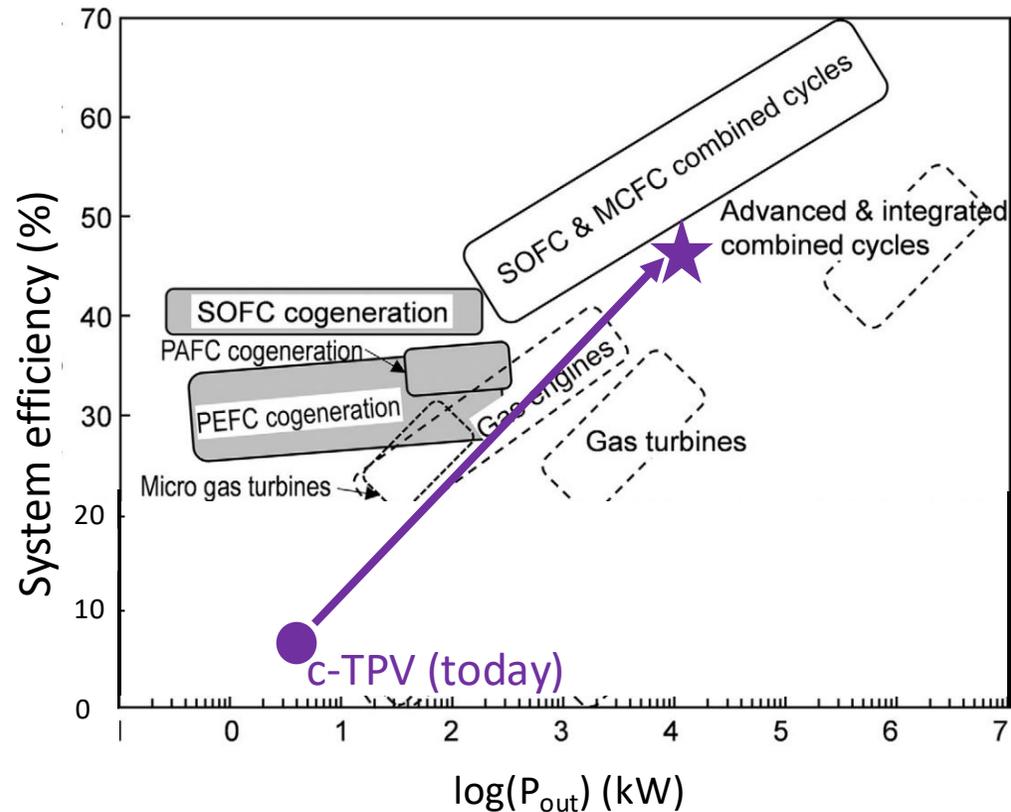
Combustor heat flux:

$$Q'' = \frac{Q_{out}}{A_{comb}}$$

P_{gen}

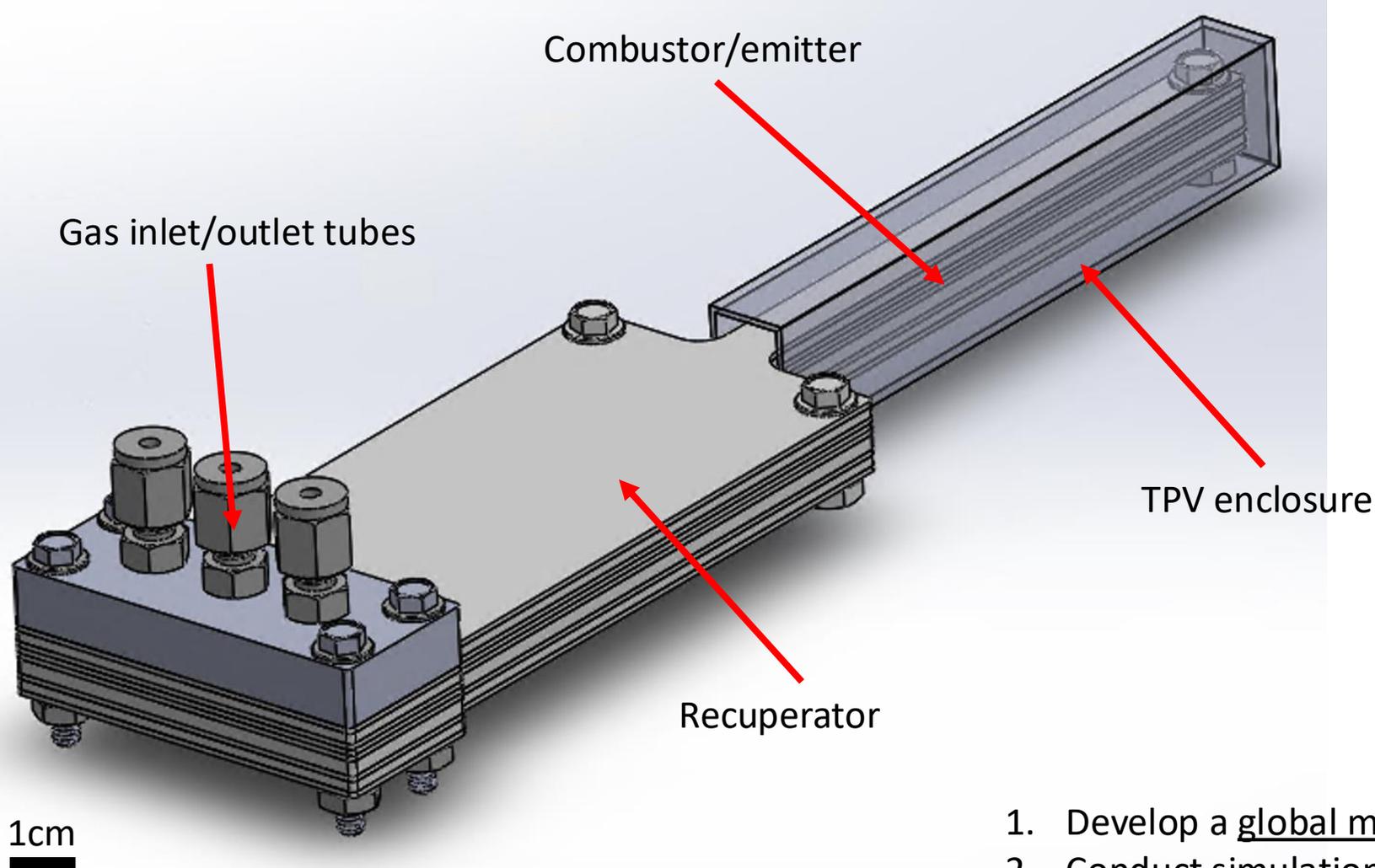
Existing c-TPV devices have low efficiency

c-TPV (today)



Material: silicon carbide (SiC)

Max temp: 1900C



If:

80% combustion efficiency,
20 W/cm² heat flux

Get:

965W thermal output,
482W electricity power output,
41% system efficiency
\$0.50/W capital cost
8¢/kWh LCOE

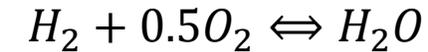
Questions:

1. How close can we get to this efficiency value?
2. What is the effect on NO_x?

1. Develop a global mechanism for accelerated simulations
2. Conduct simulations of given geometry
3. Improve geometry to maximize combustion efficiency

Developing a global mechanism

- Unique combustion conditions (highly preheated non-premixed reactants)
- Detailed: GRIMech3.0 subset:
 - 10 species, 29 reactions
- Global: From literature for single-step
- Custom: Independently generated by varying A and E_a



Name	Rate
Marinov	$5.69e11 \exp\left(-\frac{1.46e8}{RT}\right) [H_2][O_2]^{0.5}$
Zhang	$1.89e12 \exp\left(-\frac{1.64e8}{RT}\right) [H_2][O_2]^{0.5}$
Wang_1	$1.13e12 \exp\left(-\frac{1.12e8}{RT}\right) [H_2][O_2]$
Wang_2	$3.12e7 \exp\left(-\frac{6.50e7}{RT}\right) [H_2][O_2]^{0.5}$
Custom	$5.62e10 \exp\left(-\frac{1.87e8}{RT}\right) [H_2][O_2]^{0.5}$

References

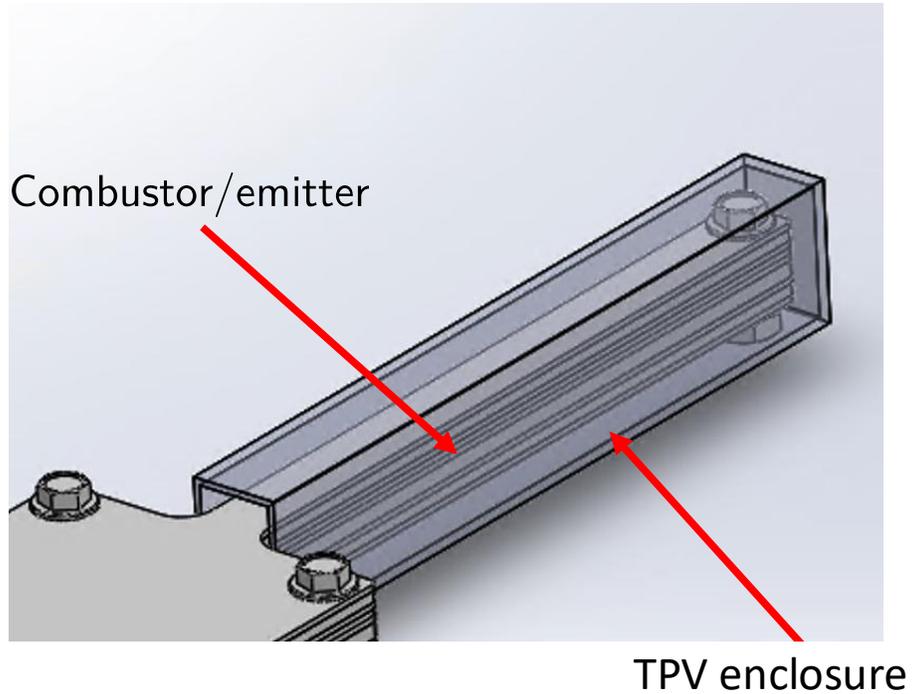
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<https://www.frontiersin.org/articles/10.3389/fenrg.2017.00031/full#F2>
<https://link.springer.com/article/10.1007/s11431-012-4932-4>
<https://www.sciencedirect.com/science/article/pii/S0360319915304973>

Comparing reduced vs. detailed mechanism

Property	Detailed	Reduced-8	Marinov	Zhang	Wang1	Wang2	Custom
Adiabatic flame temp (lean well mixed)	2201 K	2201 K	2226 K				
Adiabatic flame temp (stoich)	2935 K	2935 K	3218 K				
Ignition delay time (const P reactor)	1.06e-5 s	1.07e-5 s	3.59e-7 s	3.75e-7 s	3.28e-7 s	1e-7 s	6.09e-5 s
WSR min residence time to reach 90% of max temp	0.0977 s	0.125 s	7.87e-5 s	6.27e-5 s	2.00e-4 s	0.016 s	0.0077 s
PFR (given mdot, A) length req to reach 90% of max temp	0.128 m	0.150 m	0.0022 m	0.0022 m	0.0022 m	0.042 m	0.038 m
Laminar flame speed (premixed, 900K)	3.36 m/s	3.46 m/s	7442 m/s	2484 m/s	49853 m/s	10997 m/s	3.36 m/s
Counterflow diffusion flame (1cm sep) flame loc	2.81%	2.81%	3.43%	3.41%	3.43%	2.5%	2.96%
Counterflow diffusion flame (1cm sep) flame temp	1968 K	1967K	3405 K	3398K	3719K	1974K	2994 K

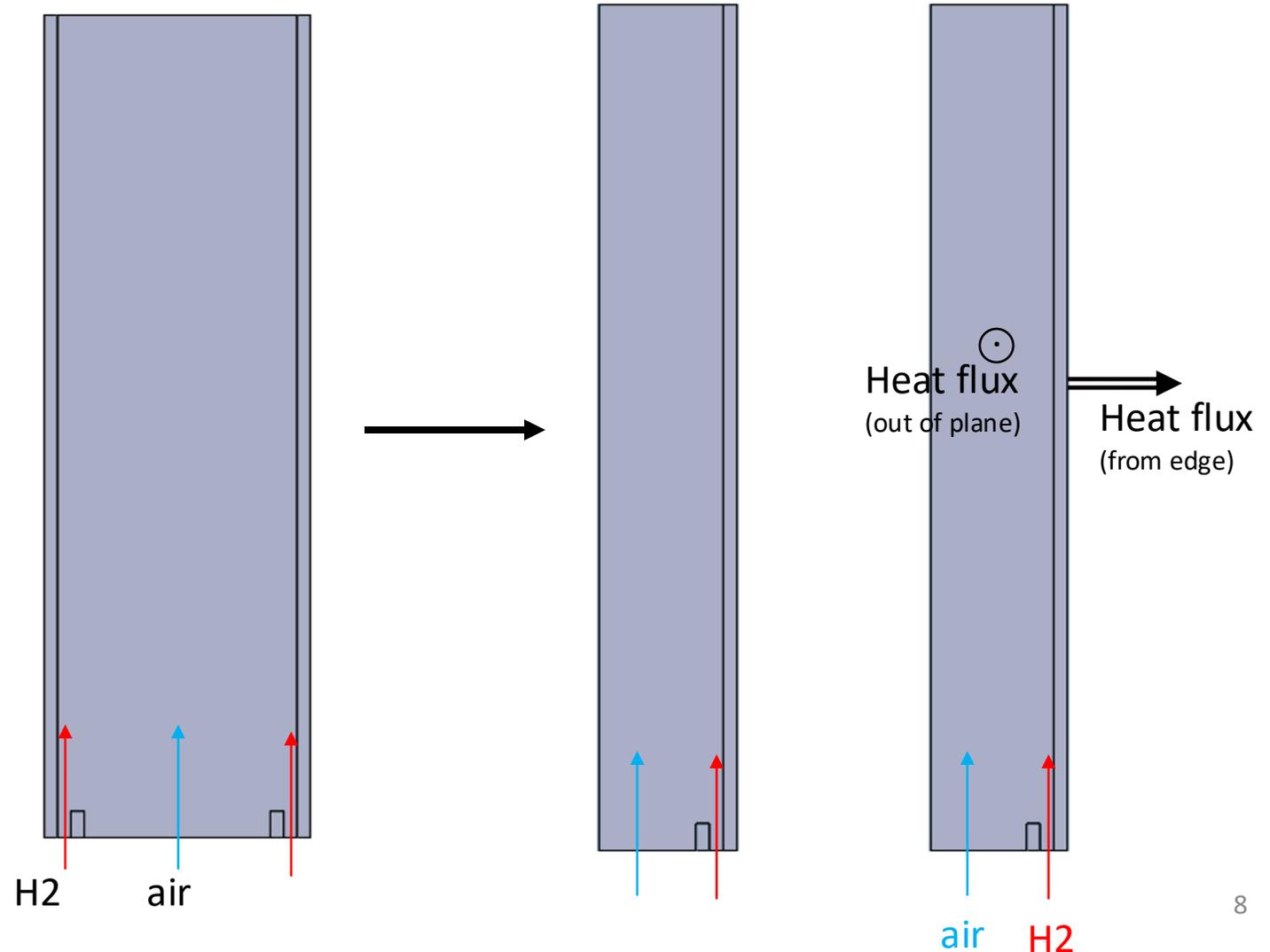
Now we have a fast and (reasonably) accurate global mechanism!

