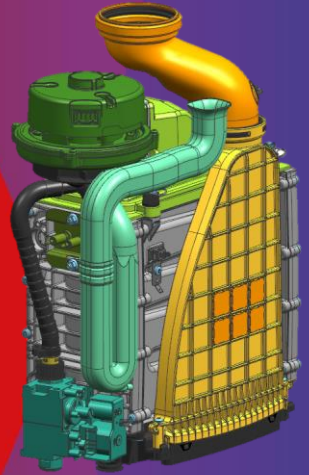
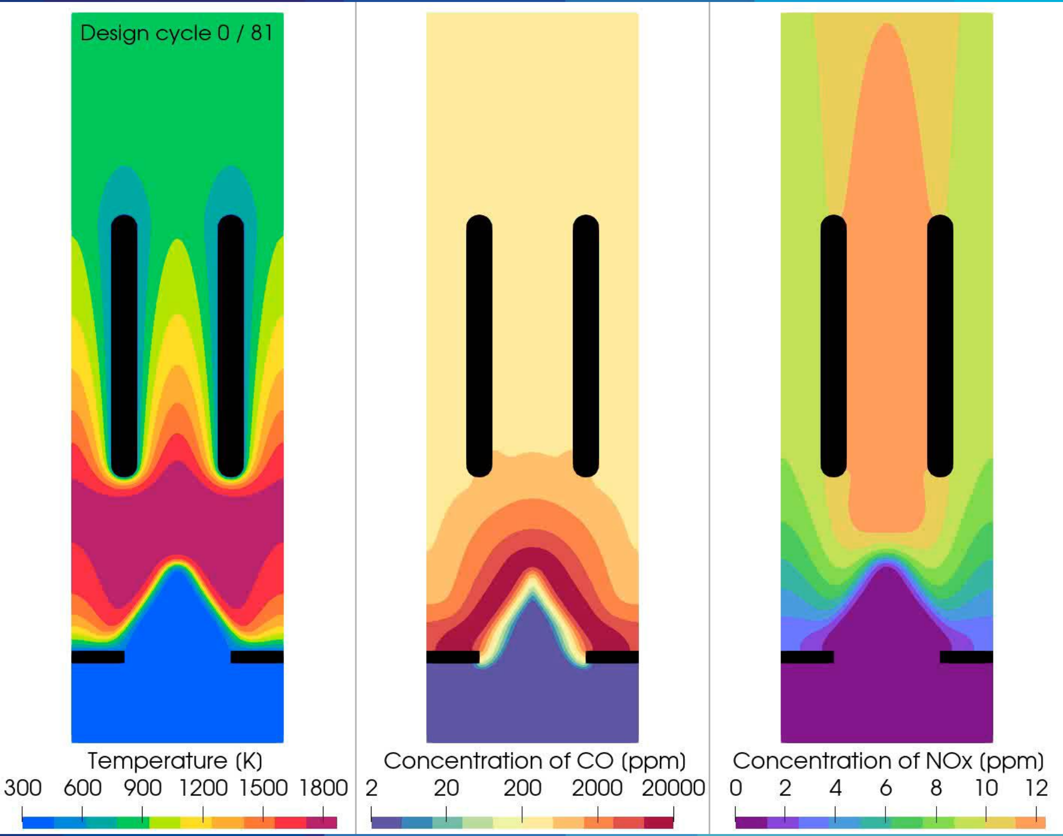
AUTOMATIC DESIGN OPTIMIZATION FOR HYDROGEN BOILERS





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EINDHOVEN UNIVERSITY OF TECHNOLOGY

BOSCH

H_2 IN THE BUILT ENVIRONMENT

H_2 VS. NATURAL GAS

MODELLING H_2

ADJOINT DESIGN OPTIMIZATION

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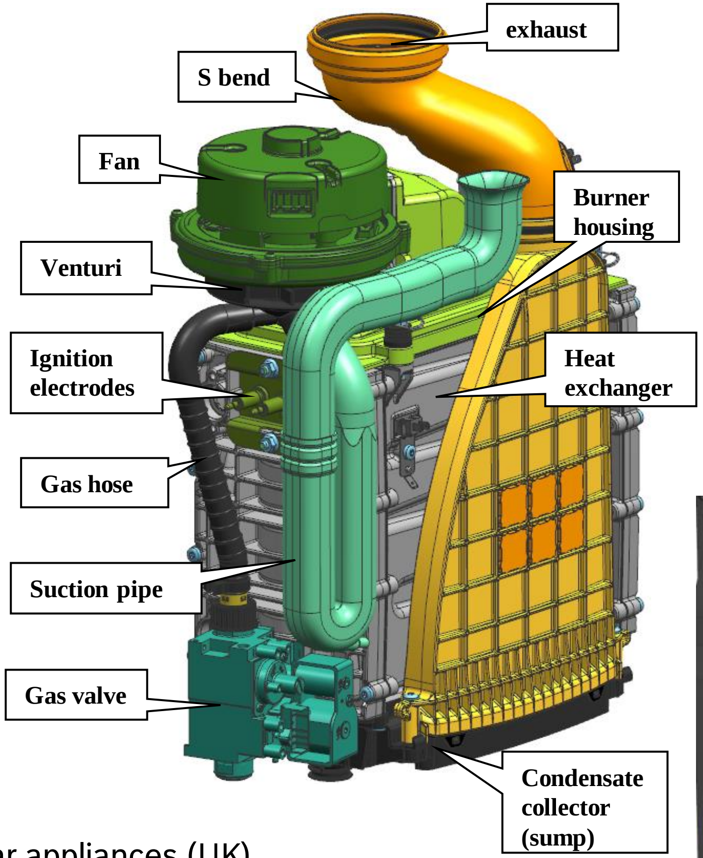
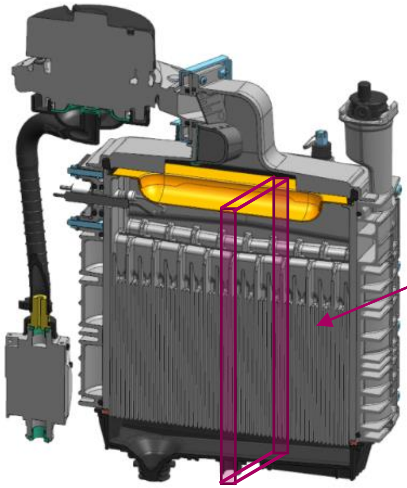
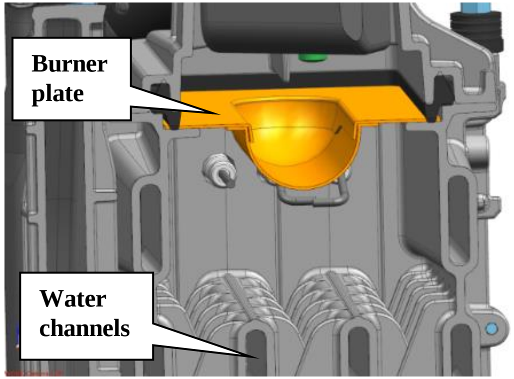
Introduction – domestic boilers





A slice of the heat exchanger is simulated to assess performance and improve design



- WB7 Heat exchanger (7-37 kW)
- Used in Trendline (NL) and Greenstar appliances (UK)

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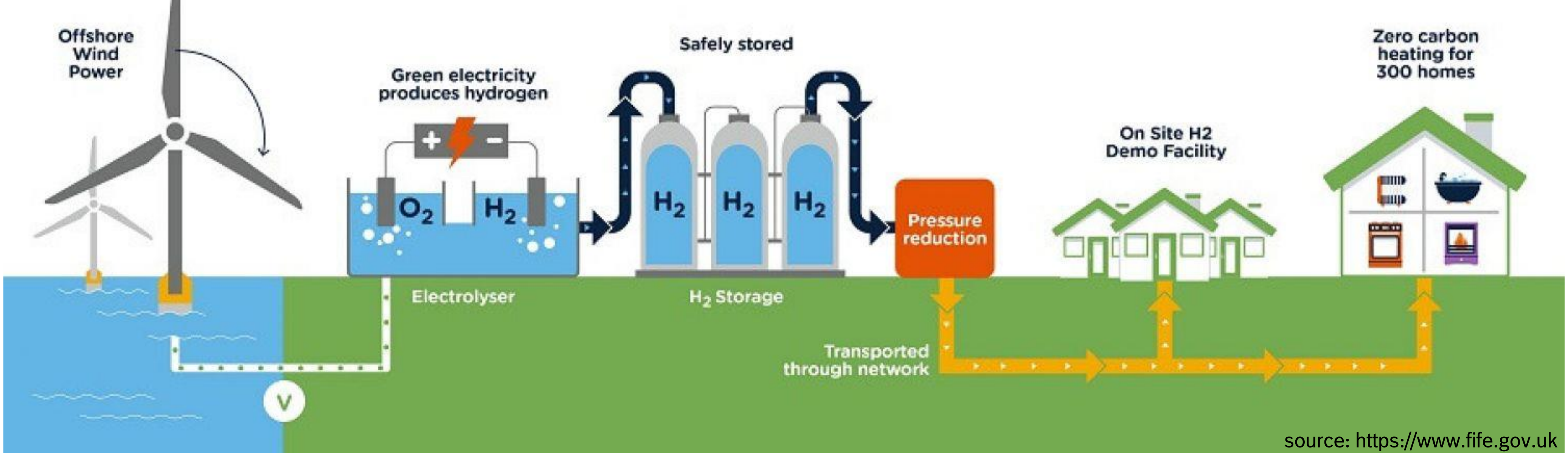
H_2 in the built environment