Calculate combustion efficiency with CFD



2D planar geometry with y-axis symmetry
Inlet temp = 1500C EAR = 4.5

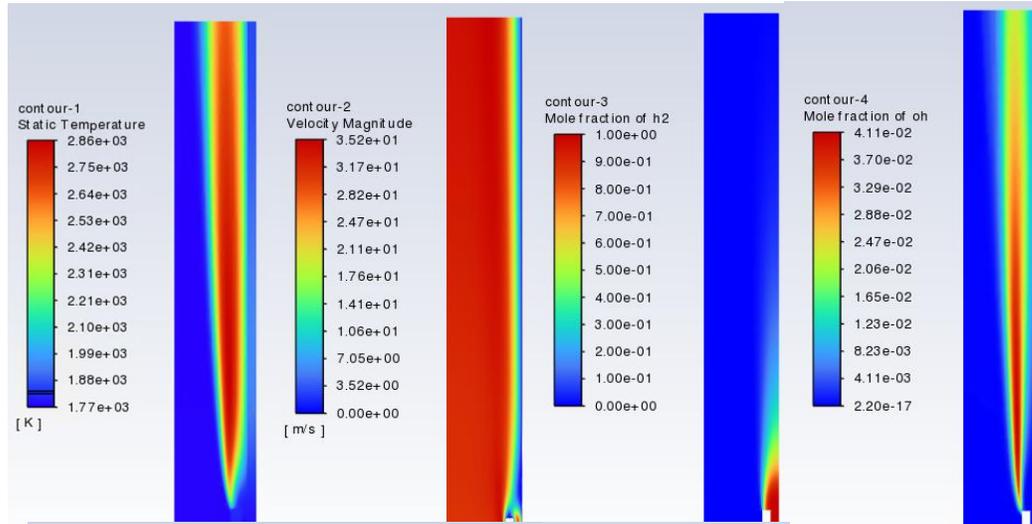
Top view of cross section



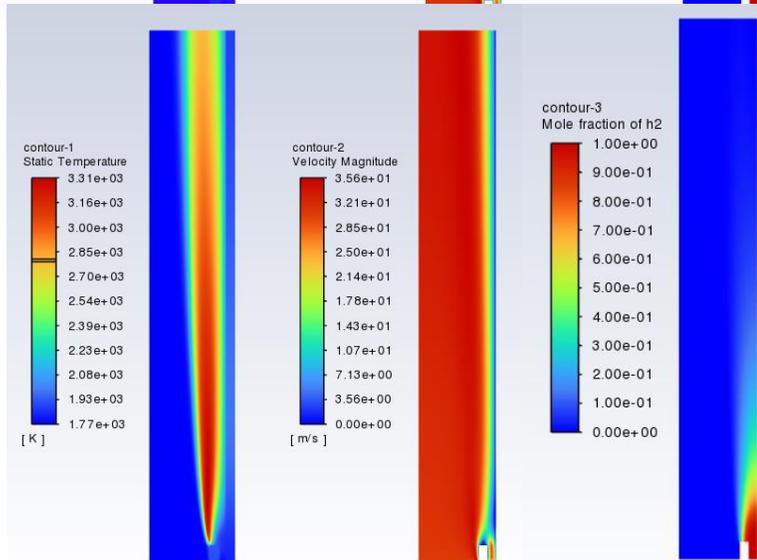
Validation of global mechanism in CFD

Temperature Velocity H2 mole frac OH mole frac

Detailed



Global

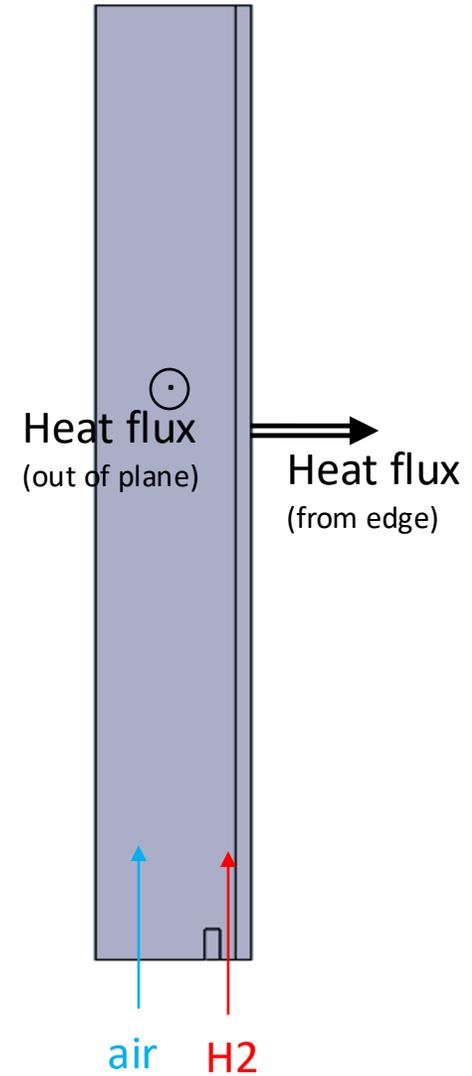
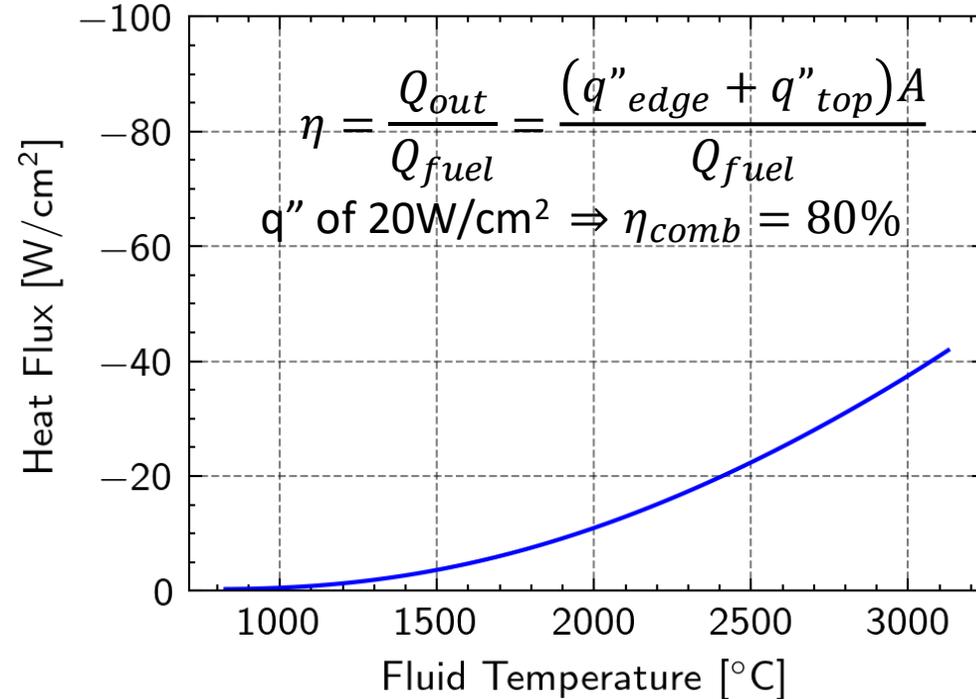
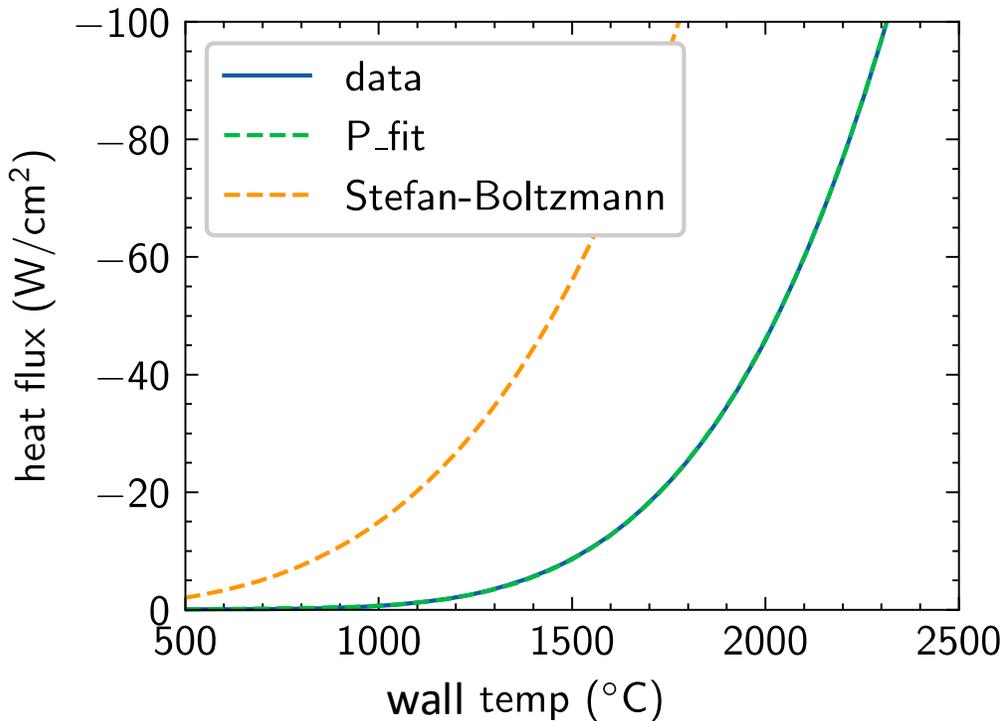


Metric	Detailed	Global
Max solid temp	1953K	1962K
Max fluid temp	2860K	3309K
Max emitter wall temp	1949K	1958K
Emitter wall delT	149K	121K
Heat out	466W	560W
Outlet temp (ma)	2107K	2053K
Time	3:30 hr	0:20 hr

$$\eta_{comb} = \frac{560W}{1e-5 \frac{kg}{s} \cdot 120e6 \frac{J}{kg}} = 47\%$$

How can we improve efficiency?

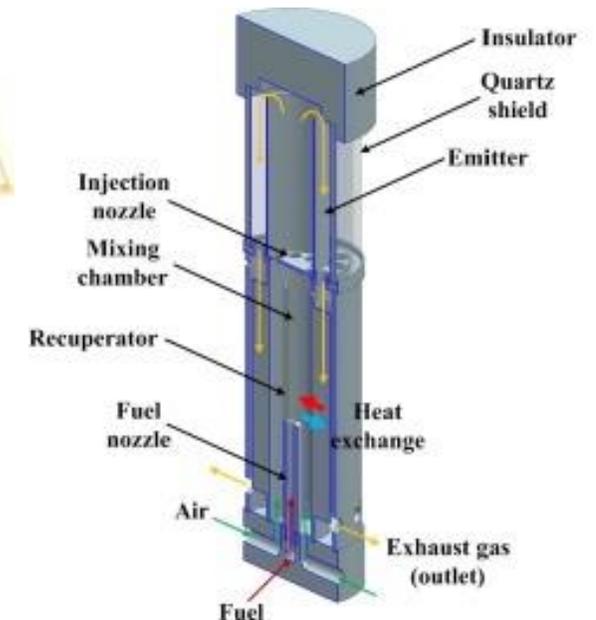
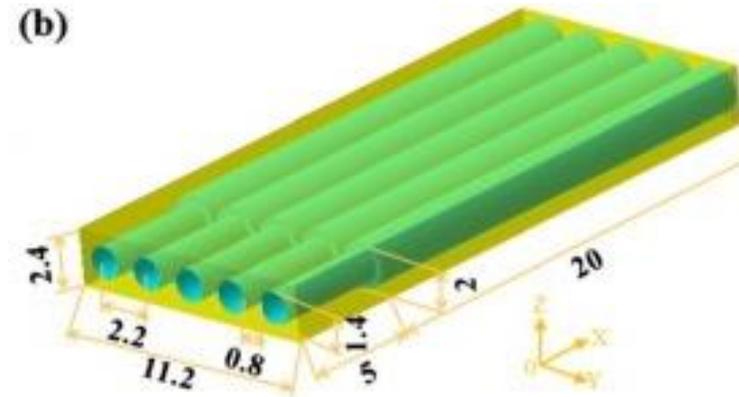
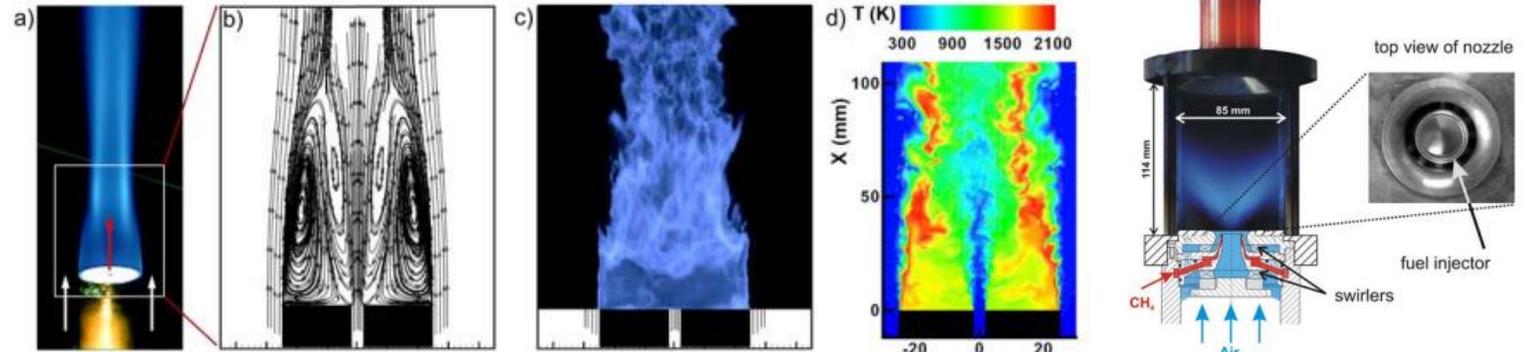
- Performance metrics:
 - High, uniform emitter temperature (~1700C) for edge heat flux
 - High, uniform fluid temperature (~2400C) for out of plane heat flux
 - ⇒ high heat flux out (20W/cm²), high combustion efficiency (>80%)



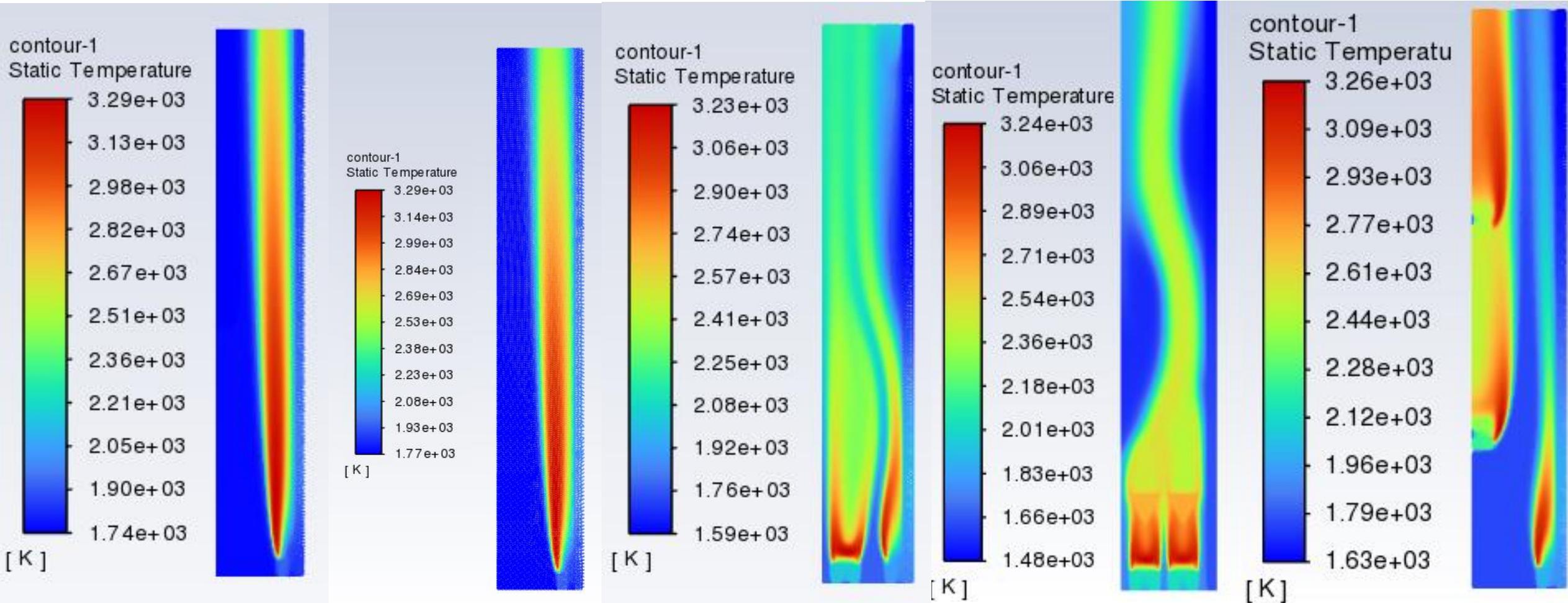
Several geometric ideas from the literature

- Geometric improvements

- Inducing turbulence
- Multi-inlet injection
- Bluff-body
- Staged injection
- Swirl combustion



Comparing different combustor geometries



Base case

Turbulence

Multi-inlet

Bluff-body

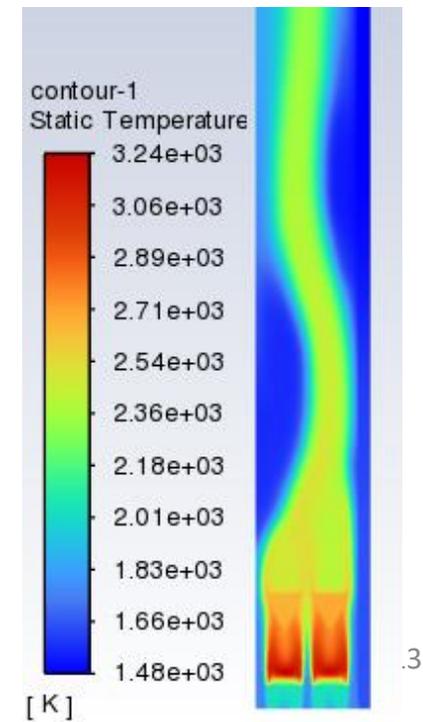
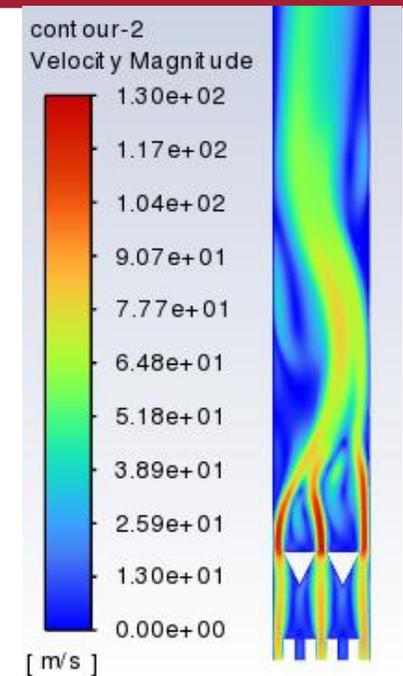
Staged

Metrics of geometries compared

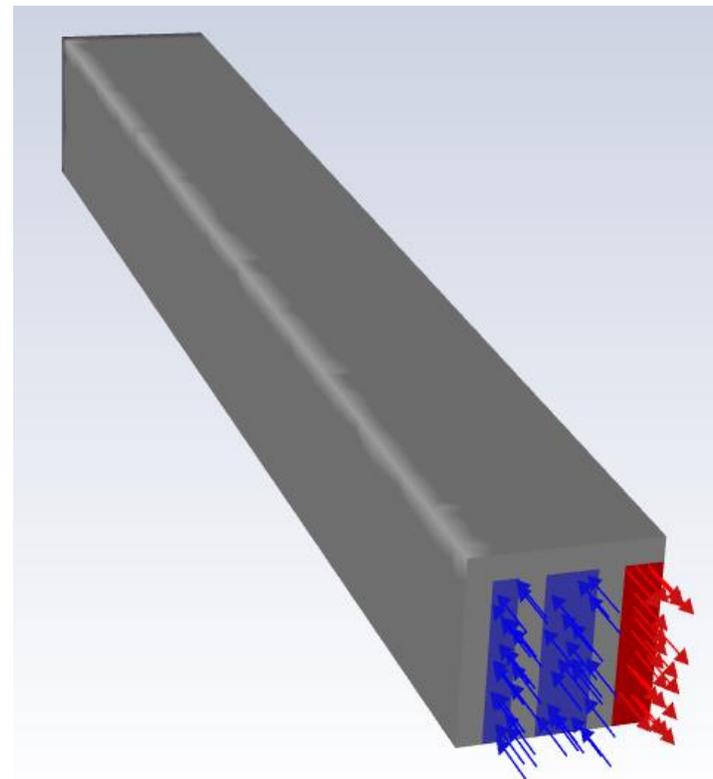
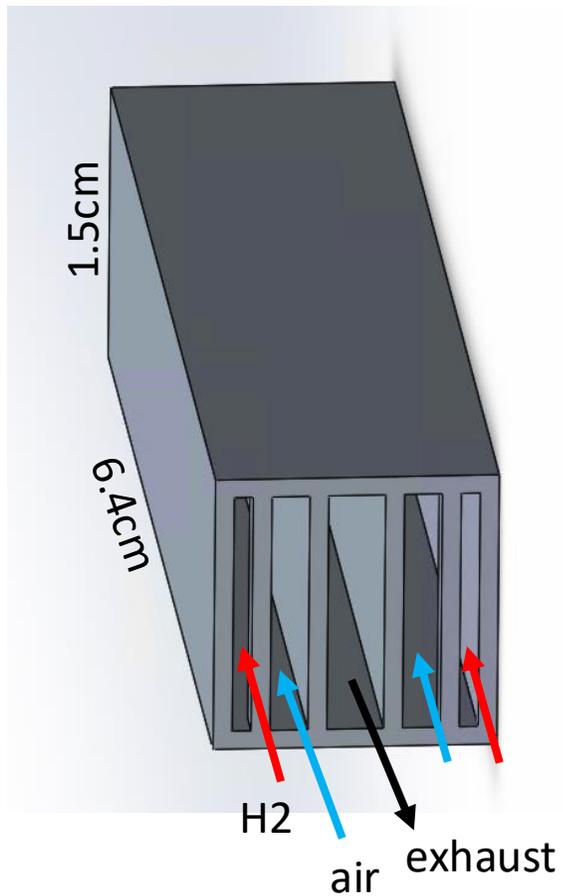
Metric	Base case	Turbulence	Multi-inlet	Bluff body	Staged
Max solid temp	1962K	2023K	2047K	2704K	2500K
Max fluid temp	3309K	3313K	3243K	3242K	3281K
Avg emitter wall temp	1898K	1943K	1781K	1570K	1811K
Heat out	560W	596W	440W	470W	538W
Efficiency	47%	50%	37%	39%	45%
Outlet temp (ma)	2053K	2055K	2169K	2111K	2096K
Time	0:20 hr	2:00 hr	2:00hr	1:32 hr	1:12 hr

Tradeoff between mixing and heat extraction
 Large ΔT between flame temp and wall temp
 Hard to spread heat to both side wall and top wall
 How to improve? Utilize 3D geometry