SGN
H100 Fife



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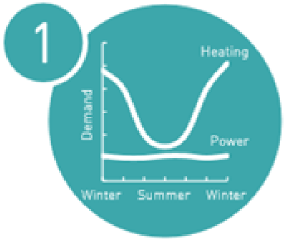
H_2 in the built environment

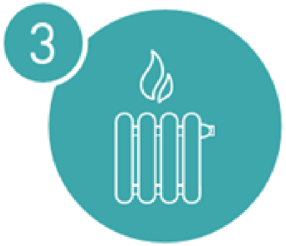


Full direct electrification of heating not feasible

Would require significant increase in power generation and grid capacity that is used only in the winter

Compatible with existing building stock compared to use of heat pumps

90% of all buildings emissions result from buildings older than 25 years



Infrastructure, skills and regulations already available and ready to be leveraged

40% of all European households have gas heating as of today making fast and convenient implementation possible

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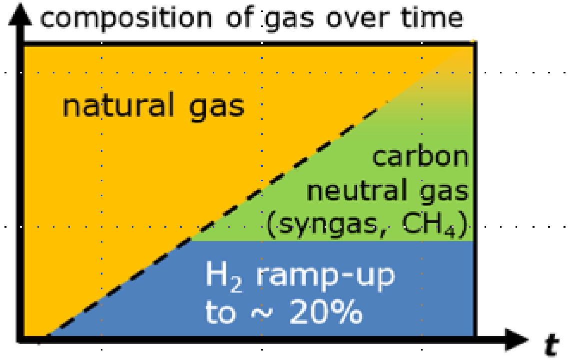
H_2 in the built environment

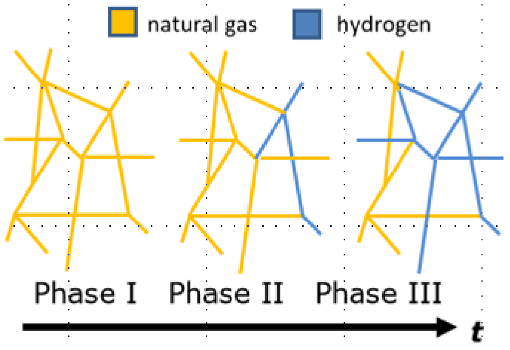
Scenario A: blending

- Use existing gas grid and make it suitable for H2NG blends
- Increase share of syngas and biomethane + Hydrogen
- Use existing combustion technology and validate it against new gas quality spec.



Scenario B: H_2-islands

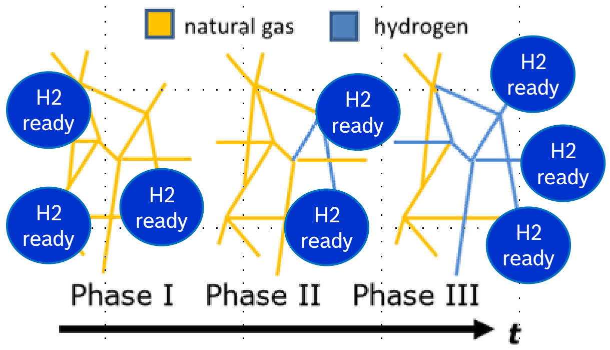
- Successive upgrade of existing gas grid sections to closed local hydrogen nets.
- Increase islands step by step
- Boundary: H2 supply & CAT 1 product installation at the same time



CAT 1= gas application Hydrogen only

Scenario C: H_2-ready products

- Gas applications are designed for pure hydrogen combustion, but installed in natural gas setting: CAT 2 application
- Gas grid is upgraded step by step, installed stock is prepared



CAT 2= gas application Hydrogen ready, factory setting natural gas

There are 3 scenarios to use hydrogen in the heating market to reduce CO_2 emissions.

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H_2 IN THE BUILT ENVIRONMENT