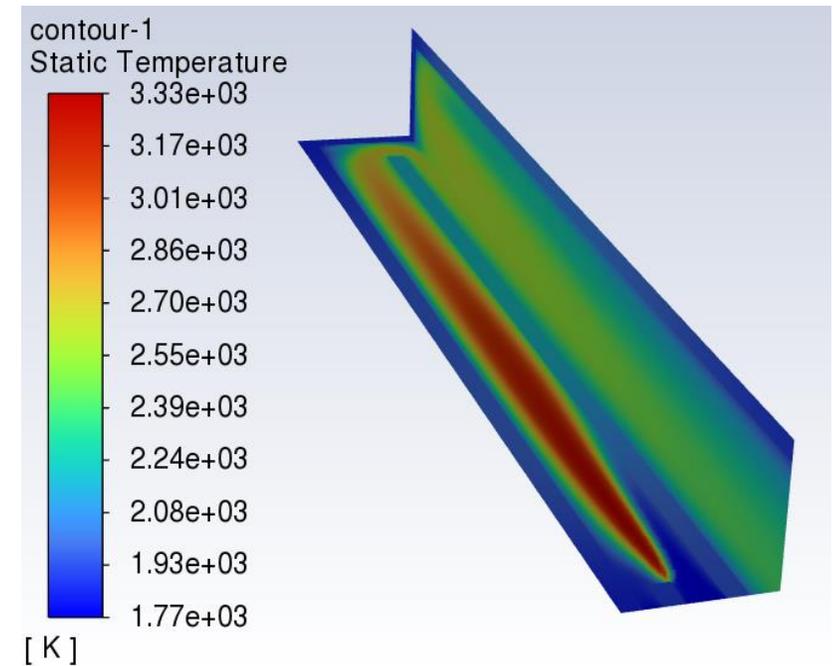
$$\eta_{comb} = \frac{Q_{out}}{\dot{m}HV}$$



Moving to 3D allows addition of heat spreading features



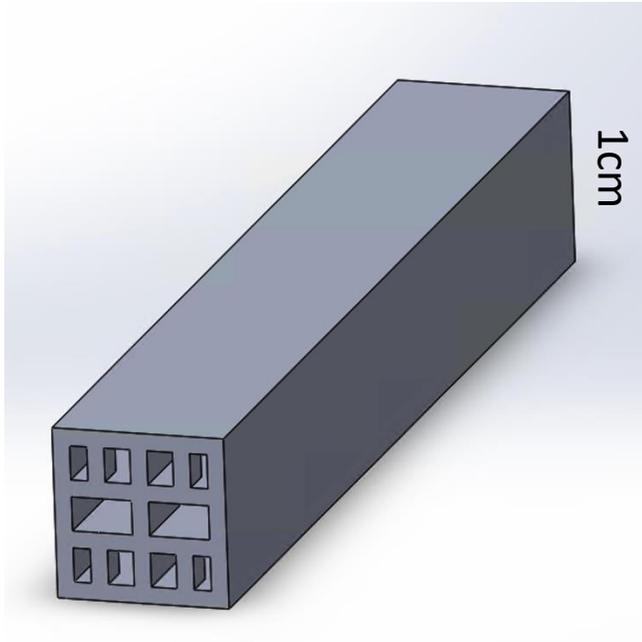
Utilize symmetry to
accelerate computation



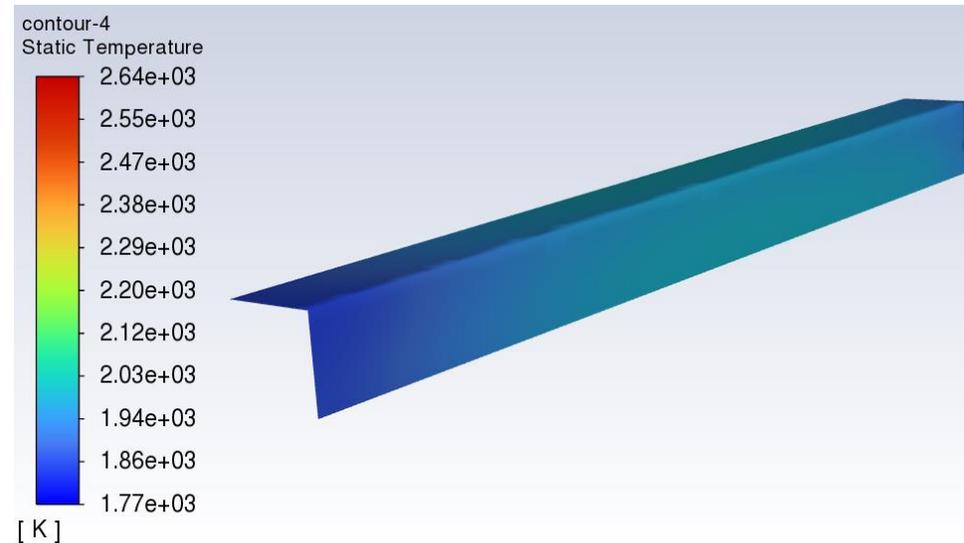
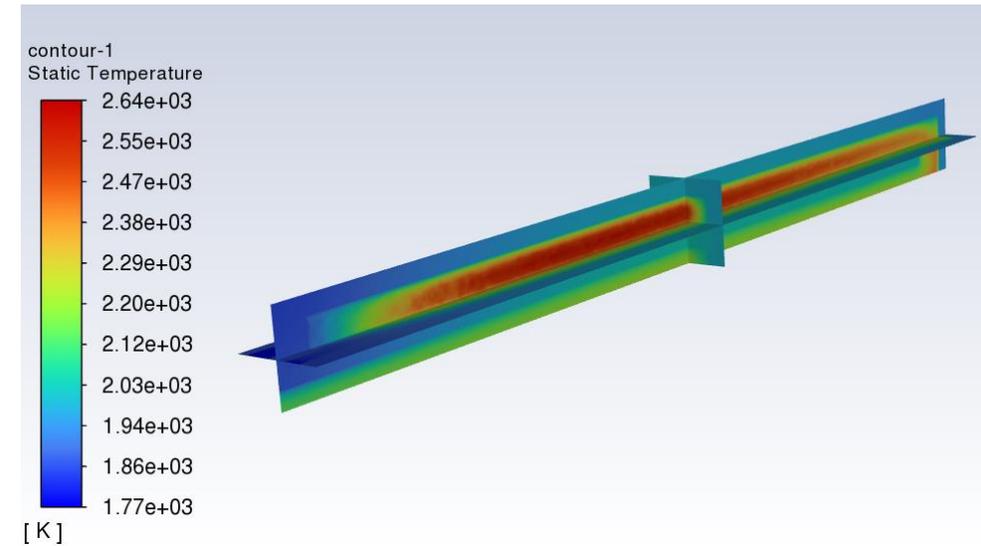
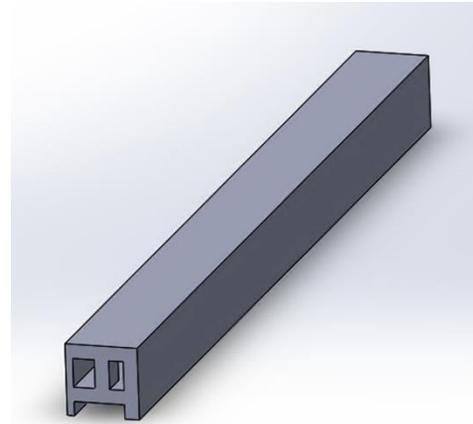
79% efficiency
17.4 W/cm²
177W out
Max solid temp = 2000C (too high)

Further optimization of heat spreading

(Sliced design)



Add additional heat spreading fins

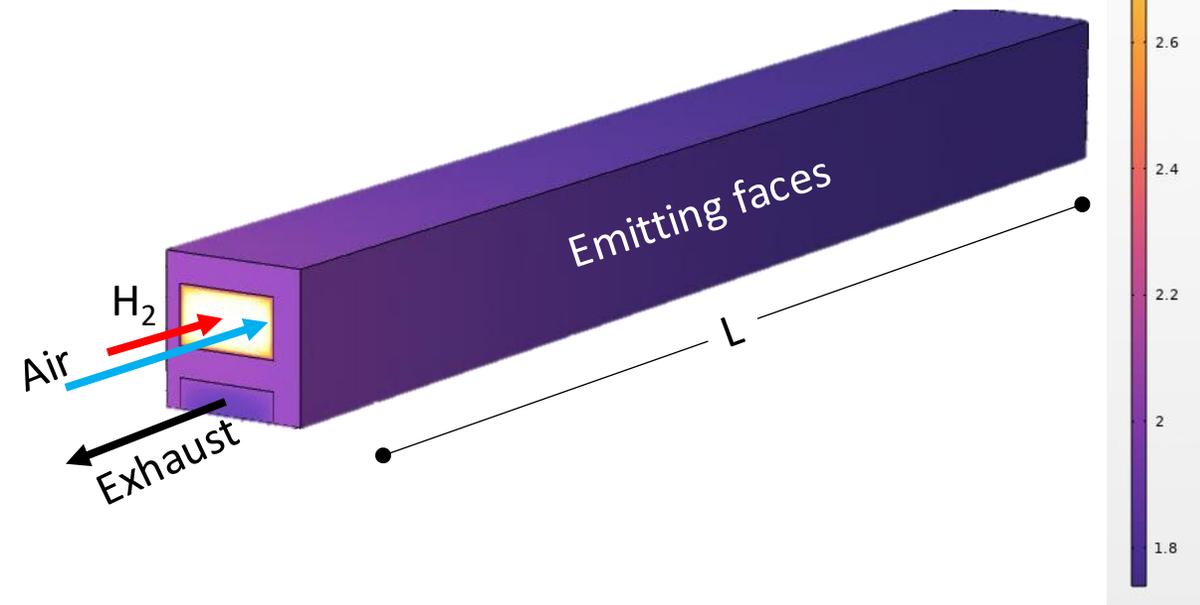


Combustion efficiency = 80%
17.9W/cm²
Heat out = 120W
Max solid temp = 1780C

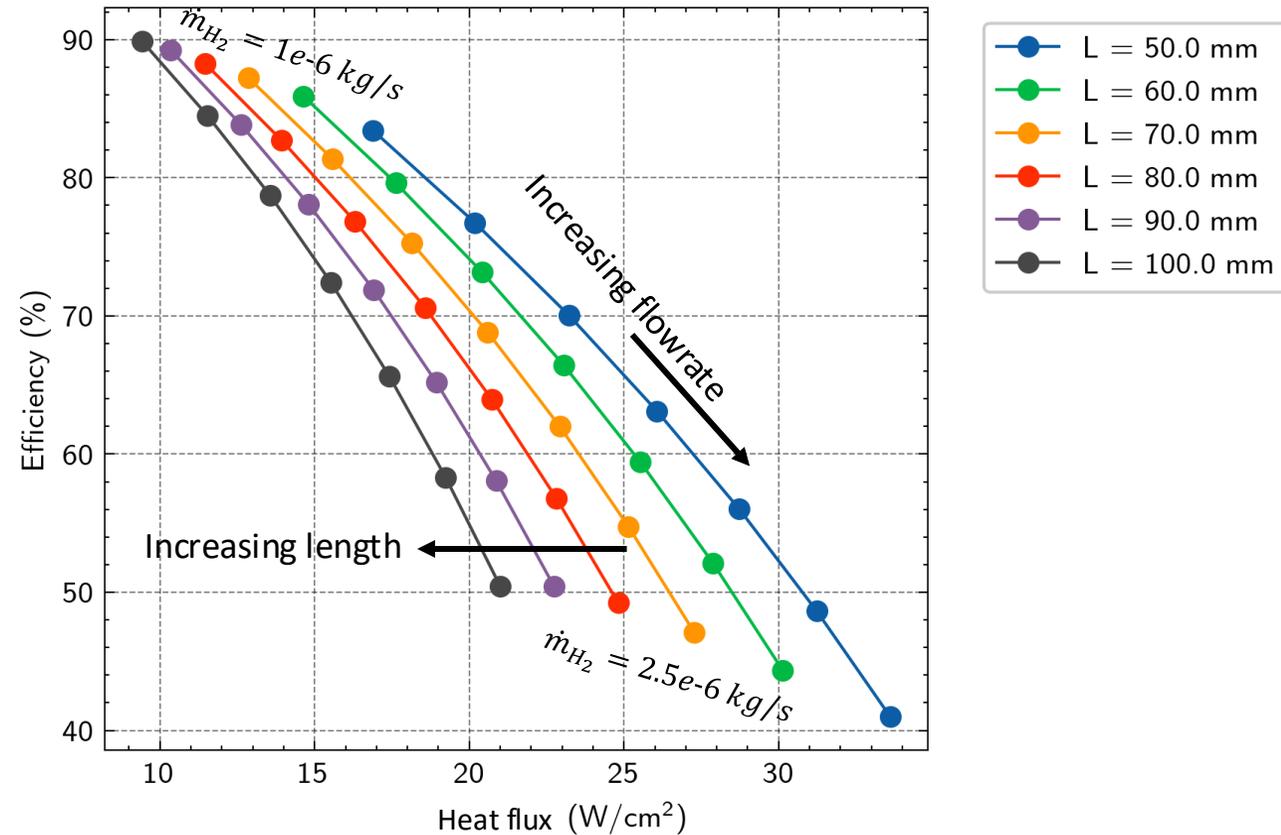
Tradeoff between efficiency and heat flux

$$\eta = \frac{Q_{out}}{Q_{fuel}} = \frac{q''A}{\dot{m}HV}$$

dictated by exhaust temp
 q'' dictated by emitter temp



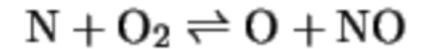
Vary flowrate and combustor length



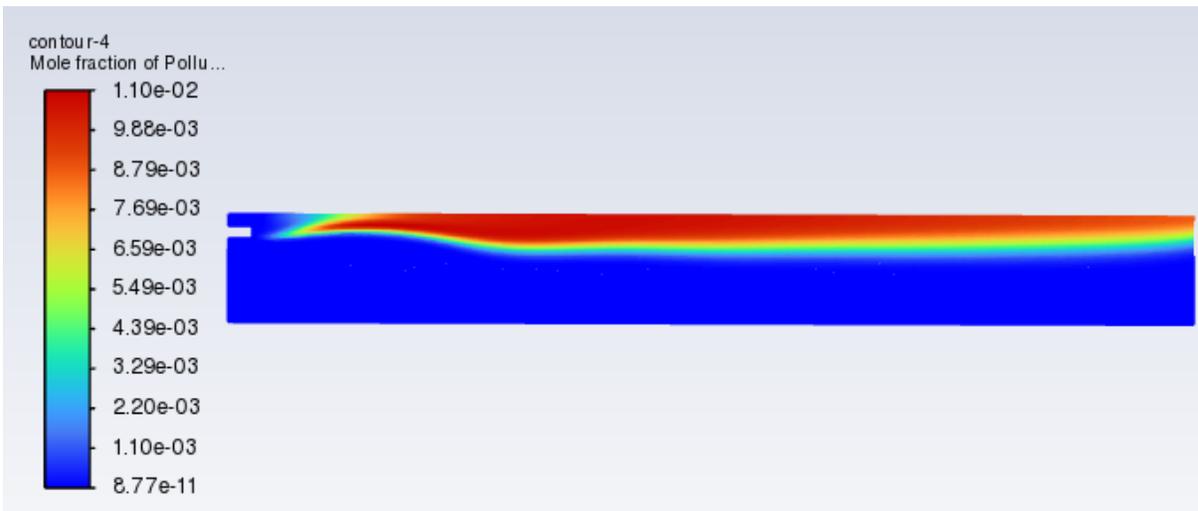
Question 1: high efficiency and heat flux

NOx emissions characterization

- Implement Zeldovich mechanism



$$\frac{d[\text{NO}]}{dt} = k_{f,1}[\text{O}][\text{N}_2] + k_{f,2}[\text{N}][\text{O}_2] + k_{f,3}[\text{N}][\text{OH}] - k_{r,1}[\text{NO}][\text{N}] - k_{r,2}[\text{NO}][\text{O}] - k_{r,3}[\text{NO}][\text{H}]$$



To decouple from combustion, use (partial) equilibrium model:

$$[\text{O}] = 3.97 \times 10^5 T^{-1/2} [\text{O}_2]^{1/2} e^{-31090/T} \quad \text{gmol/m}^3$$

$$[\text{OH}] = 2.129 \times 10^2 T^{-0.57} e^{-4595/T} [\text{O}]^{1/2} [\text{H}_2\text{O}]^{1/2} \quad \text{gmol/m}^3$$

NOx = 3,581 ppm

High (as expected)

How to control NOx?

1. Post-combustion
2. Oxy-combustion

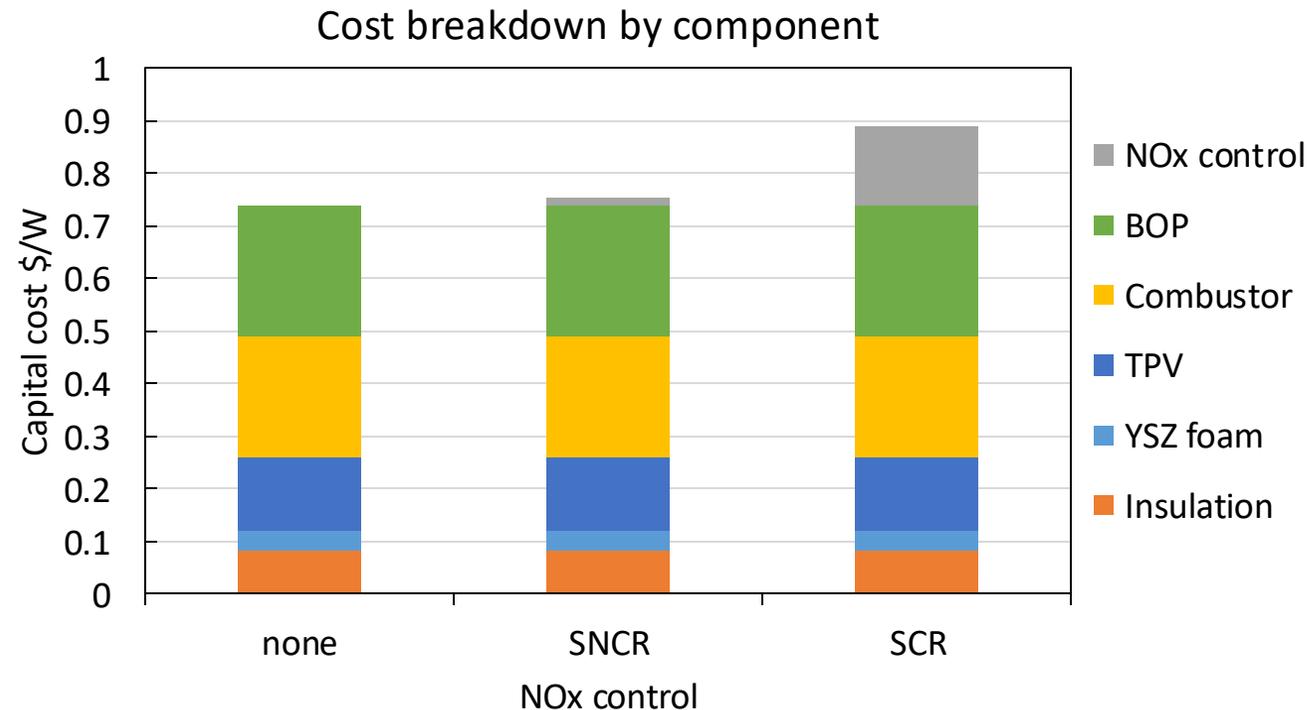
Post-combustion NOx control technologies

Selective non-catalytic reduction

- Ammonia/urea injection to react with NO
- 30-45% reduction in NOx
- 7-15 \$/kW

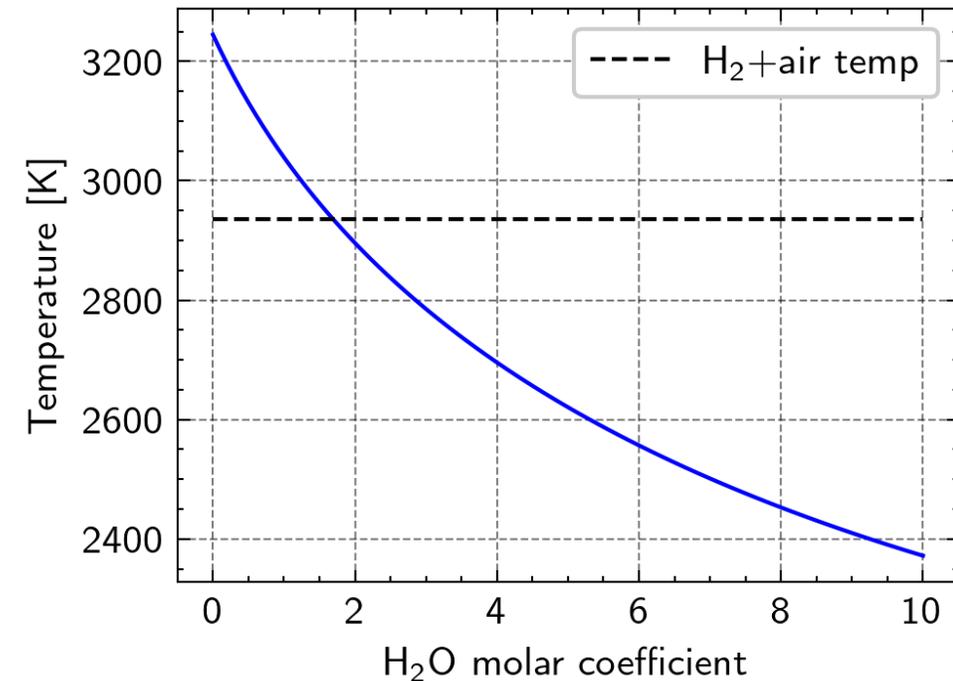
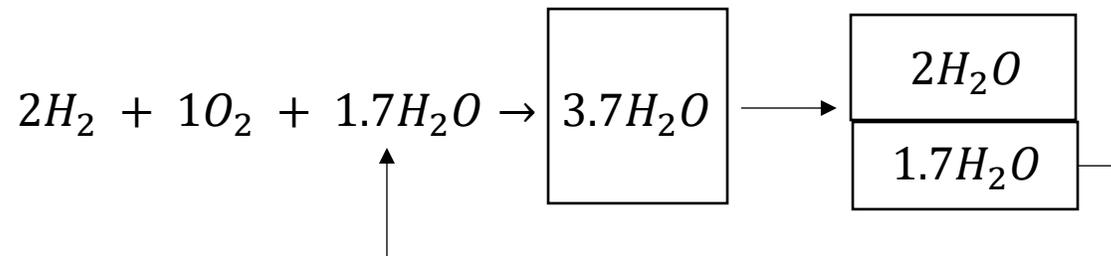
Selective catalytic reduction

- Catalytic (often vanadia-titania oxide)
- 90+% reduction in NOx
- 40-100 \$/kW

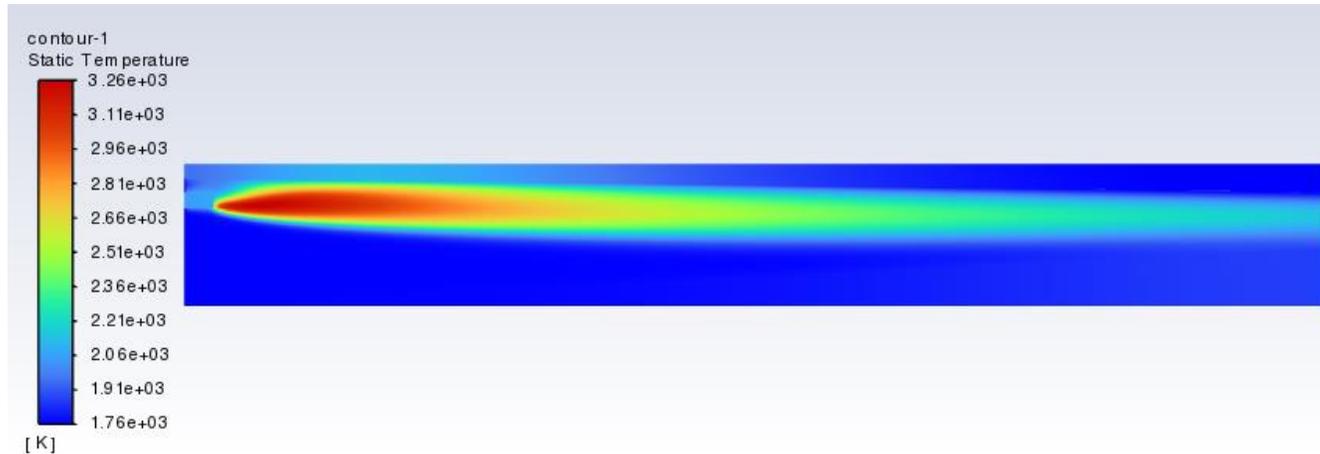


Oxy-combustion of hydrogen with steam as a diluent

- How much water/steam to match stoich adiabatic flame temp of air combustion?
 - $O_2:H_2O$ ratio of 1:1.7 $2H_2 + 10O_2 + 1.7H_2O \rightarrow 3.7H_2O$
- How to generate O_2 and steam?
 - O_2 : many H_2 production methods generate O_2
 - From water/steam
 - Electrolysis, thermochemical, photoelectrochemical
 - Steam: Flue gas recirculation



Air vs. oxy combustion preliminary CFD

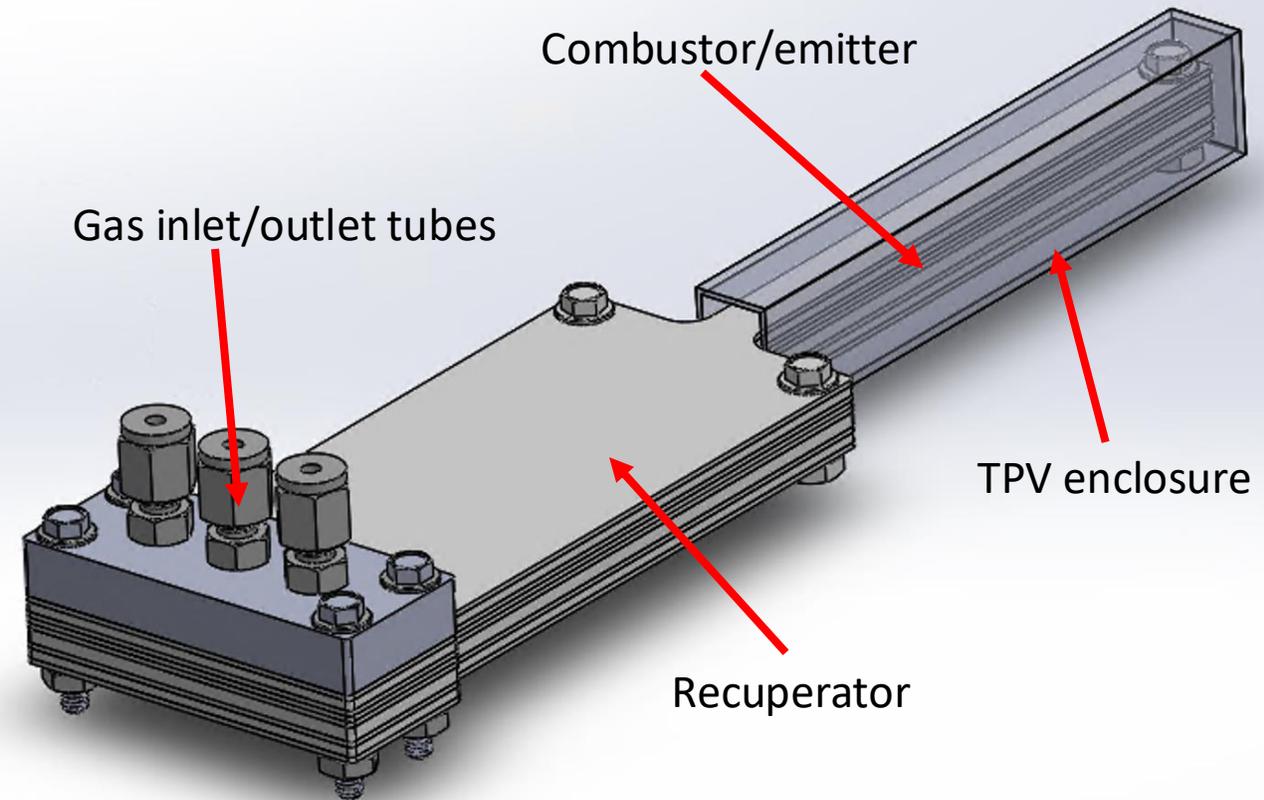
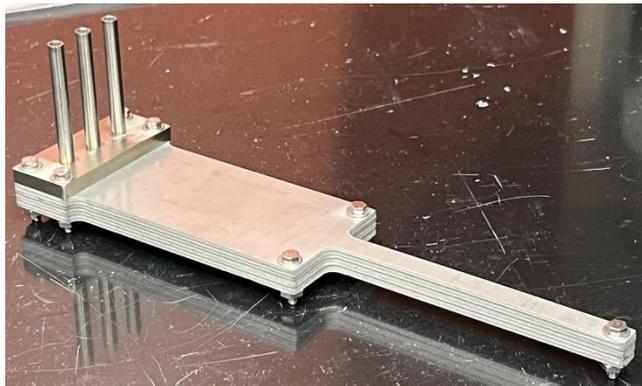


Metric	Air	Oxy
Efficiency (%)	87	91
Power density (W/cm ²)	16.1	17.2
Max wall temperature (°C)	1750	1850

Q2: low NO_x emissions

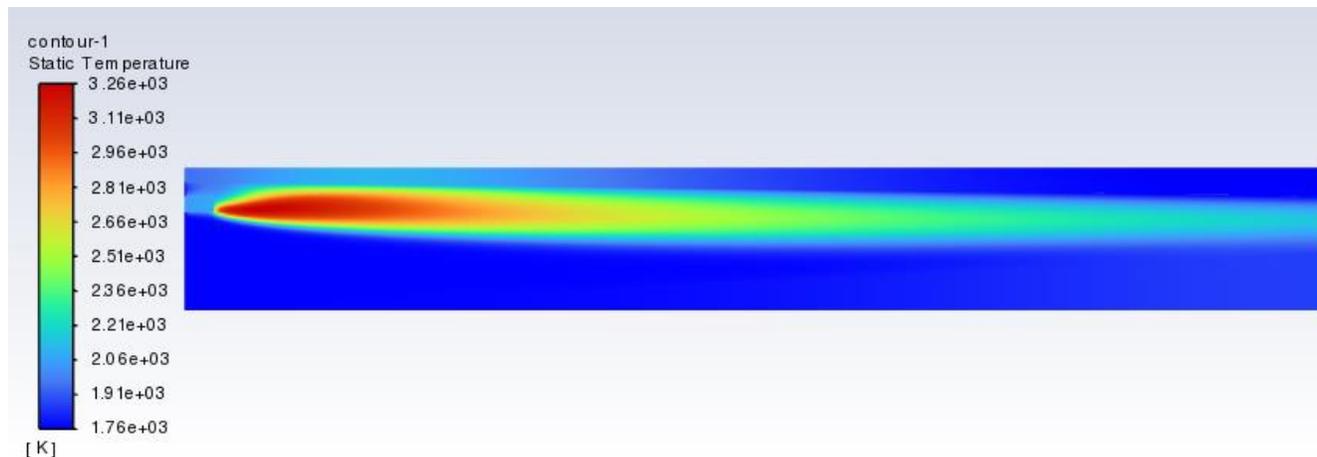
Conclusions and future work for heat extraction

- 3D geometries critical for heat spreading
 - High k of SiC
- Can design for desired efficiency vs. power density for given application
- Future work
 - Include radiation
 - Manufacturing!



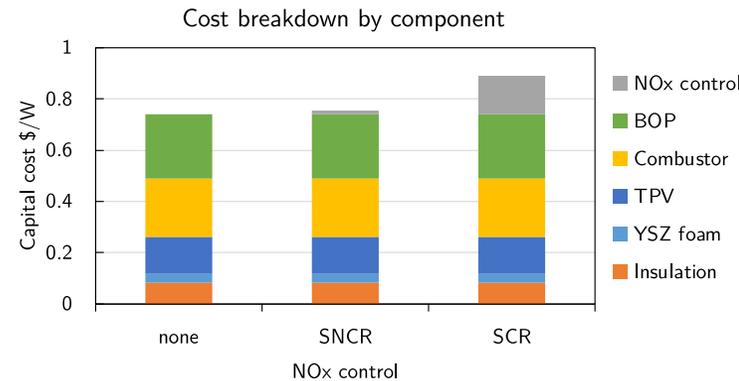
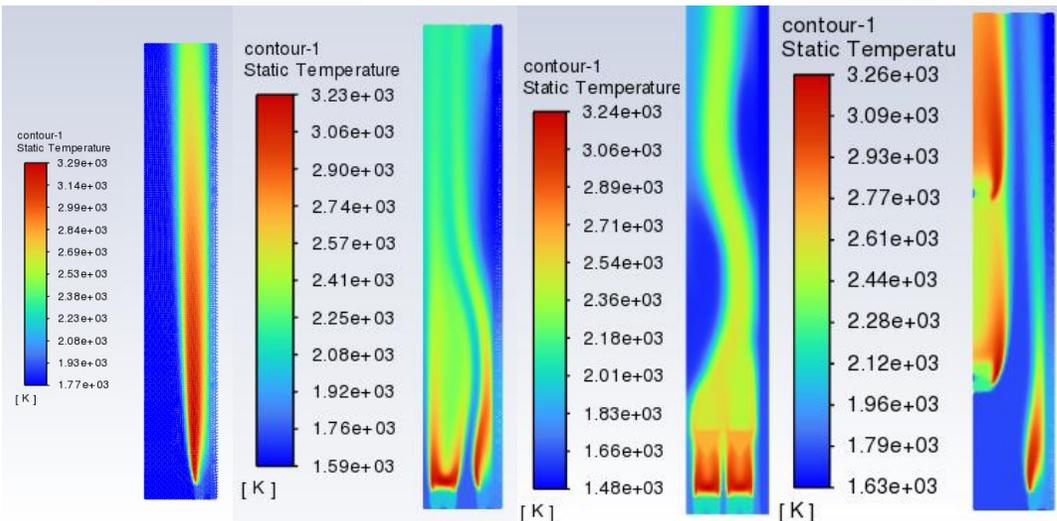
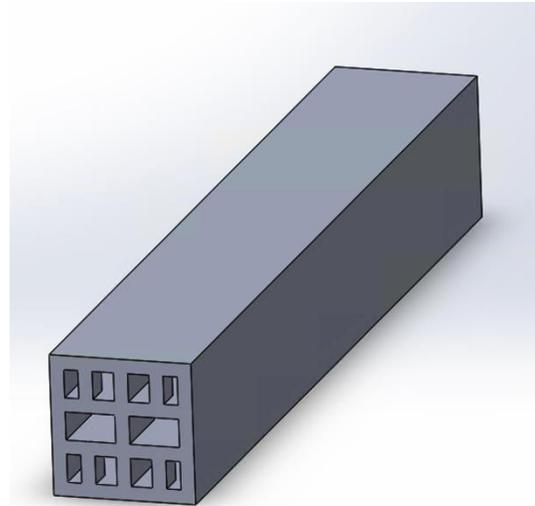
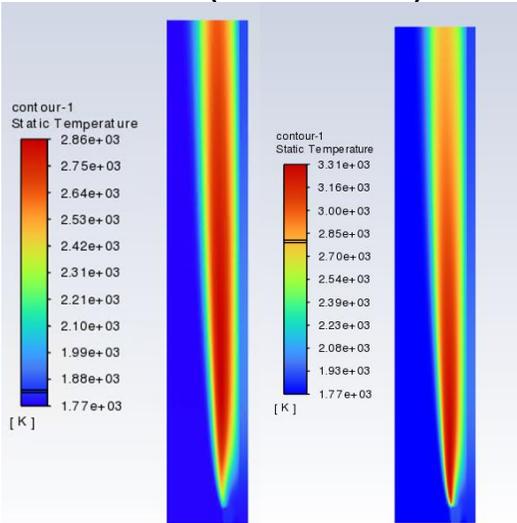
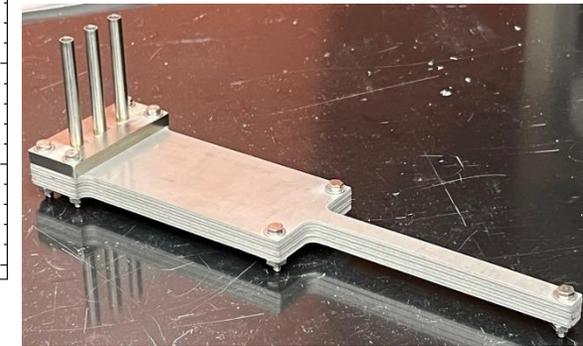
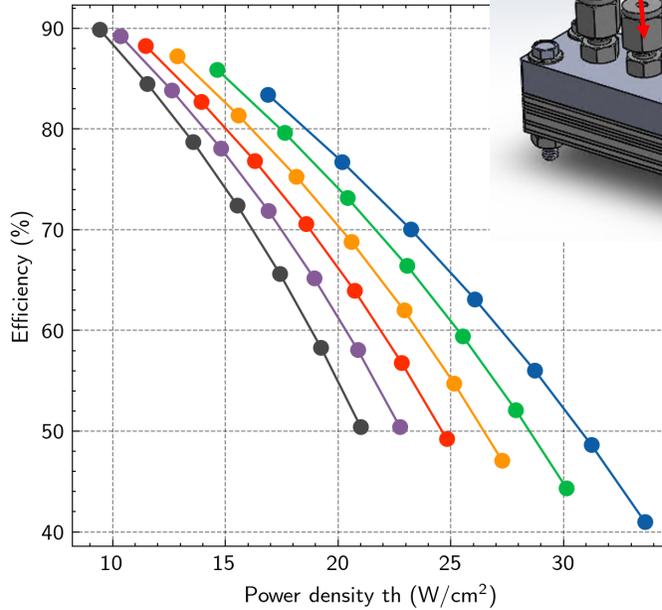
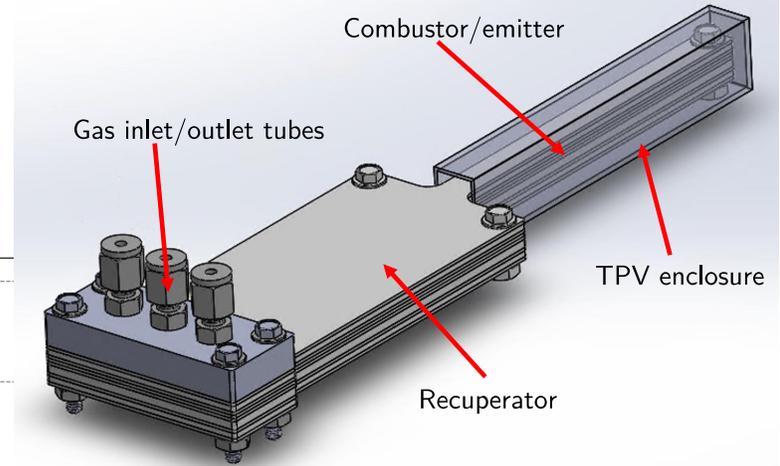
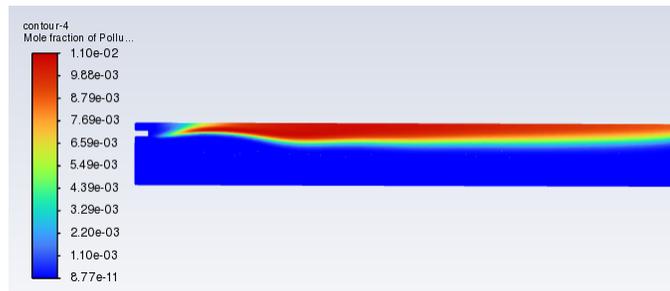
Conclusions and future work for NOx control