H_2 VS. METHANE

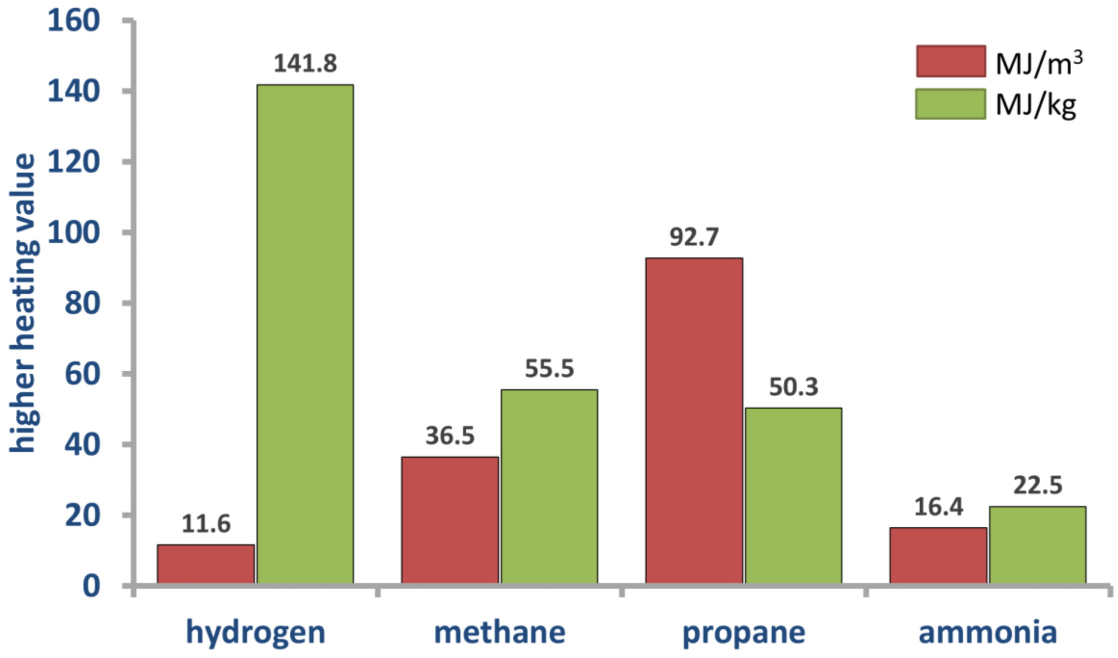
MODELLING H_2

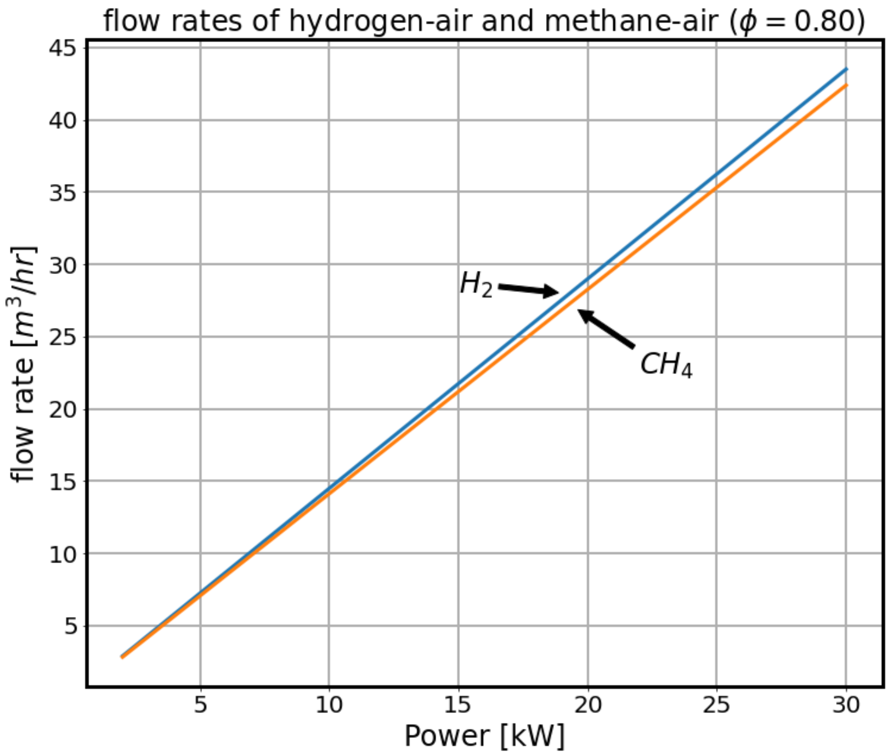
ADJOINT DESIGN OPTIMIZATION

Hydrogen vs. methane

$CH_4 + 2O_2 \rightarrow CO_2 + 2H_2O$

$H_2 + ½\ O_2 \rightarrow H_2O$





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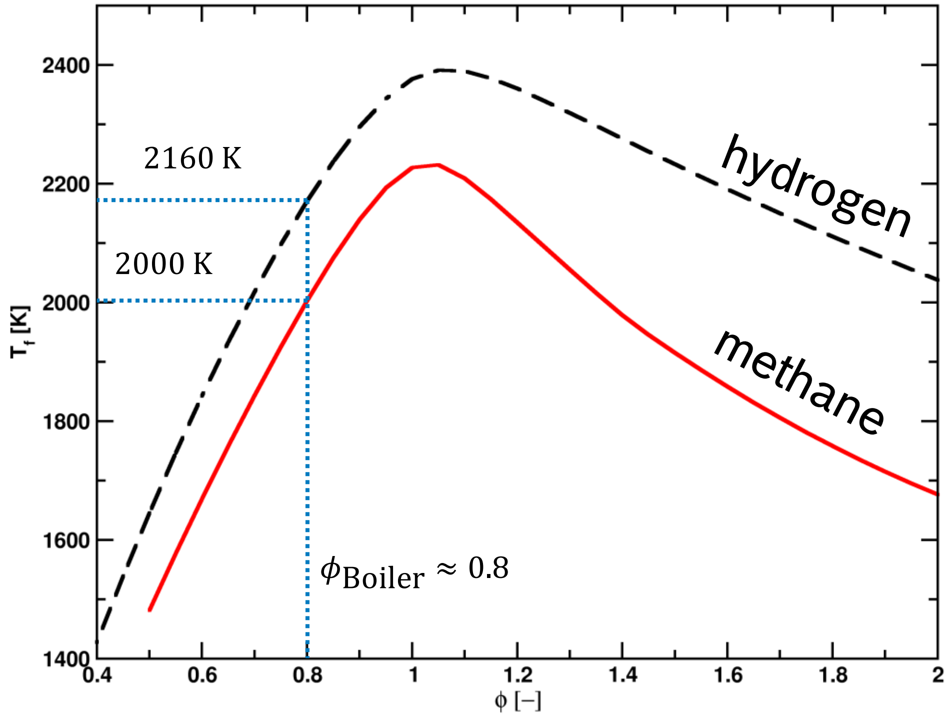
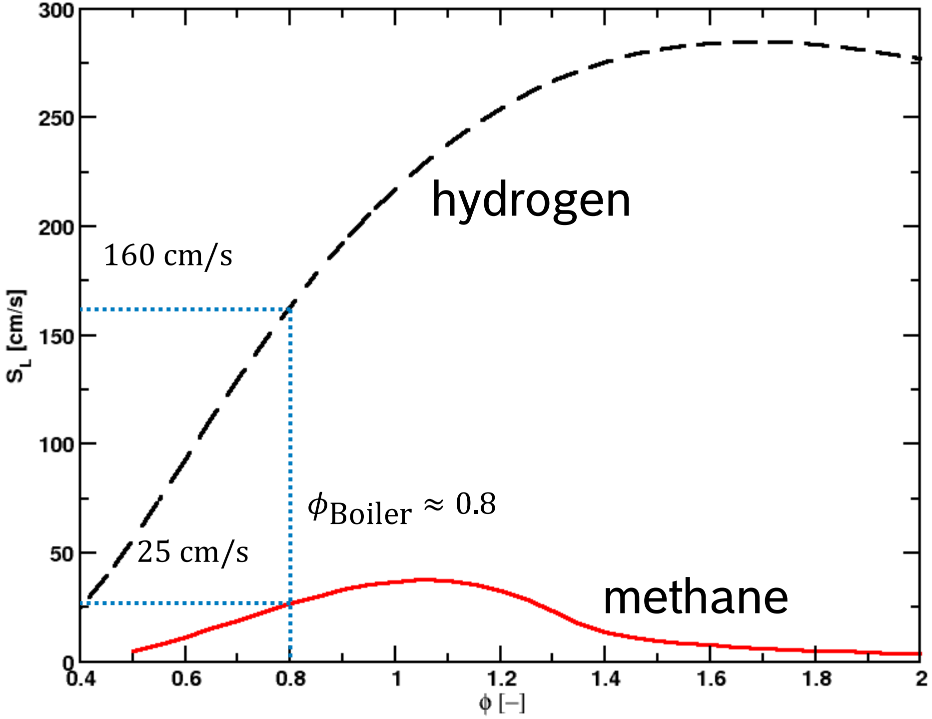
Hydrogen vs. methane

Flame temperature



Flame speed



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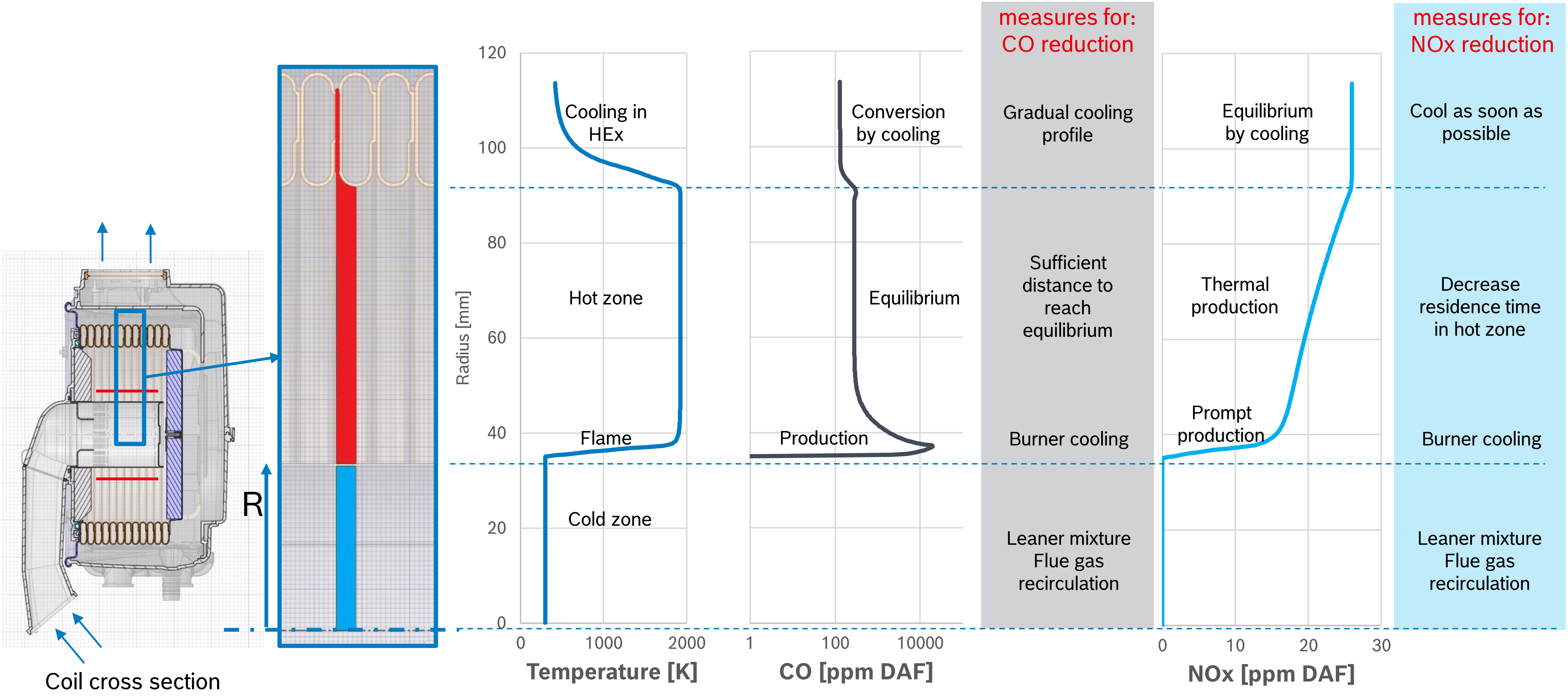
Hydrogen vs. methane - emissions