- High H₂ flame temp \Rightarrow oxy-combustion required
- Can dilute O₂ stream with recirculated H₂O
- Future work
 - Continued CFD simulations
 - Costs and full TEA of H₂+O₂ production
 - Environmental degradation of SiC



Summary

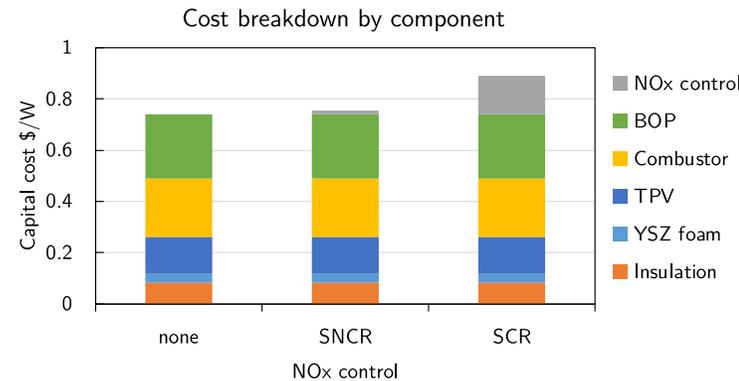
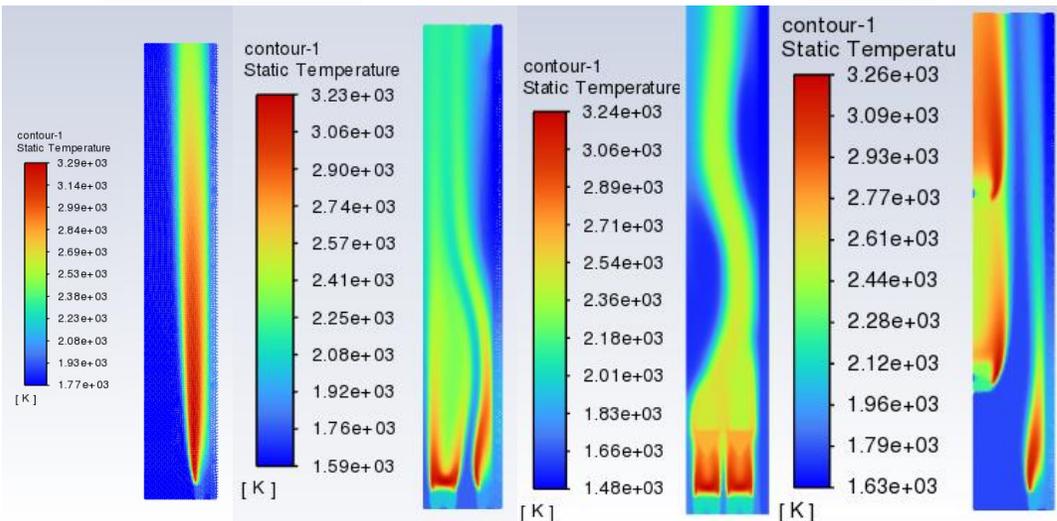
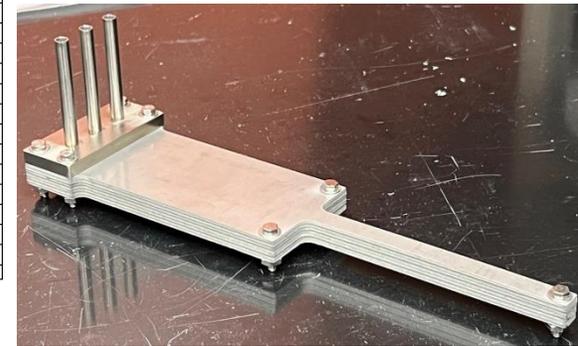
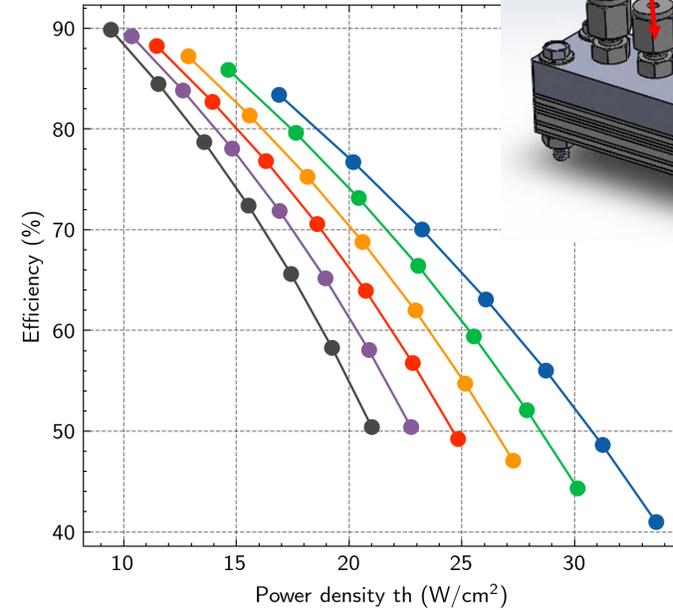
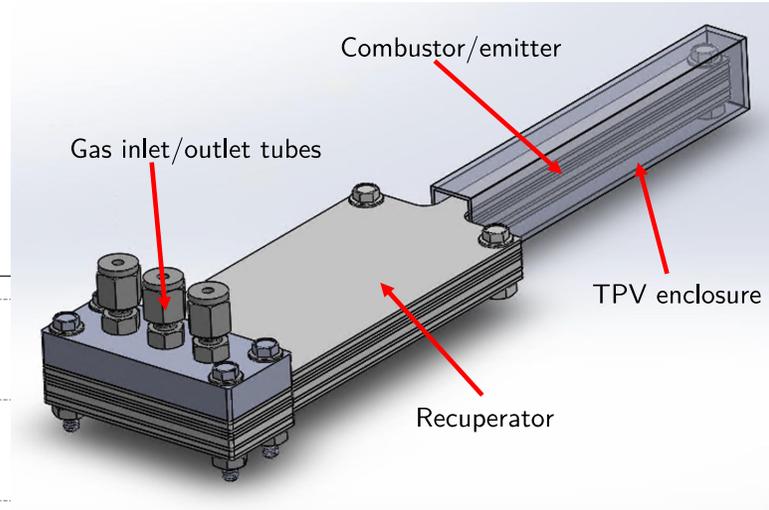
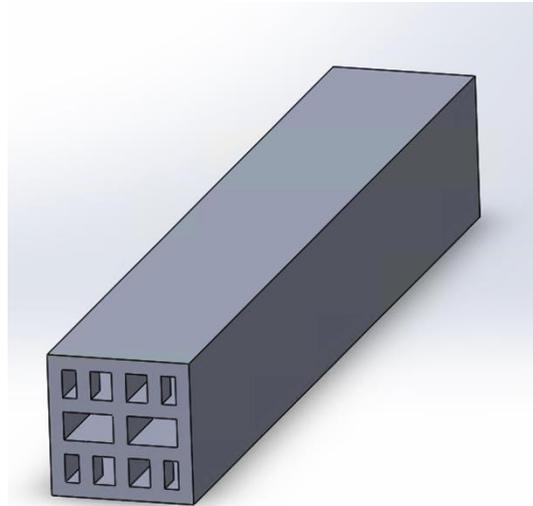
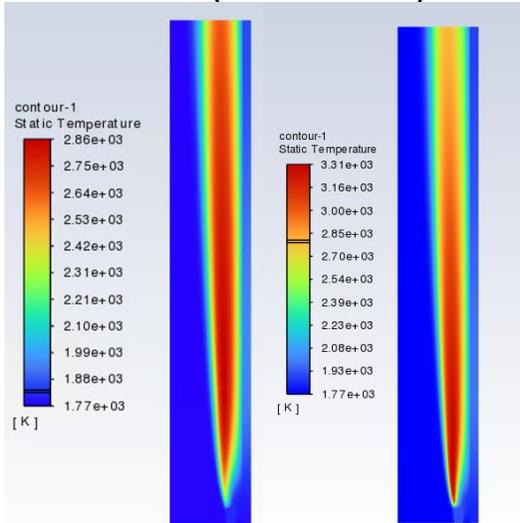
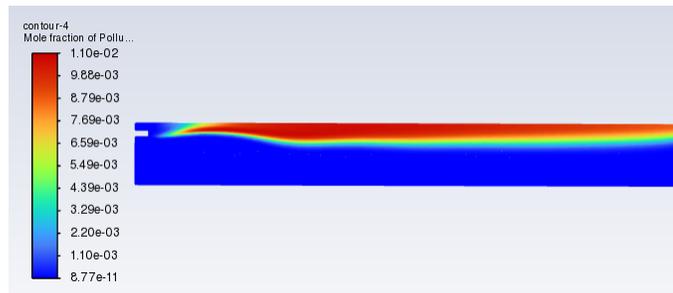
$$5.62e10 \exp\left(-\frac{1.87e8}{RT}\right) [H_2][O_2]^{0.5}$$



$\eta_{comb} = 80\%$
 NOx emissions <3ppm
 Cost below \$1/W
 LCOE below 10¢/kWh
 Dispatchable
 No moving parts

Thanks! Q&A

$$5.62e10 \exp\left(-\frac{1.87e8}{RT}\right) [H_2][O_2]^{0.5}$$



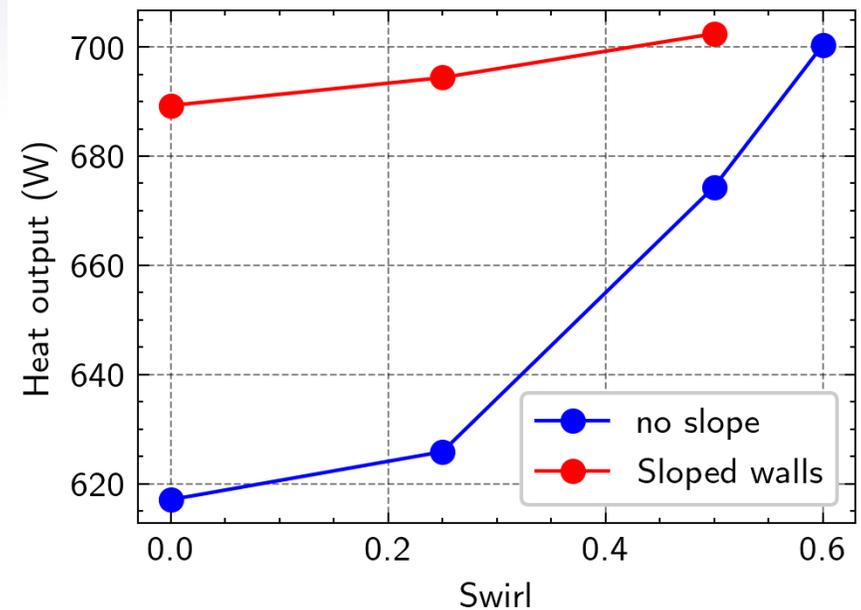
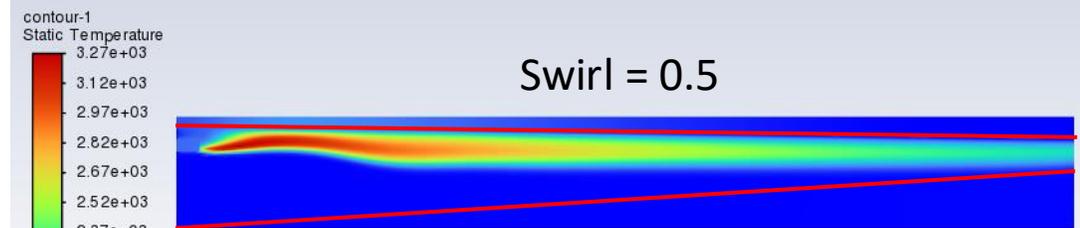
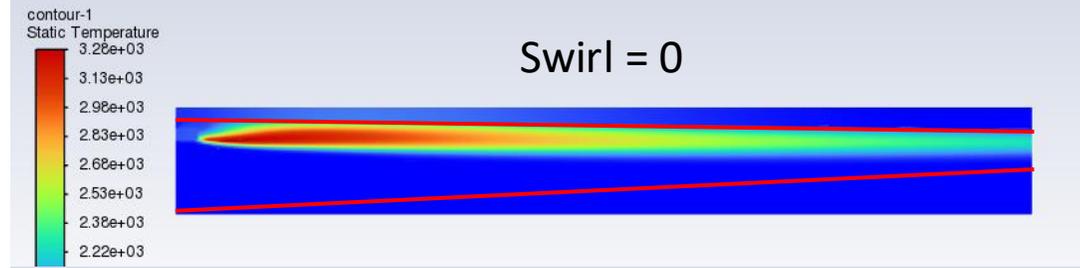
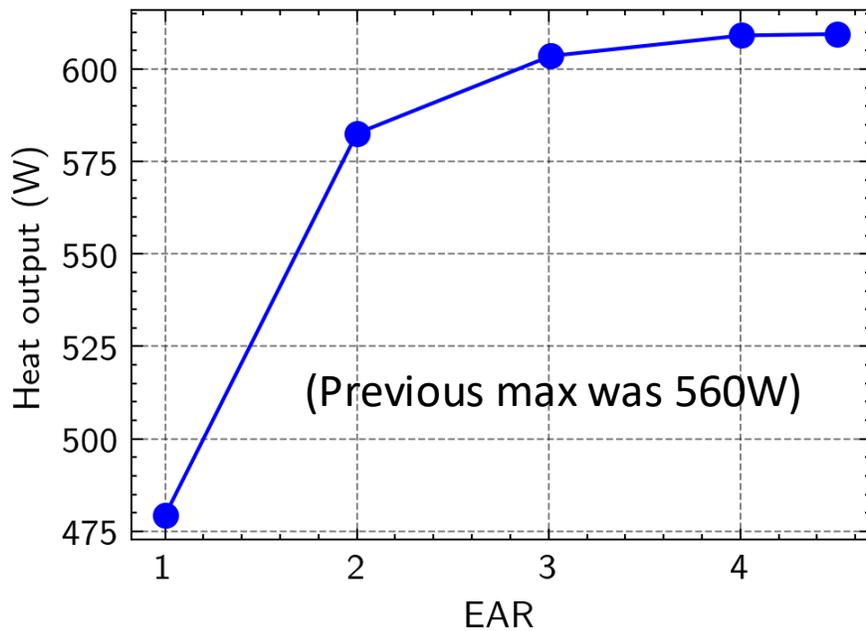
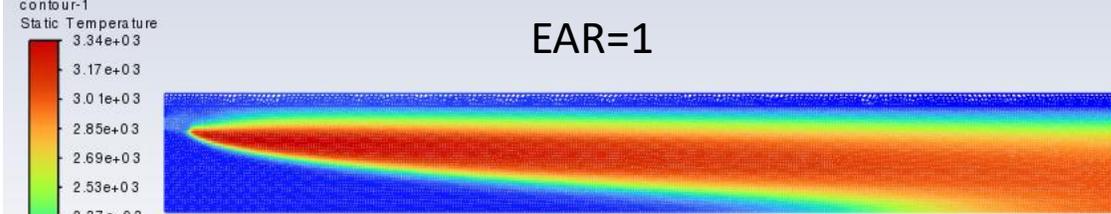
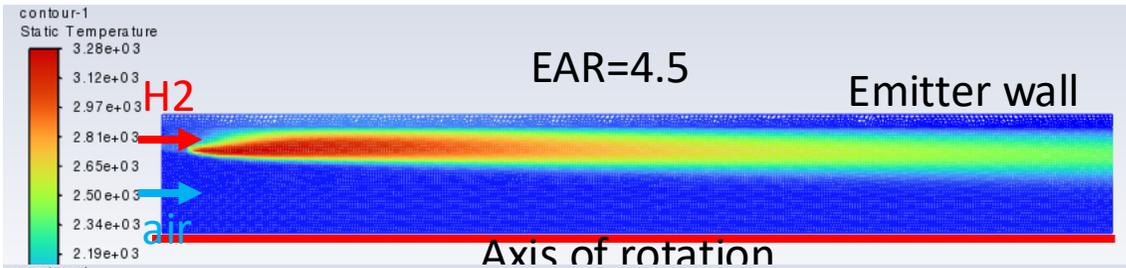
$\eta_{comb} = 80\%$
 NOx emissions <3ppm
 Cost below \$1/W
 LCOE below 10¢/kWh
 Dispatchable
 No moving parts

Backup Slides

How to fix stoich temp of custom mechanism?

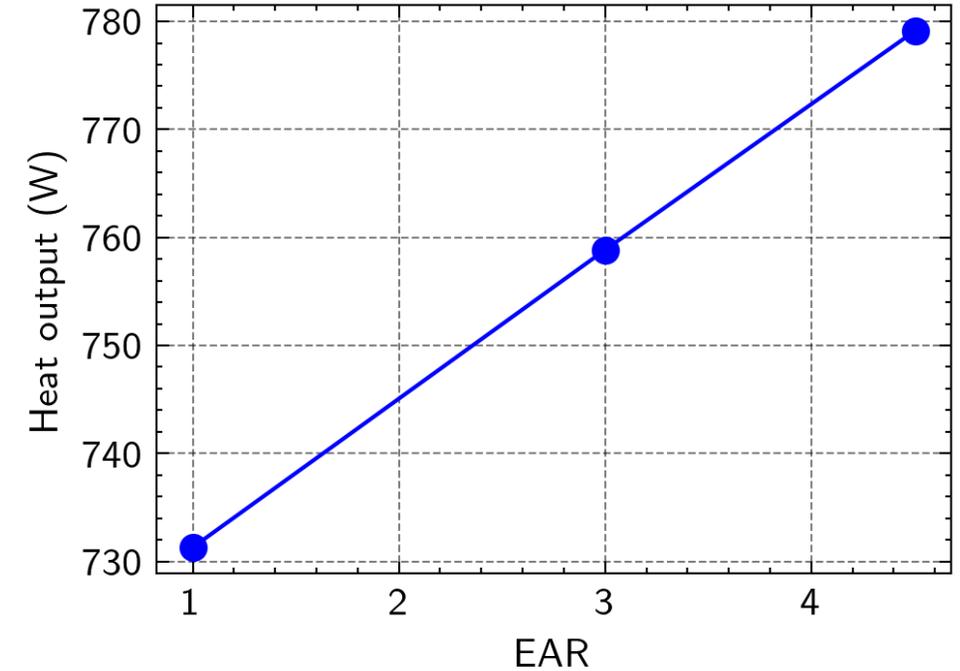
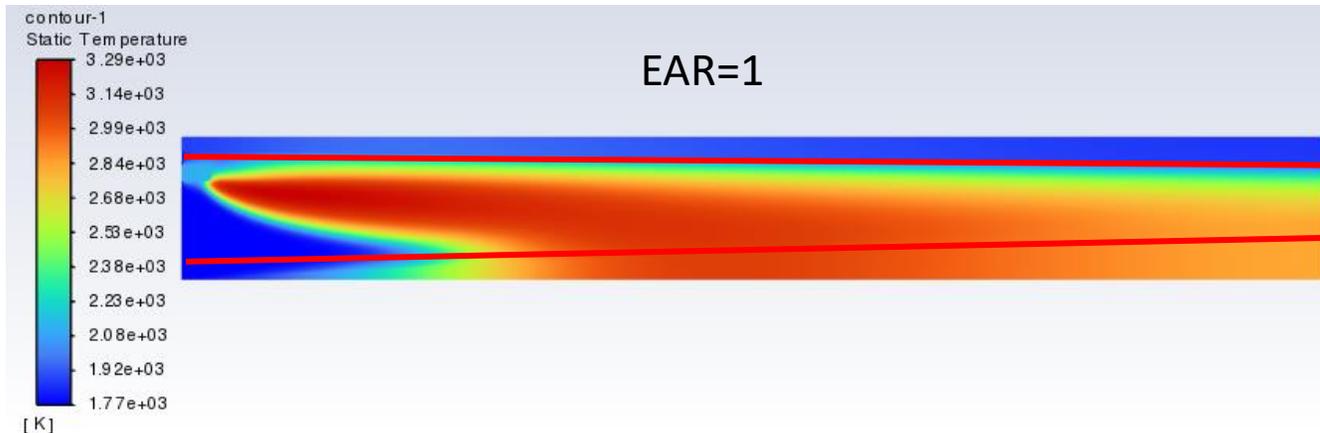
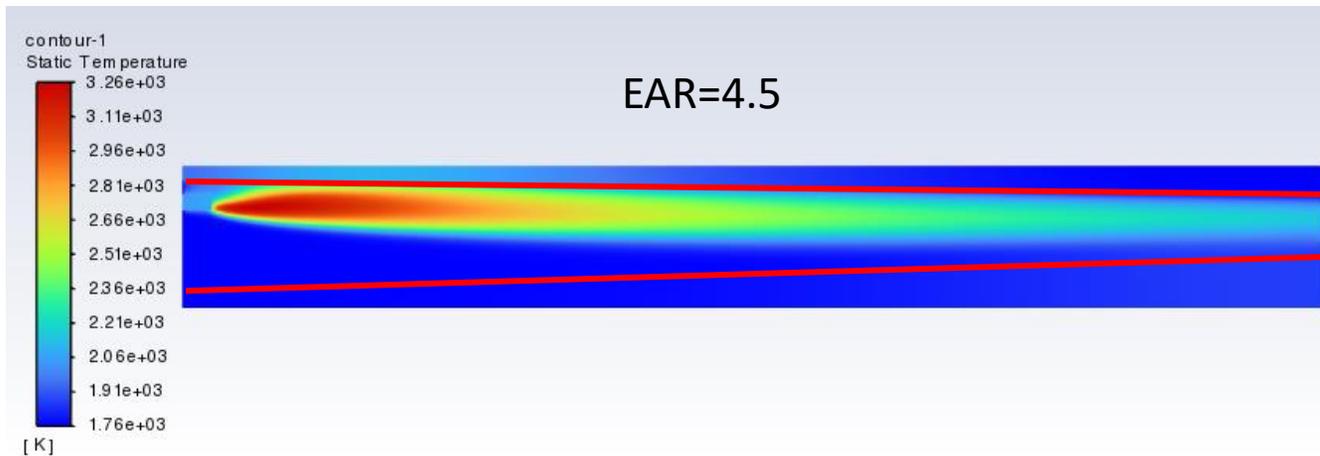
- Adiabatic flame temp of stoich mixture determined by equilibrium between products and reactants
- Equilibrium determined by entropy
- Inaccuracy caused by fewer products in the global reaction mechanism
- Need to change thermo – difficult without impacting other aspects

Switching to an axisymmetric design improves efficiency

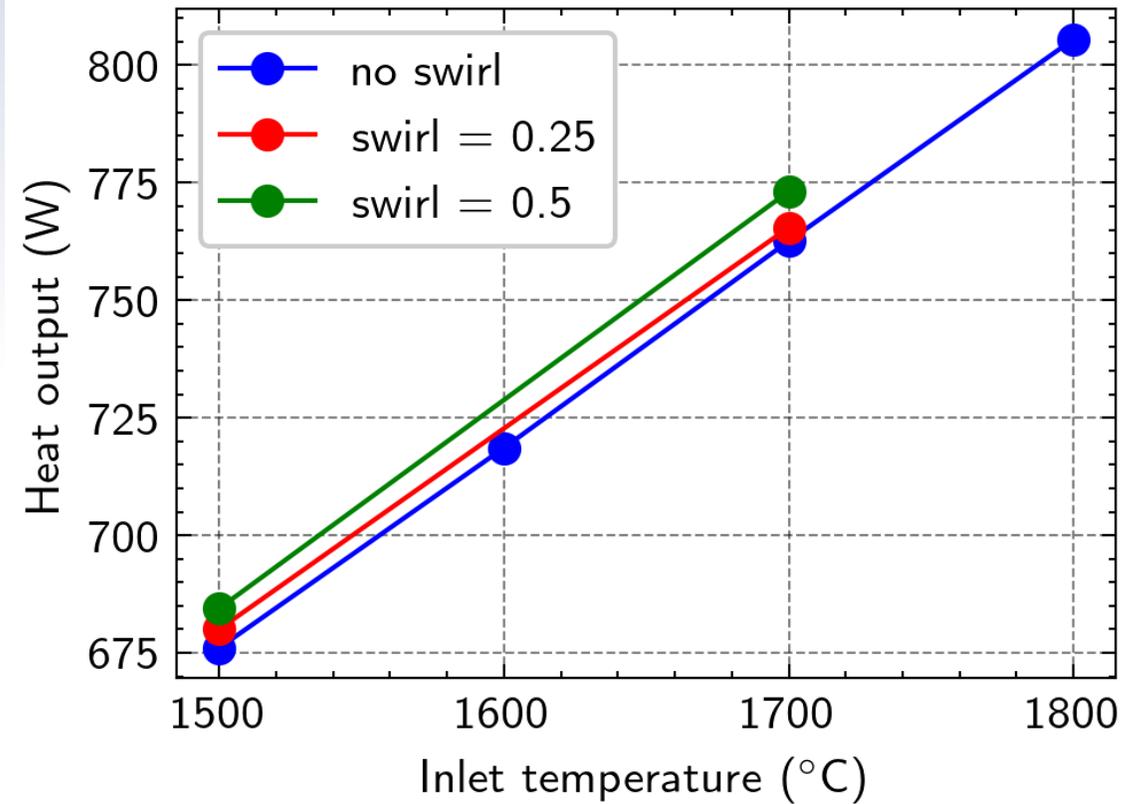
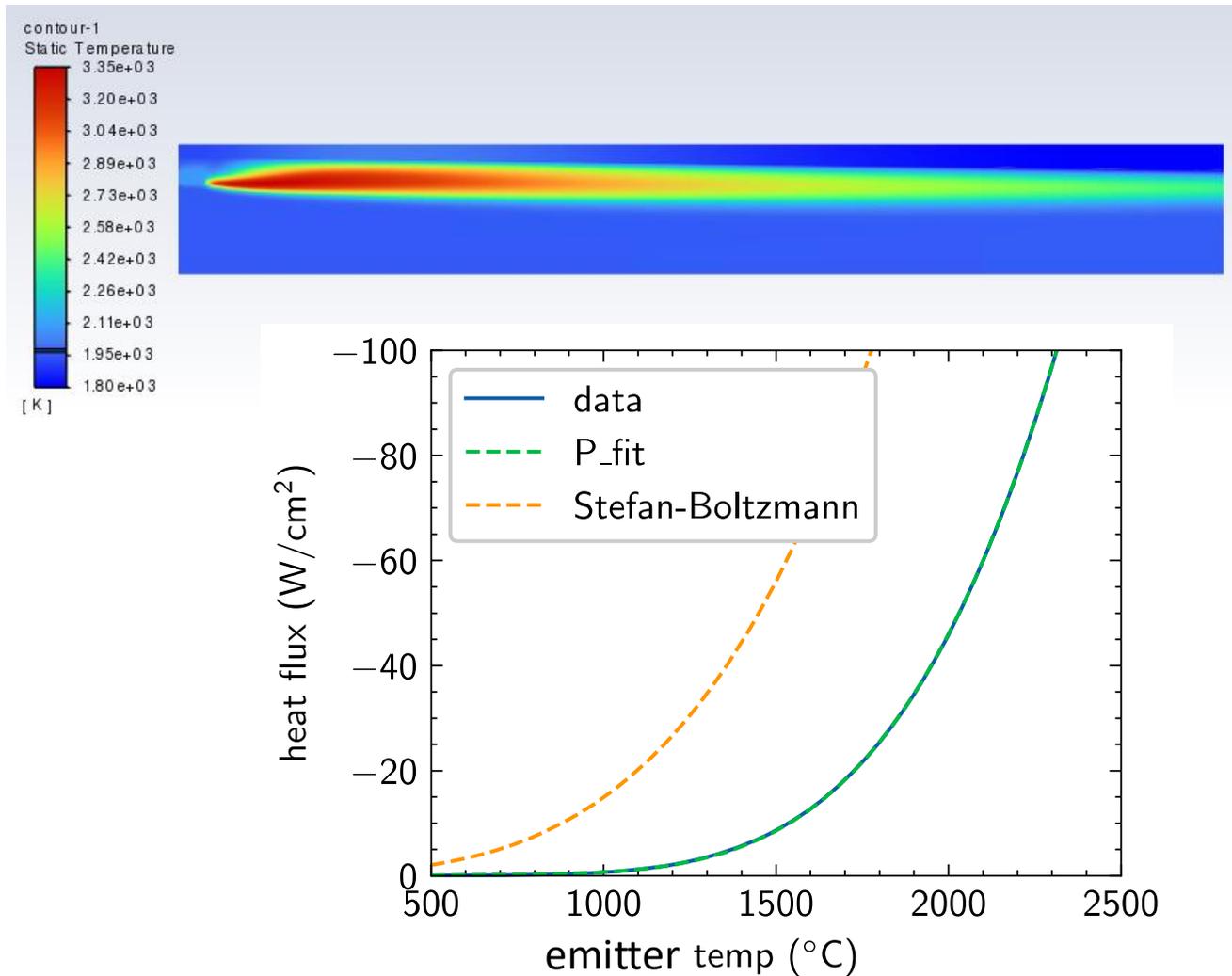


Oxy-combustion with steam as a diluent – CFD simulations

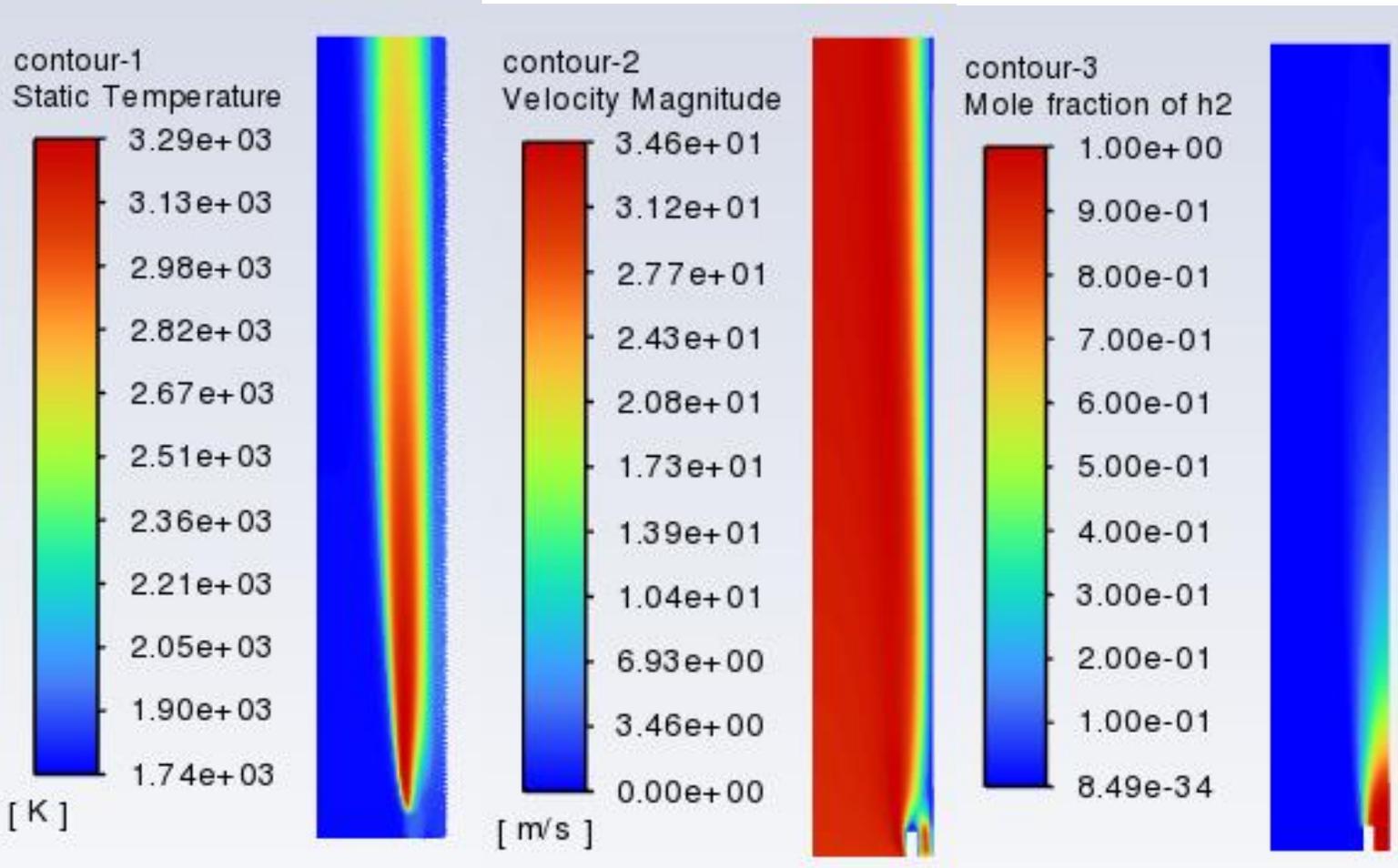
Still need to run lean to keep flame at wall



Effect of increasing inlet temperature



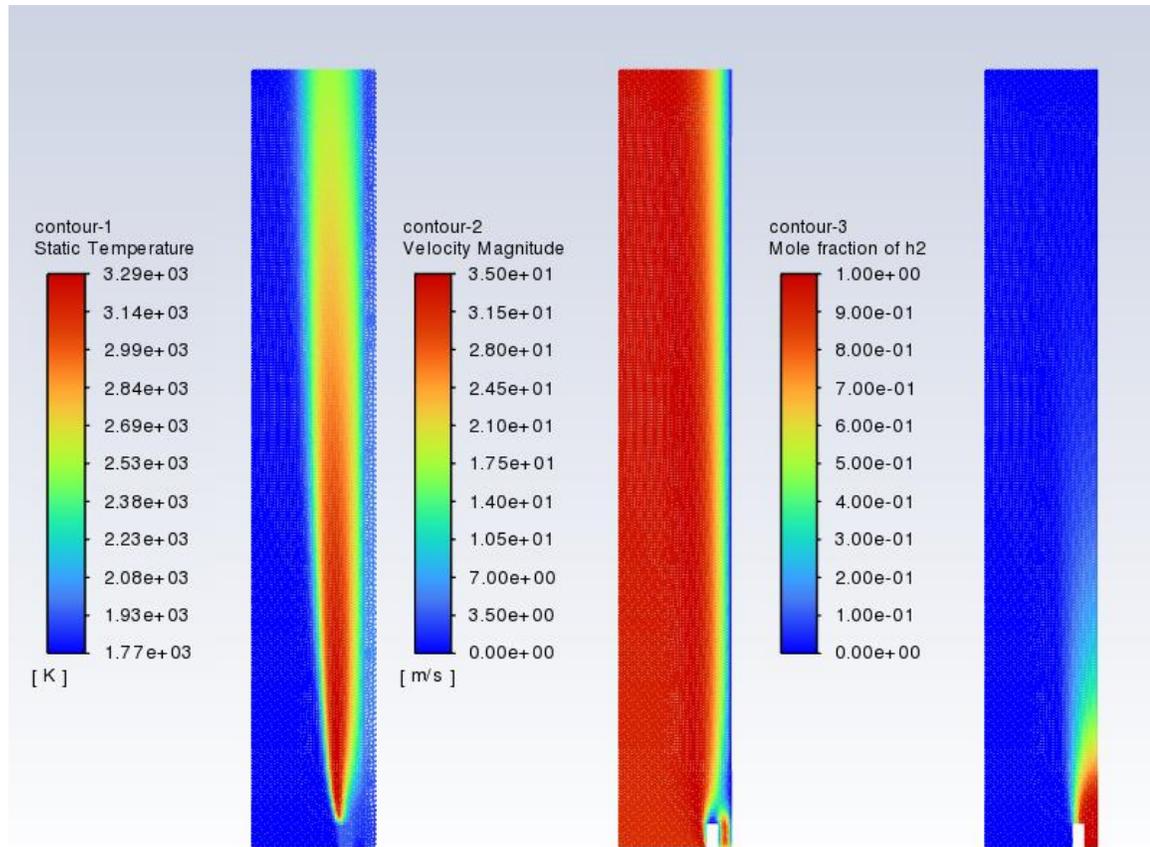
Base case for comparison



Metric	Value
Max solid temp	1962K
Max fluid temp	3309K
Max emitter wall temp	1958K
Emitter wall delT	121K
Heat out	560W
Outlet temp (ma)	2053K
Time	0:20 hr

$$\eta_{comb} = \frac{560W}{1e-5 \frac{kg}{s} \cdot 120e6 \frac{J}{kg}} = 47\%$$

Inducing turbulence in inlet streams



Metric	Value
Max solid temp	2023K
Max fluid temp	3313K
Max emitter wall temp	2018K
Emitter wall delT	154K
Heat out	596W
Outlet temp (ma)	2055K
Time	2:00 hr