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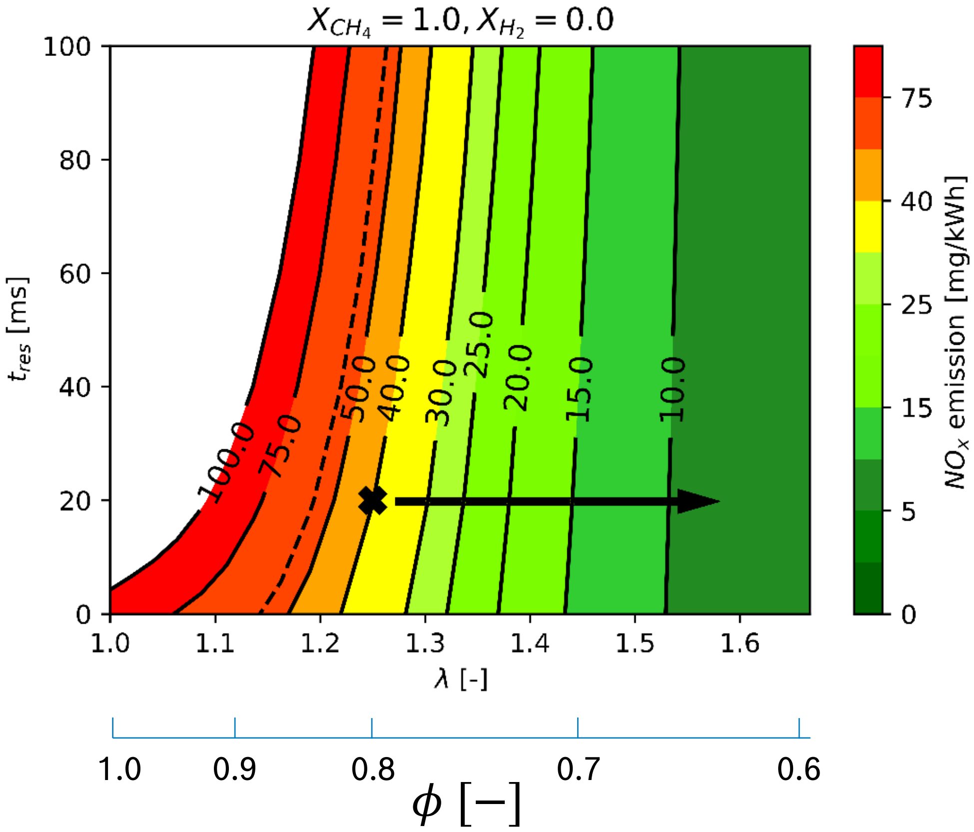
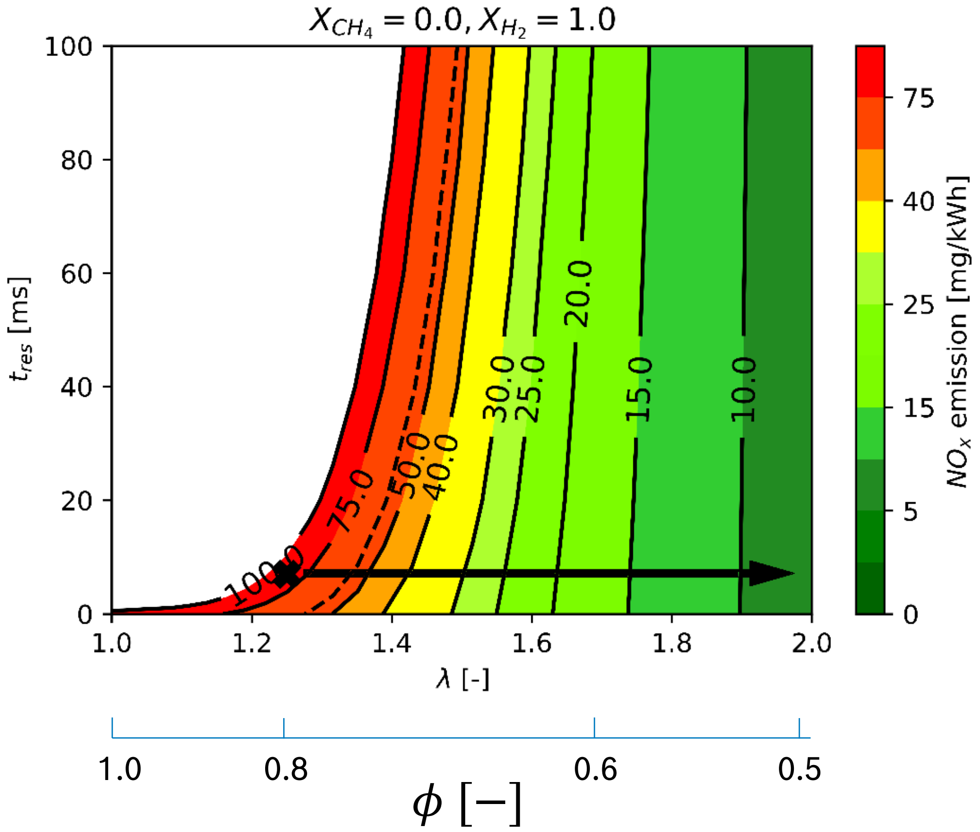
Hydrogen vs. methane
NO_x emissions





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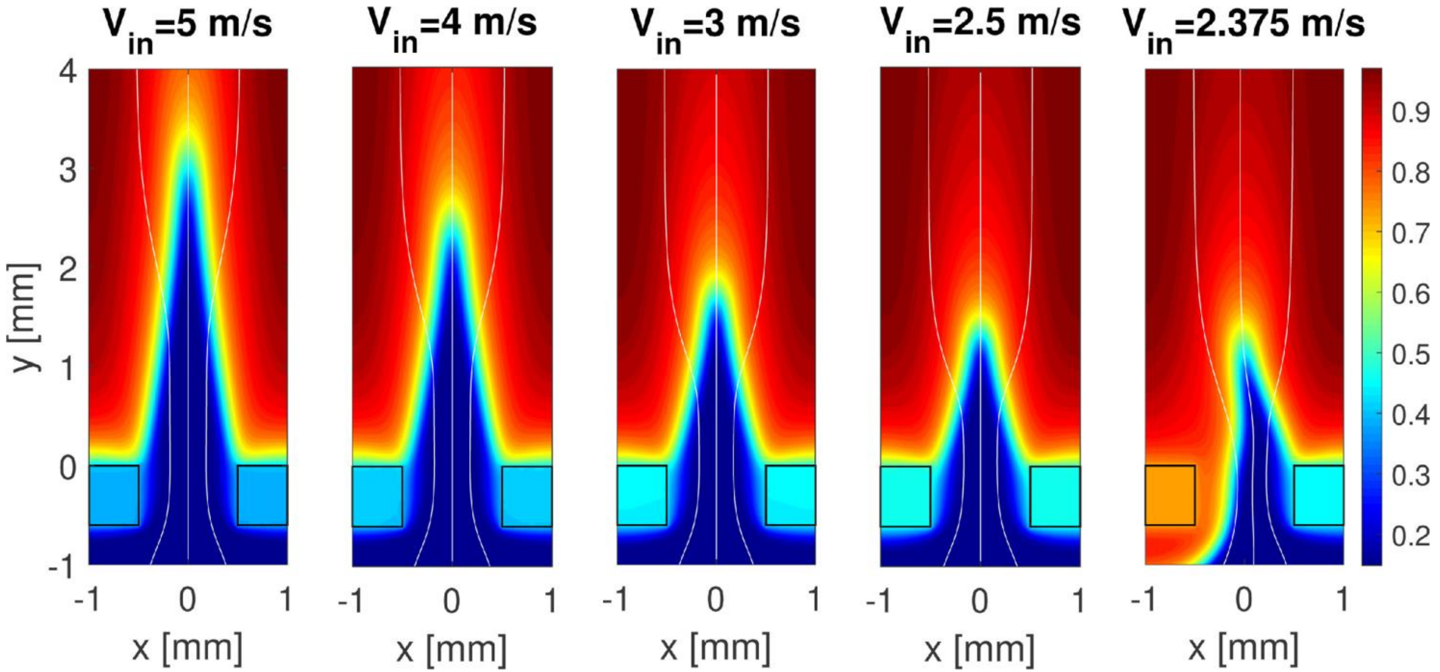
Hydrogen vs. methane
Hydrogen flash back



Vance et al. *Combust. flame* (2022)

For more on hydrogen flash-back, see the presentation of Sikke Klein

H_2 IN THE BUILT ENVIRONMENT
H_2 VS. NATURAL GAS
MODELLING H_2
ADJOINT DESIGN OPTIMIZATION

Modelling H_2
For combustion simulations we need the chemical reactions

One step reaction: $H_2 + ½ O_2 \rightarrow H_2O$

But: Detailed description of hydrogen-air combustion consists of many reactions involving many species being produced during the reaction, e.g. The mechanism from Galway:

44 SPECIES: AR N2 HE H2 H O2 O H2O OH OHV H2O2 HO2 CO CO2 HOCO CH4 CH3 OCHO C2H6 N NO NOV NO2 N2O NH3 HNO HON HONO H2NO NNH NH2 NH HNOH NO3 HONO2 HNO3 N2H2 N2H3 N2H4 H2NN NH2OH HNO2 N2O4 N2O3

- **251 reactions:**
- (1) $H_2 + M \leftrightarrow H + H + M$
- (2) $H_2 + O \leftrightarrow H + OH$
- (3) $H_2 + OH \leftrightarrow H + H_2O$
- ...
- (251) $H_2NN + NH_2 \leftrightarrow NNH + NH_3$

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Modelling H_2
Detailed chemistry simulations

Conservation equations:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \boldsymbol{u}) = 0,$$

$$\frac{\partial (\rho \boldsymbol{u})}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} \otimes \boldsymbol{u}) + \nabla p - \nabla \cdot \boldsymbol{\tau} = 0,$$

Species transport

$$\frac{\partial (\rho Y_i)}{\partial t} + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{u} Y_i) + \boldsymbol{\nabla} \cdot (\rho \boldsymbol{V}_i Y_i) = \dot{\omega}_i,$$

$$\frac{\partial (\rho c_p T)}{\partial t} + \nabla \cdot (\rho \boldsymbol{u} c_p T) - \nabla \cdot (\lambda \nabla T) + \rho \nabla T \cdot \sum_{i=1}^{n} c_{p,i} Y_i \boldsymbol{V}_i = \dot{\omega}_T$$

Coupled system:

$$\dot{\omega}_i = W_i \sum_{r=1}^{n_r} \nu_{i,r} K_r \prod_{j=1}^{n_{sp}} \left(\frac{\rho Y_j}{W_j} \right)^{\nu'_{j,r}}$$

difficulty:

- large number of equations
- stiffness of equations
- small mesh size (thin reaction zones)

} high computational cost

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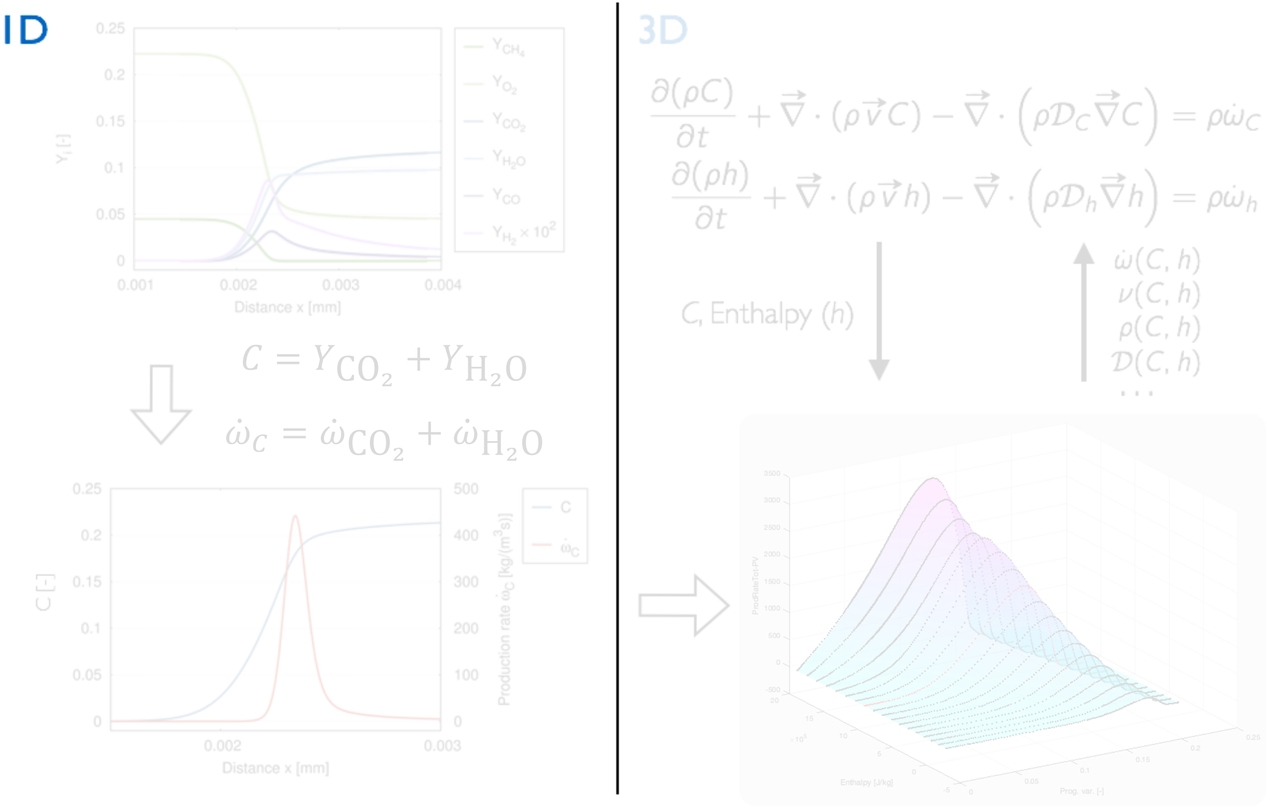
Modelling H_2
Combustion modeling: The flamelet approach

Idea: Map detailed 1D simulation results in 3D space using problem specific parameters:

here: progress variable ***C*** and enthalpy ***h***

- Compute 1D simulations
- Tabulate 1D solutions as functions of progress variable *C* and enthalpy *h*
- Solve 3D transport equations for *C* and *h* using table look-ups to obtain values for source terms and physical quantities



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Modelling H_2
Emission models

Accuracy of Y_{CO} and Y_{NO} in the lookup table can be low for strong cooling.

➔ Transport equations for Y_{CO} and Y_{NO} with source term correction[2]

Consider generic reaction equation for emission consumption:

Reaction # c: $EM + B \rightarrow C + D$, with $EM = \{\mathrm{CO}, \mathrm{NO}\}$

$$\dot{\omega}_{EM} = W_{EM} \sum_{r=1}^{n_r} \nu_{EM,r} K_r \prod_{j=1}^{n_{sp}} \left(\frac{\rho Y_j}{W_j}\right)^{\nu'_{j,r}} = \underbrace{W_{EM} \sum_{r=1, r\neq c}^{n_r} \nu_{EM,r} K_r \prod_{j=1}^{n_{sp}} \left(\frac{\rho Y_j}{W_j}\right)^{\nu'_{j,r}}}_{\dot{\omega}^{+}_{EM}} + \underbrace{W_{EM} K_c \rho^2 \frac{Y_{EM}}{W_{EM}} \frac{Y_B}{W_B}}_{\dot{\omega}^{-}_{EM}}$$

$$\dot{\omega}^{3\mathrm{D}}_{EM} = \dot{\omega}^{+,1\mathrm{D}}_{EM} + \frac{\dot{\omega}^{-,1\mathrm{D}}_{EM}}{Y^{1\mathrm{D}}_{EM}} Y^{3\mathrm{D}}_{EM}$$

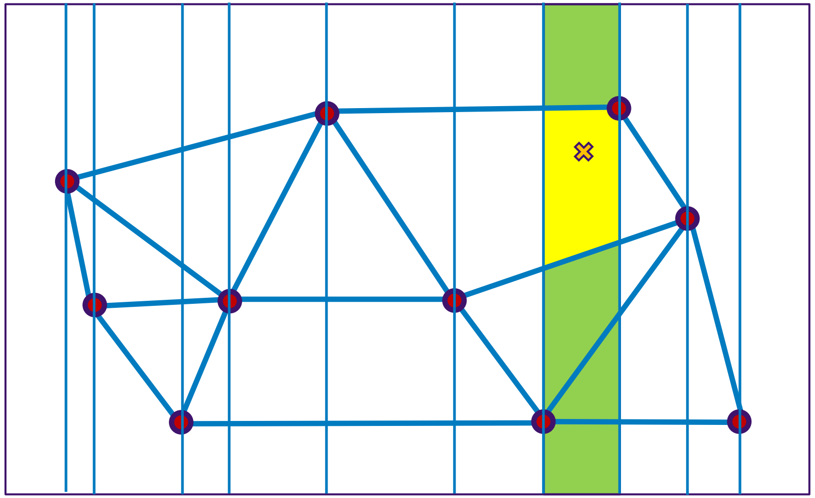
Stored in chemistry table

Solved using transport equation

[2]: M. Ihme, H. Pitsch, Physics of Fluids 20, 055110 (2008)

Modelling H_2
tabulation: slab approach

- We need point location in a table
- We want to be smarter than loop over all cells and check if the point is inside
- first idea: partition into vertical slabs
  - find correct slab (binary search over the slabs)
  - loop over the segments inside the slab to determine point location (also binary search)
  - time to find cell: $O(\log(n))$
  - memory requirement: worst case $O(n^2)$



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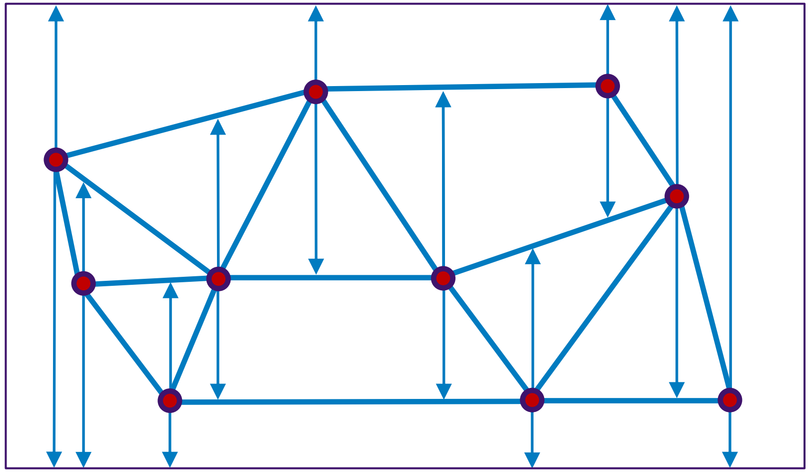
Modelling H_2
smarter tabulation: trapezoidal map