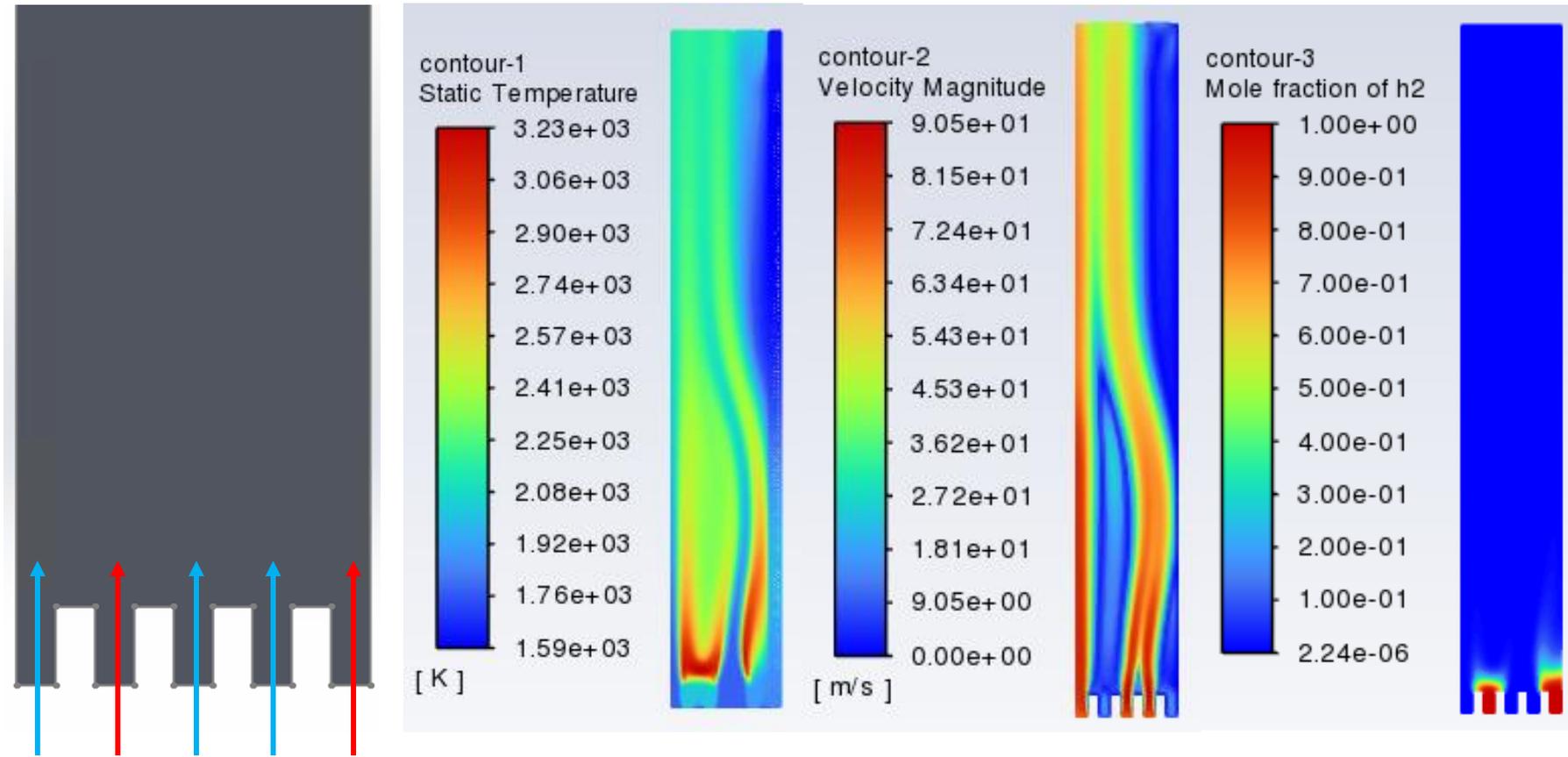
$$\eta_{comb} = \frac{596W}{1200W} = 50\%$$

Turbulent streams (5% intensity)

Future work: use non-premixed combustion module in fluent for species transport

But Re is so low unlikely to be turbulent flow anyway

Adding multiple inlet points

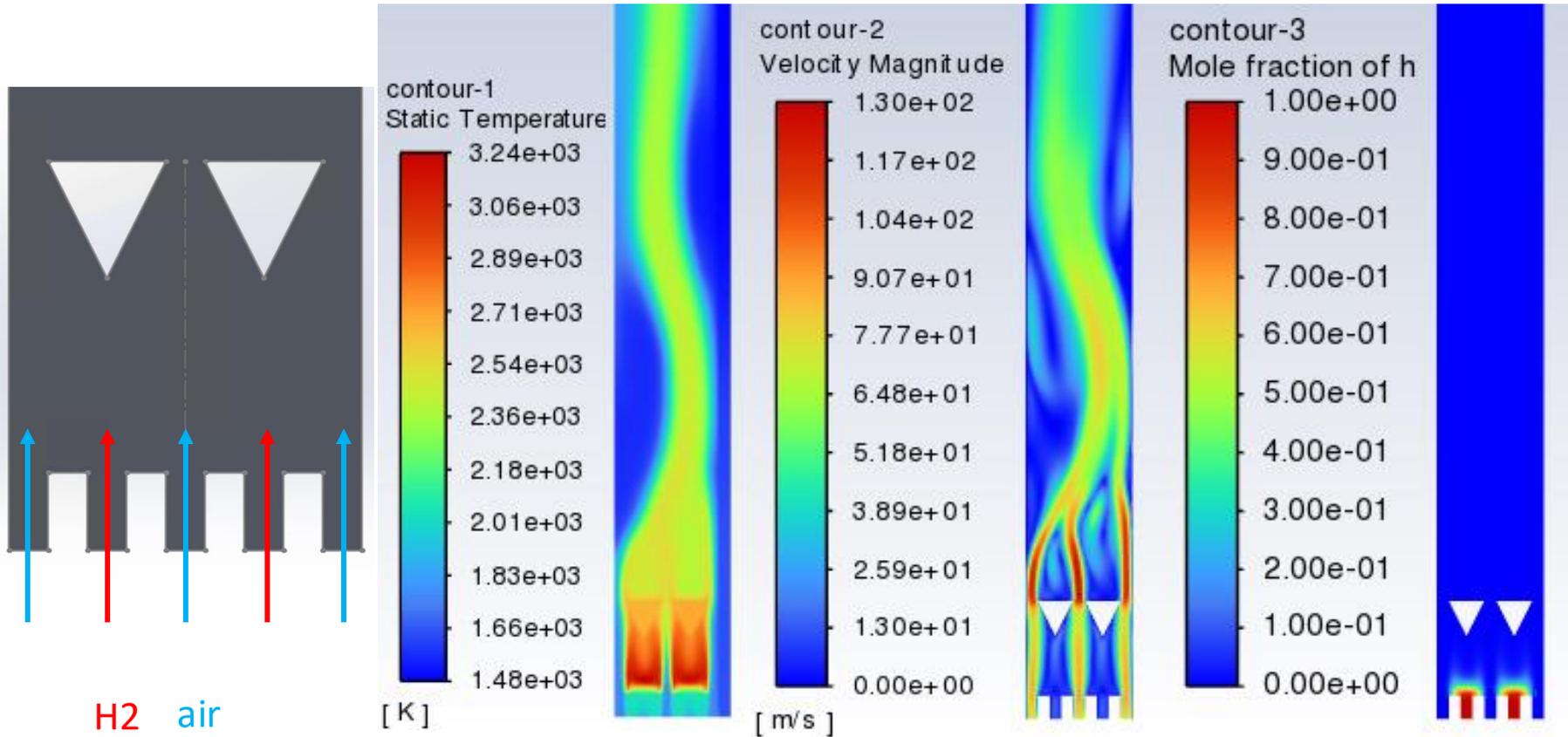


Metric	Value
Max solid temp	2047K
Max fluid temp	3243K
Max emitter wall temp	1980K
Emitter wall delT	388K
Heat out	440W
Outlet temp (ma)	2169K
Time	2:00hr

$$\eta_{comb} = \frac{440W}{1200W} = 37\%$$

H2 air

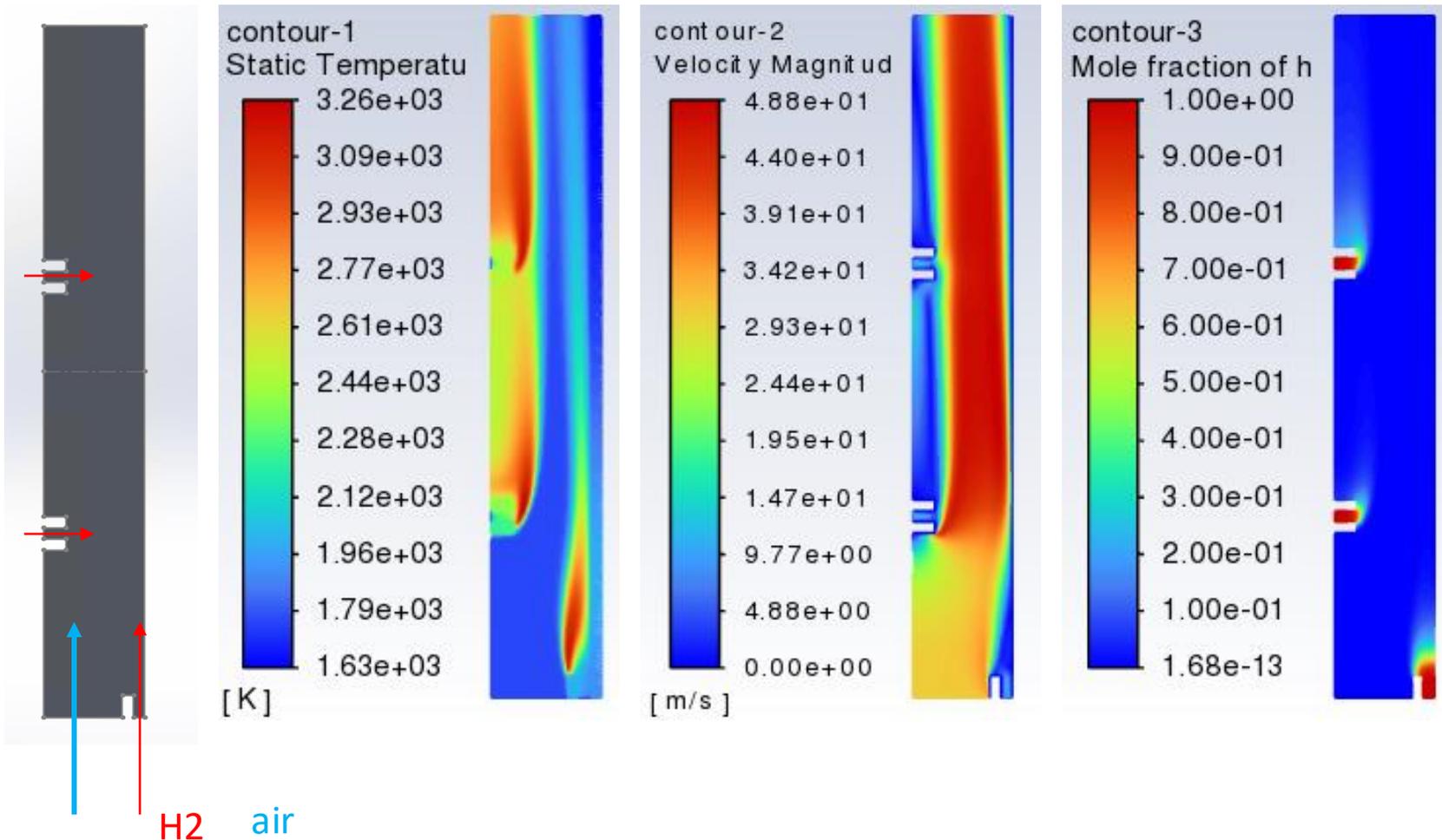
Adding 2 bluff bodies for reactant mixing



Metric	Value
Max solid temp	2704K
Max fluid temp	3242K
Max emitter wall temp	1660K
Emitter wall deIT	180K
Heat out	470W
Outlet temp (ma)	2111K
Time	1:32 hr

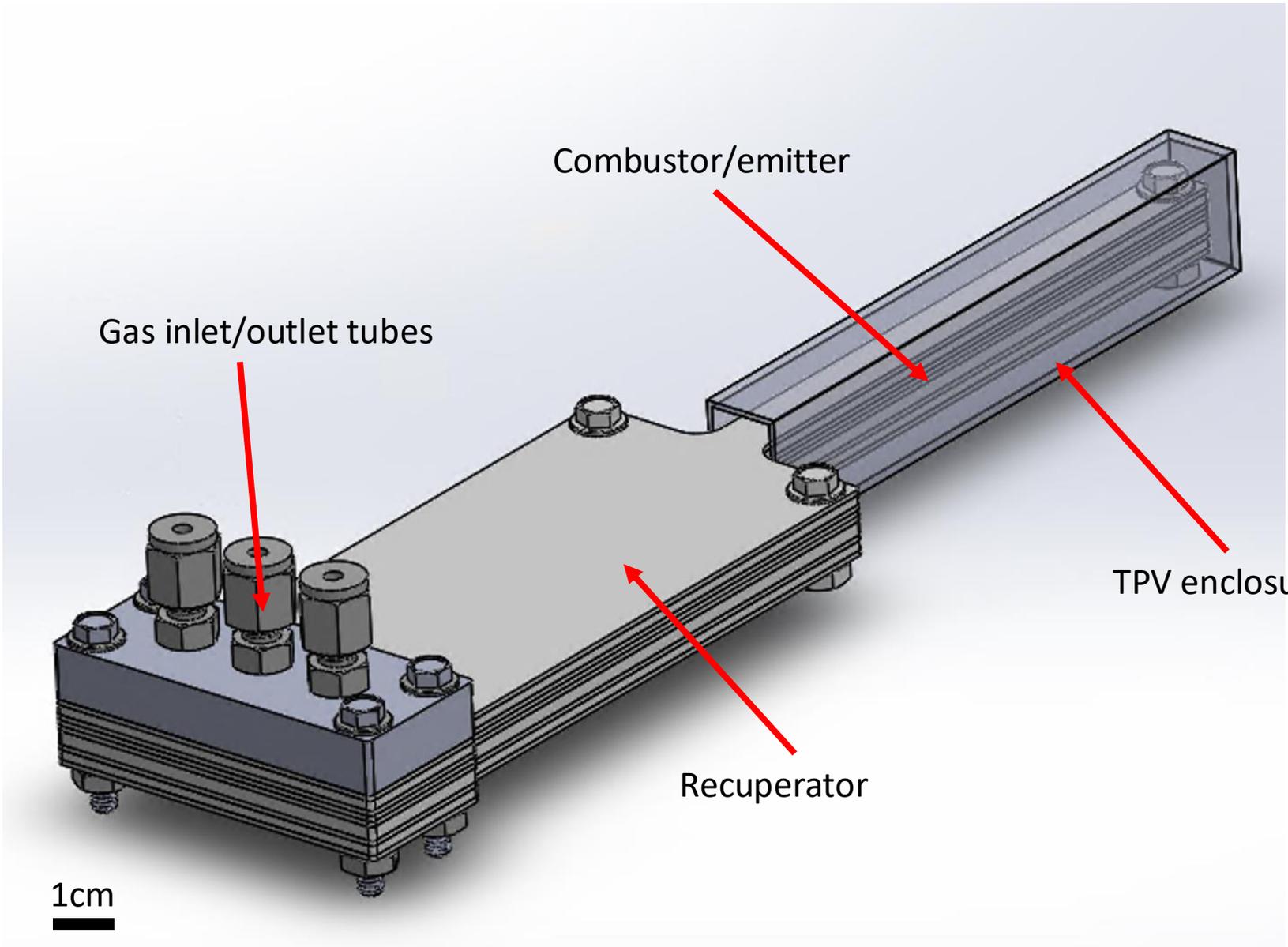
$$\eta_{comb} = \frac{470W}{1200W} = 39\%$$

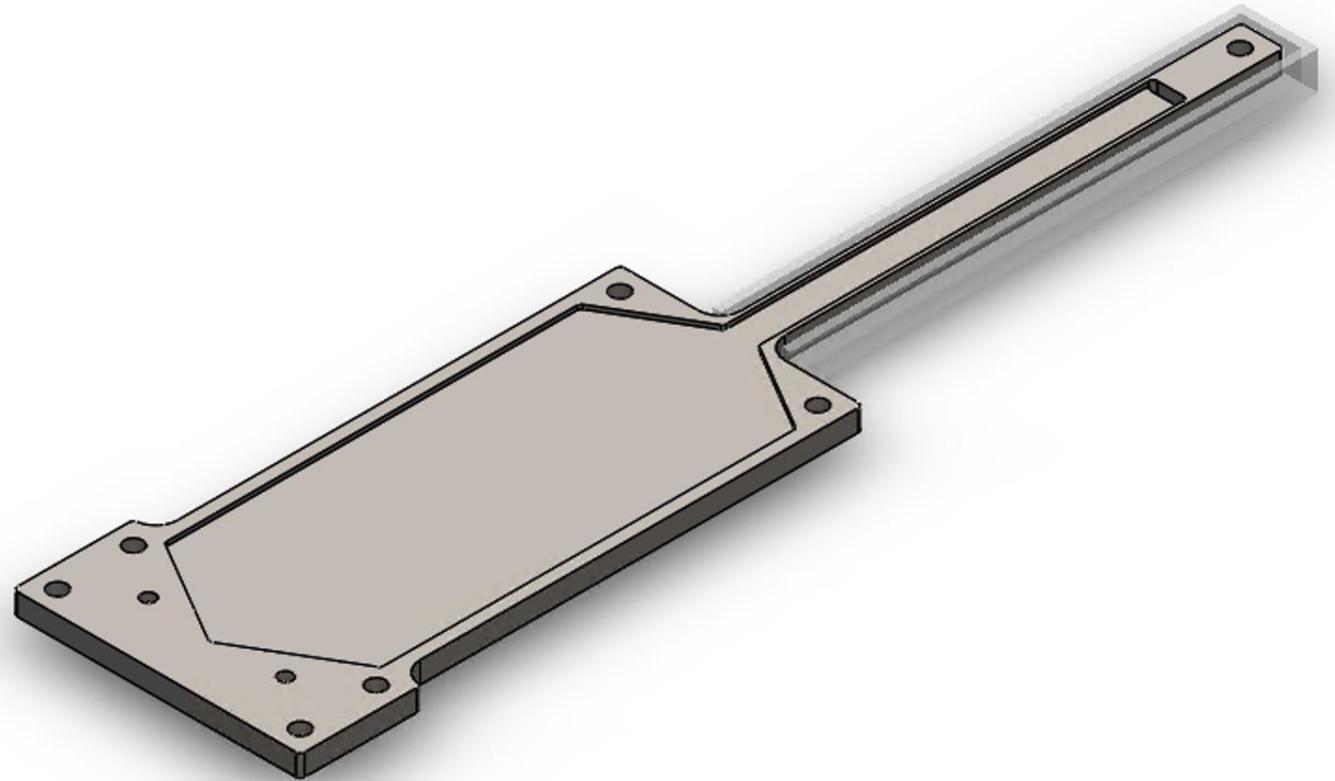
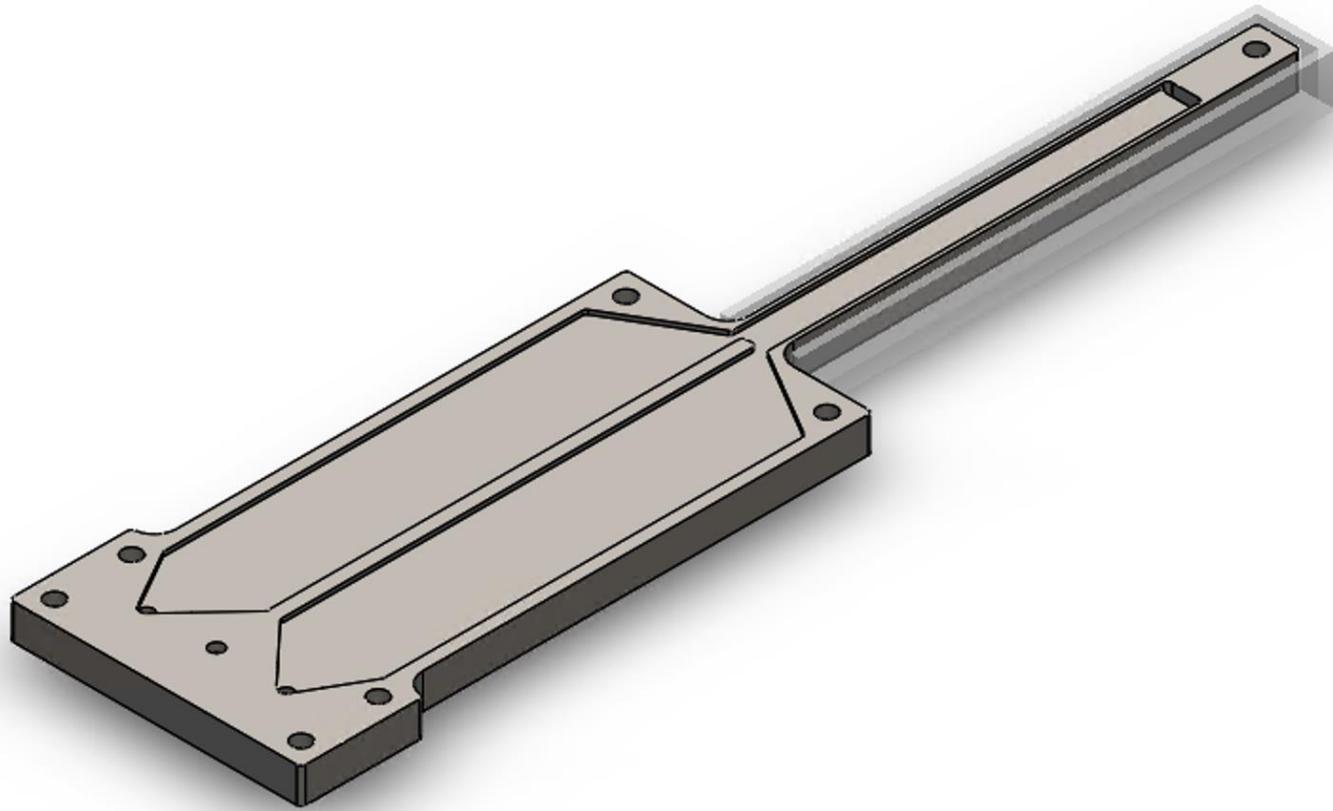
Staged injection for distributing heating



Metric	Value
Max solid temp	2500K
Max fluid temp	3281K
Max emitter wall temp	1985K
Emitter wall delT	353K
Heat out	538W
Outlet temp (ma)	2096K
Time	1:12 hr

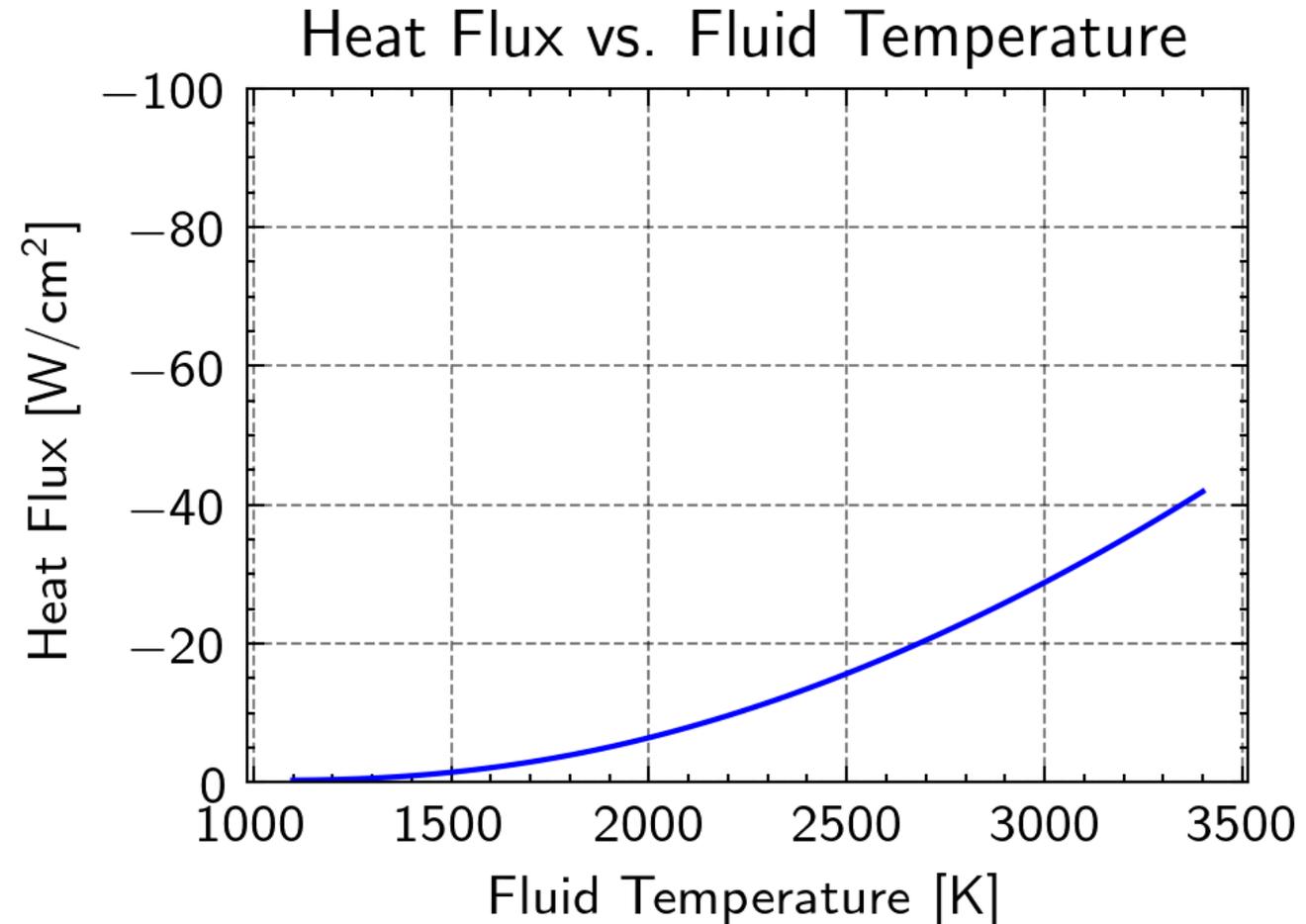
$$\eta_{comb} = \frac{538W}{600W} = 44.8\%$$



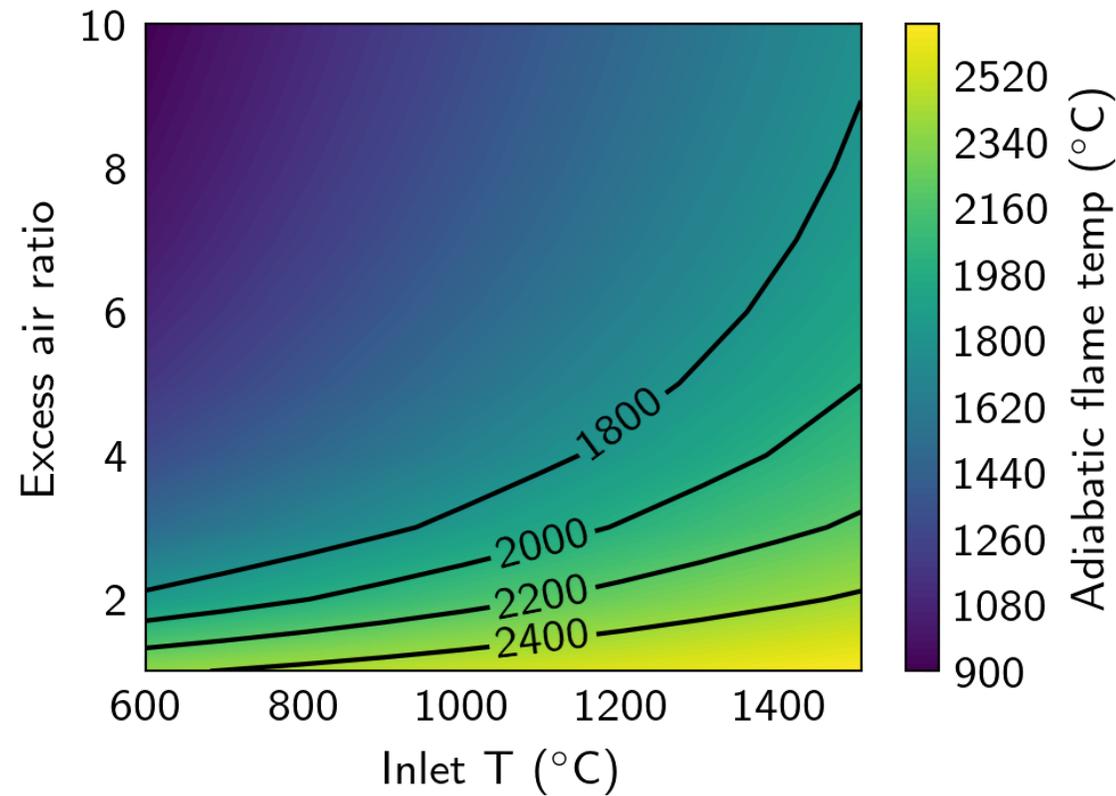


out-of-plane heat flux (theory)

- 2D geometry only has heat extraction from edges
- In reality (3D), heat extracted from top/bottom surfaces too
- Create a volumetric heat sink term as a proxy



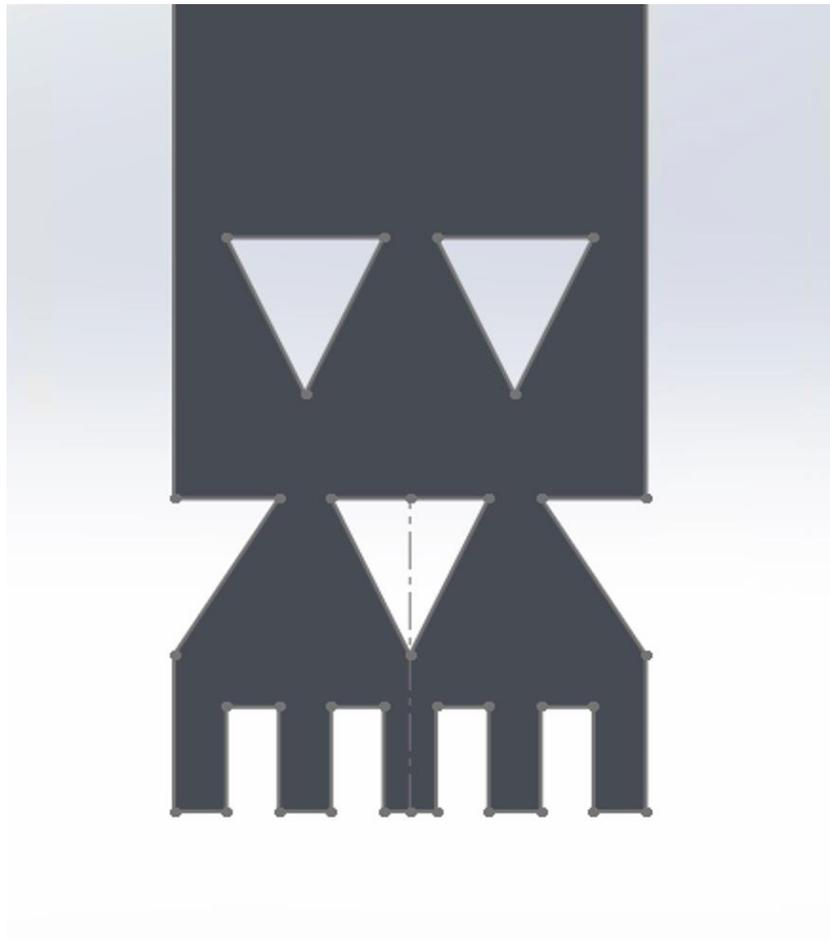
Effect of EAR on adiabatic flame temp of well-mixed reactants



Heat flux vs. wall temp

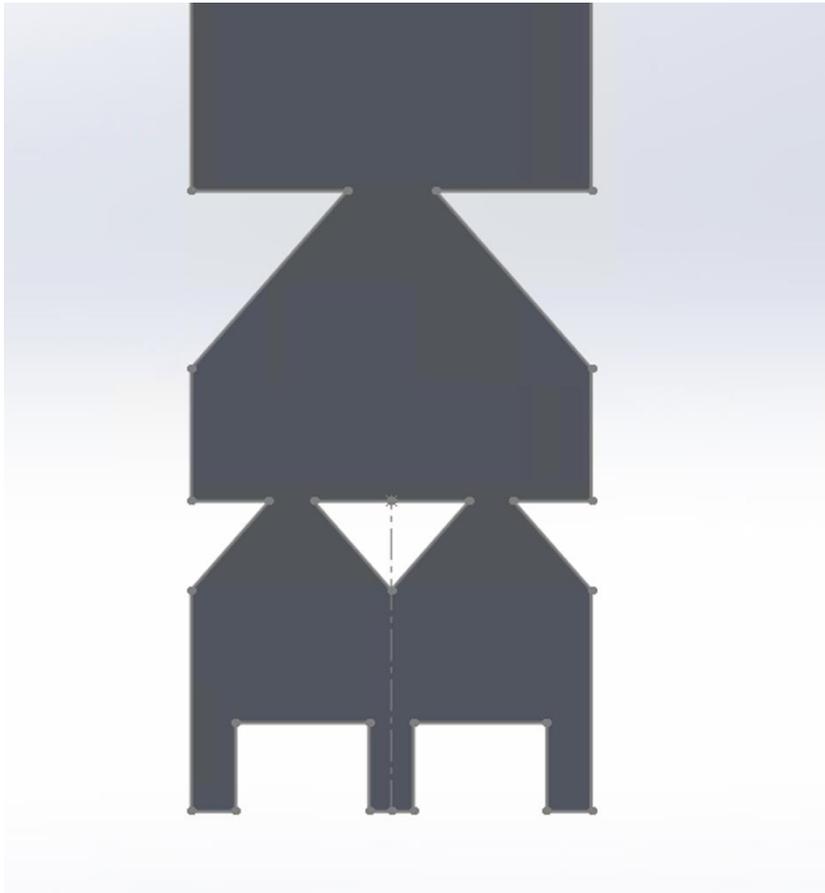
Bluff-body (5-2-3)

- CAD



Metric	Value
Max solid temp	
Max fluid temp	
Max emitter wall temp	
Emitter wall delT	
Heat out	
Outlet temp (ma)	
Time	

Bluff body (3-2-1)



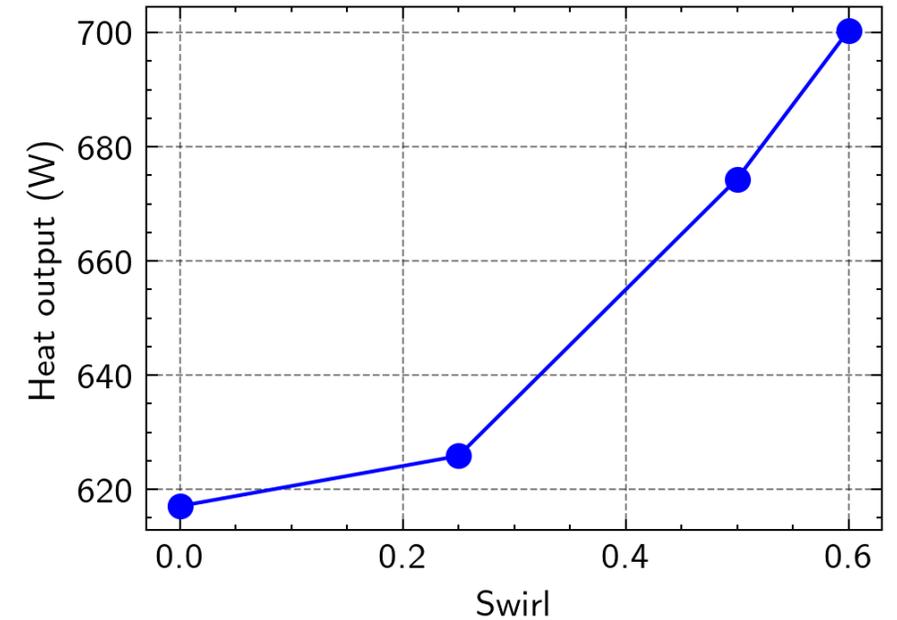
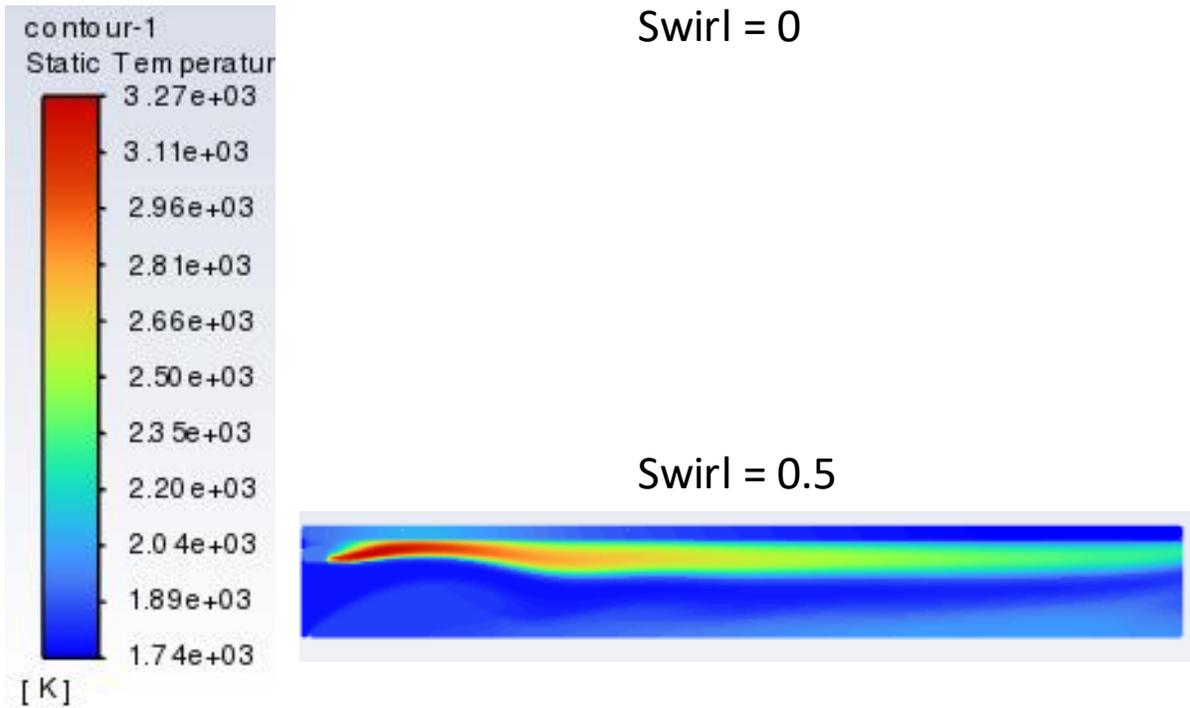
Metric	Value
Max solid temp	
Max fluid temp	
Max emitter wall temp	
Emitter wall delT	
Heat out	
Outlet temp (ma)	
Time	

Wall improvement

- CAD

Adding swirl helps increase heat output

Swirl helps flame remain close to wall



2D axisymmetric swirl with sloped wall

Preliminary technoeconomic analysis