- divide into trapezoids:
  - from each node, create a vertical edge up and down until you hit an edge
  - results in trapezoids or triangles (degenerate trapezoid)
  - Data stored in Directed Acyclic Graphs (DAG)
  - time to find cell: O(log(n))
  - lower cell count
  - memory requirement: worst case O(n)
  - Points inside a cell: interpolation using barycentric coordinates
  - Points outside the mesh: projected onto the convex hull



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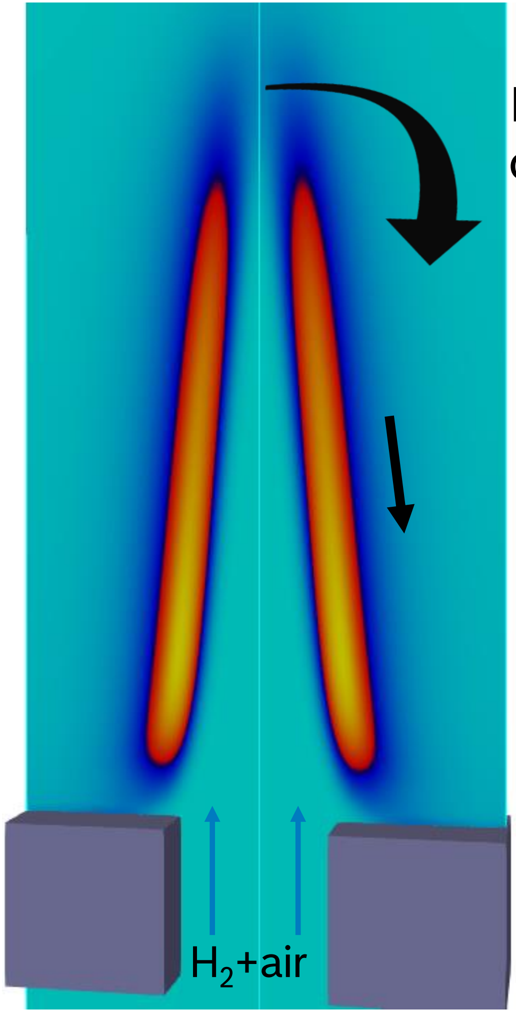
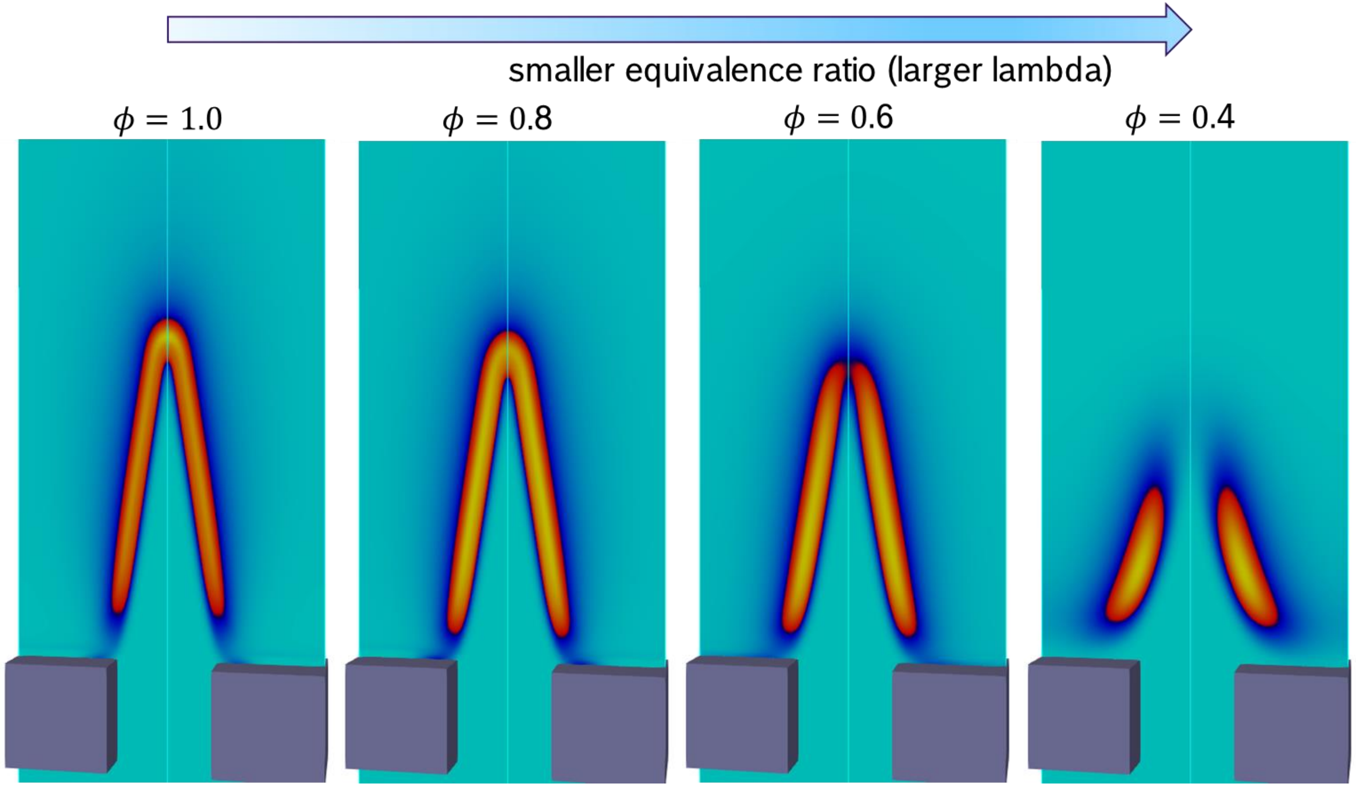
Modelling H_2 – preferential diffusion



Hydrogen diffuses out of the flame tip...

And moves towards the flame base



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Modelling H_2 - preferential diffusion

$$\frac{\partial \rho Y_k}{\partial t} + \frac{\partial}{\partial x_i}\left(\rho\left(u_i + V_{k,i}\right)Y_k\right) = \dot{\omega}_k, \qquad k = 1, \dots, N$$

diffusion velocity

Fick's law of binary diffusion:

$$Y_1 \overline{V}_1 = -D_{12} \nabla_x Y_1$$

binary diffusion of species 1 into species 2

Stefan-Maxwell equation:

$$\nabla_x X_i = \sum_{j=1}^{N} \frac{X_i X_j}{D_{ij}} \left(\overline{V}_j - \overline{V}_i\right), \qquad i = 1..N$$

$$X_k = \frac{W}{W_k} Y_k$$

binary diffusion of species *i* into species *j*

first order approximation: $X_k \overline{V}_k = -D_k \nabla_x Y_k$

Curtiss- Hirschfelder

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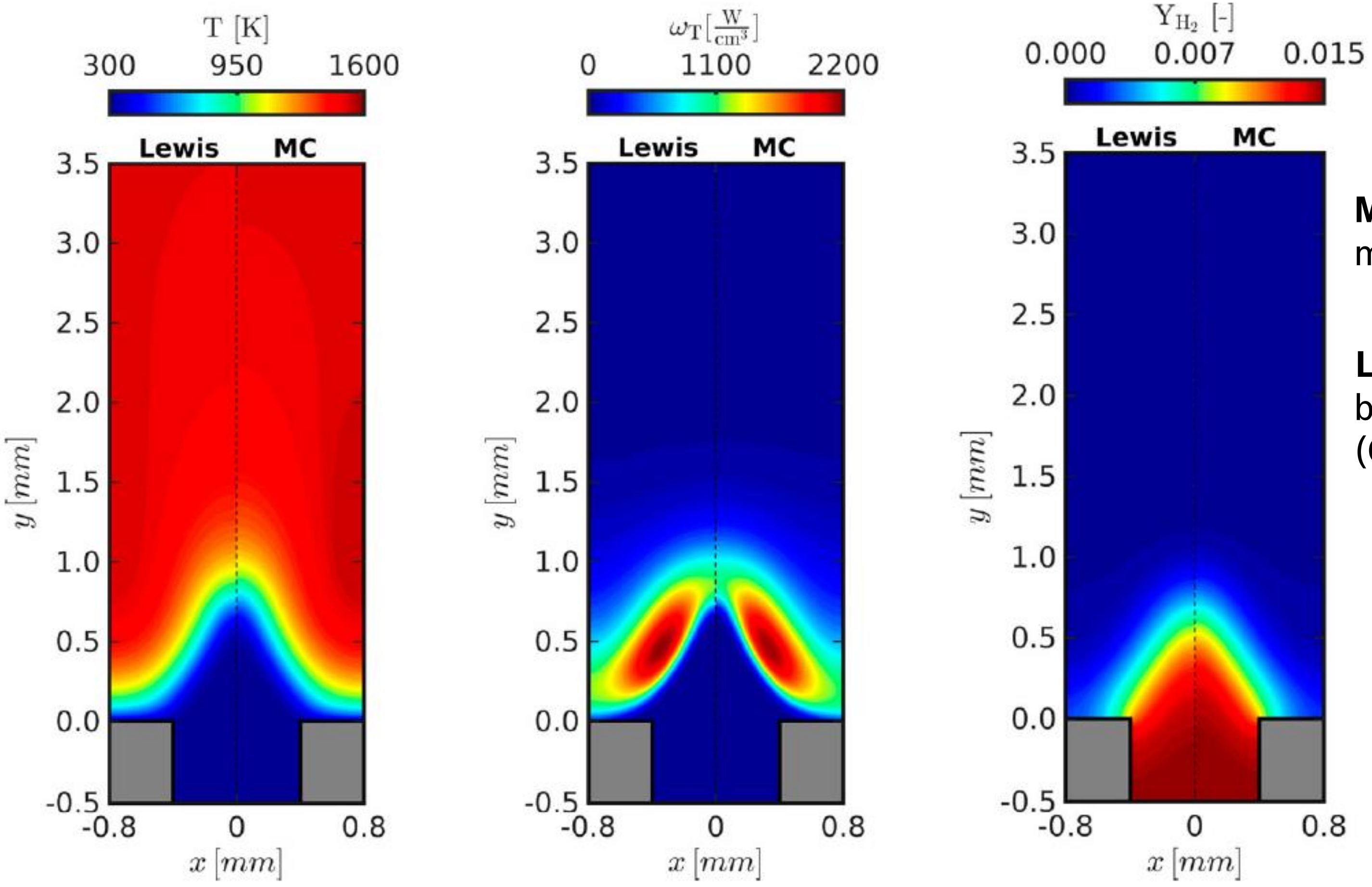
Modelling H_2 – preferential diffusion



MC: **m**ulti**c**omponent diffusion model (Stefan-Maxwell equations)

Lewis: Lewis number is constant but varying for each of the species (Curtiss-Hirschfelder approximation)

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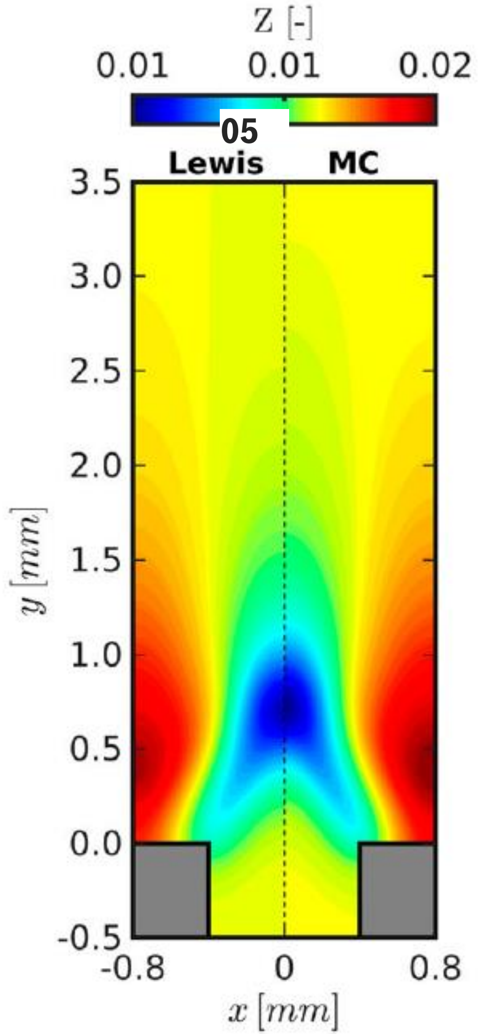
Modelling H_2 – preferential diffusion



Mixture fraction Z: mixedness of the fuel and air

Z = 0 : pure air

Z = 1 : pure fuel

Z = constant everywhere: perfectly premixed and constant fuel/air ratio (= constant equivalence ratio)

Z ≠ constant: new independent variable!

$$\frac{\partial \rho Z}{\partial t} + \nabla \cdot (\rho \mathbf{u} Z) - \nabla \cdot \left(\frac{\lambda}{c_p} \nabla \beta_Z \right) = 0,$$

$$\frac{\partial \rho h}{\partial t} + \nabla \cdot (\rho \mathbf{u} h) - \nabla \cdot \left(\frac{\lambda}{c_p} \beta_{h1} \nabla T + \frac{\lambda}{c_p} \nabla \beta_{h2} \right) = 0,$$

$$\frac{\partial \rho C}{\partial t} + \nabla \cdot (\rho \mathbf{u} C) - \nabla \cdot \left(\frac{\lambda}{c_p} \nabla \beta_C \right) = \omega_C$$

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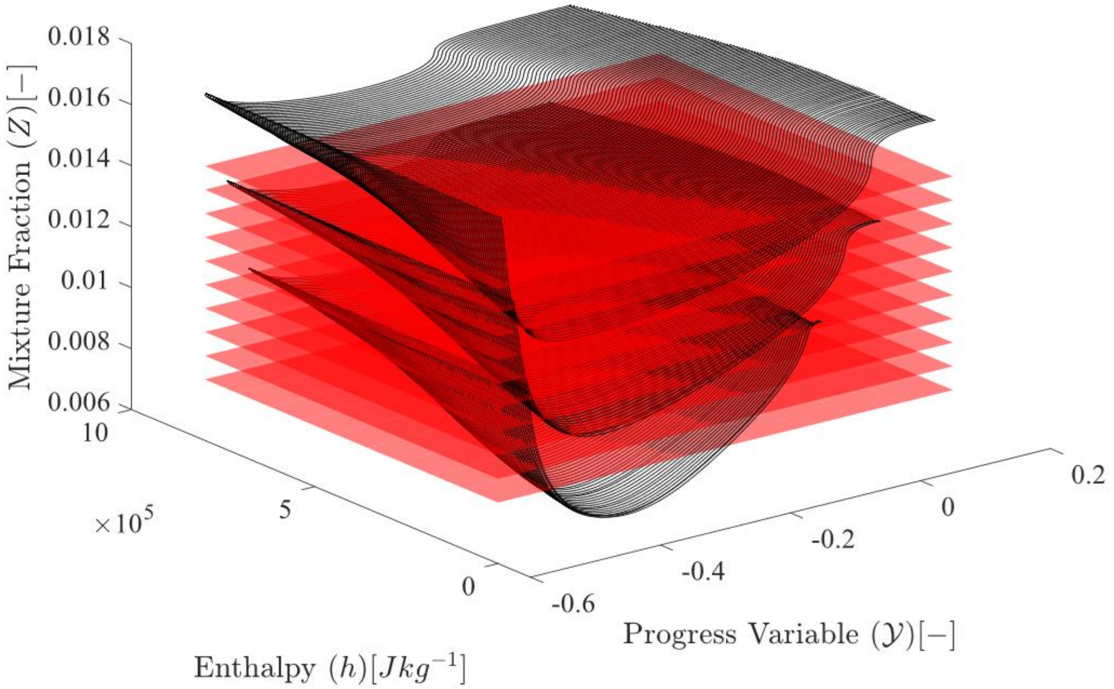
Modelling H_2
FGM - Extension to hydrogen combustion

General global reaction equation

$$\nu'_F \, C_m H_n + \nu'_{O_2} O_2 \rightarrow \nu''_{CO_2} \, CO_2 + \nu''_{H_2O} \, H_2O$$

$$Z = \frac{\frac{1}{mW_C} Z_C + \frac{1}{nW_H} Z_H + \frac{1}{\nu'_{O_2} W_O}\left(Y_{O_2,2} - Z_O\right)}{\frac{1}{mW_C} Z_{C,1} + \frac{1}{nW_H} Z_{H,1} + \frac{1}{\nu'_{O_2} W_O} Y_{O_2,2}}$$



➔ The equation for Z is fuel dependent. Current implementation includes equations for CH_4 and H_2.

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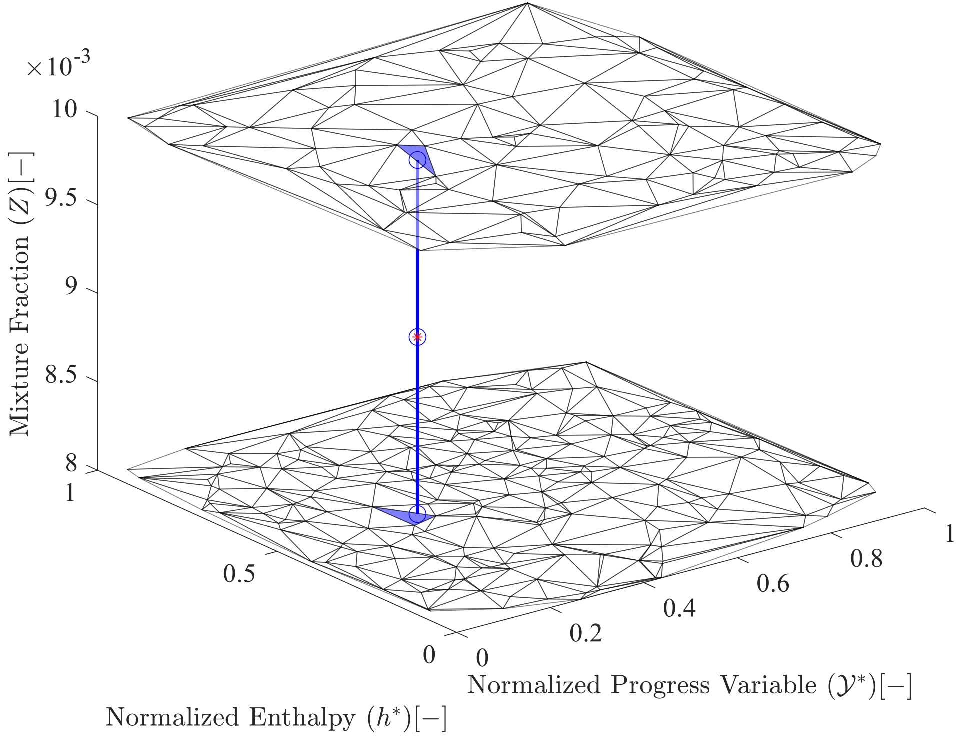
Modelling H_2
FGM – extension to hydrogen combustion

- 3D quasi-unstructured lookup:
  1. Find inclusion cells on mixture fraction levels.
  2. 2D data interpolation in inclusion triangles.
  3. Linear data interpolation along mixture fraction direction.



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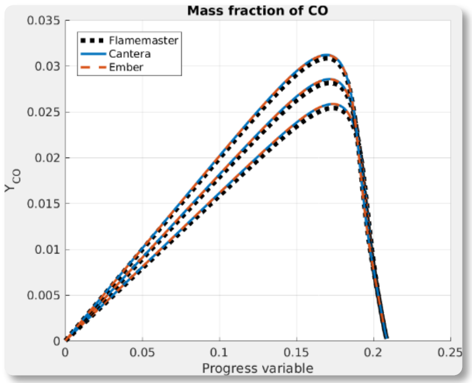
Modelling H_2
Combustion modeling: Tool chain

1. Perform 1D simulations with detailed chemistry

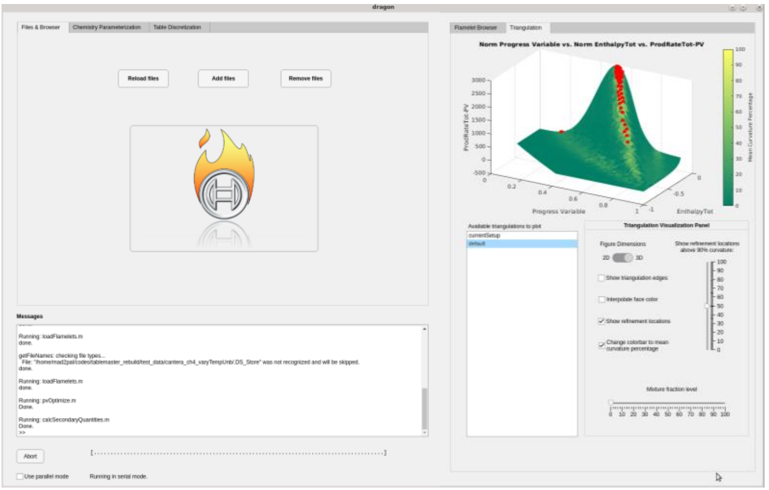
- Chem1D, Cantera & Ember
- Typically: ~50 PDEs coupled through ~300 coupled nonlinear reaction equations

Cantera / Ember
Chemical Kinetics • Thermodynamics • Transport Processes



2. Tabulate 1D solutions in look-up tables

- Tabulate as $f(C, Z, H)$
- Unstructured discretization
  - Local refinement for memory reduction
- In house developed MATLAB tool



3. Solve 3D transport equations

- SU2 solver suite
- Just 5 additional PDEs, reaction source terms from look-up tables
- C++ code base
- Automatic differentiation for adjoint gradients using CoDiPack

SU2

https://su2code.github.io/

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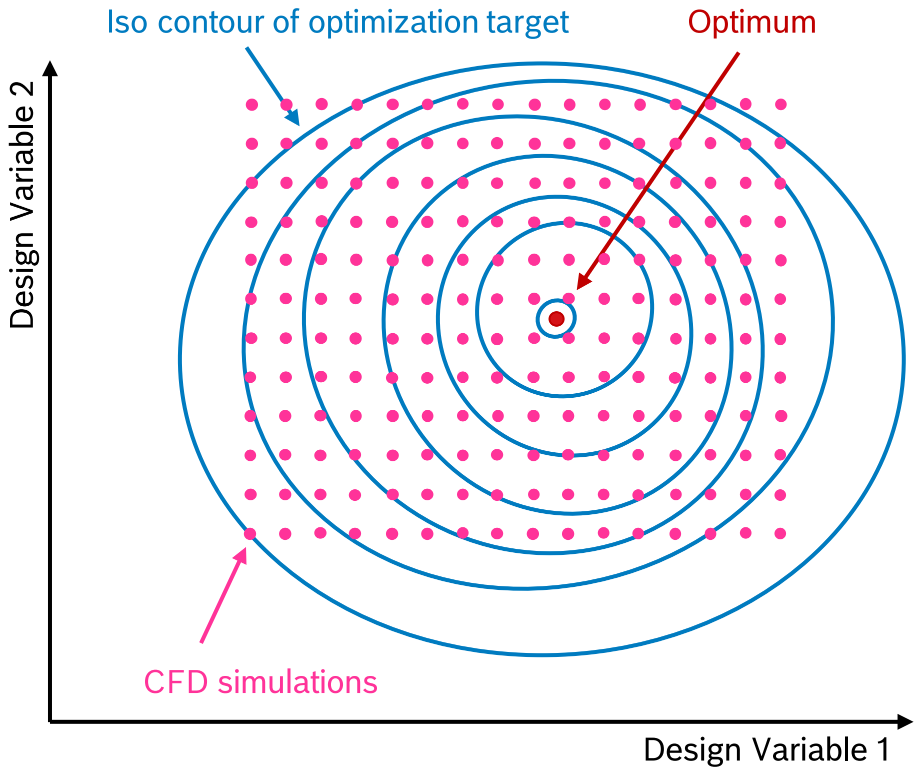
ADJOINT DESIGN OPTIMIZATION

Adjoint design optimization
Design of Experiments (DOE)



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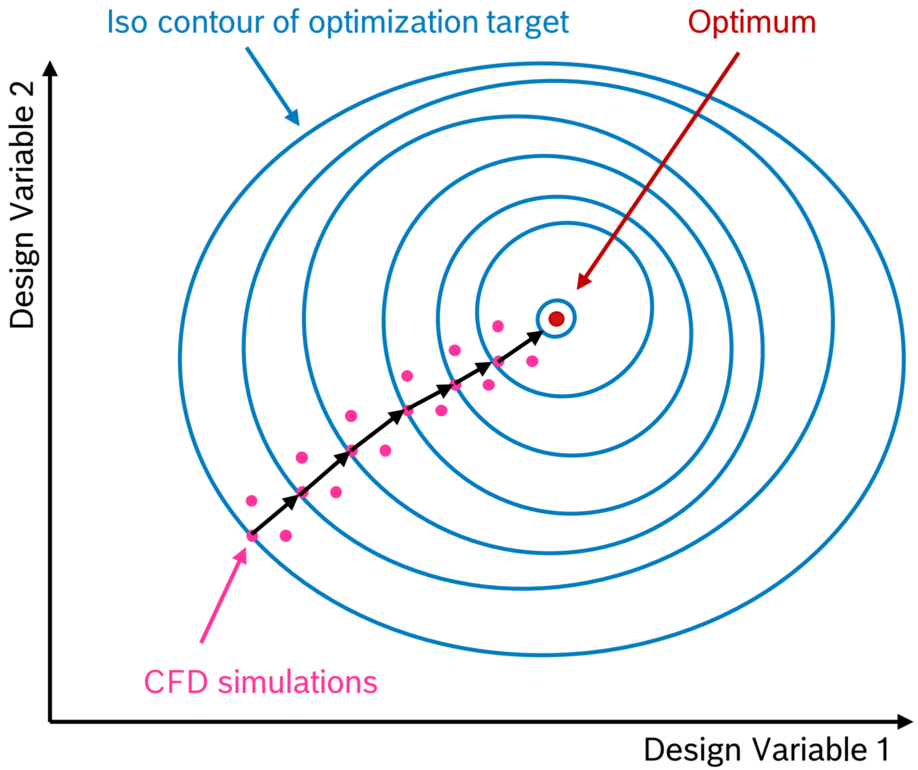
Adjoint design optimization
Gradient-based shape optimization



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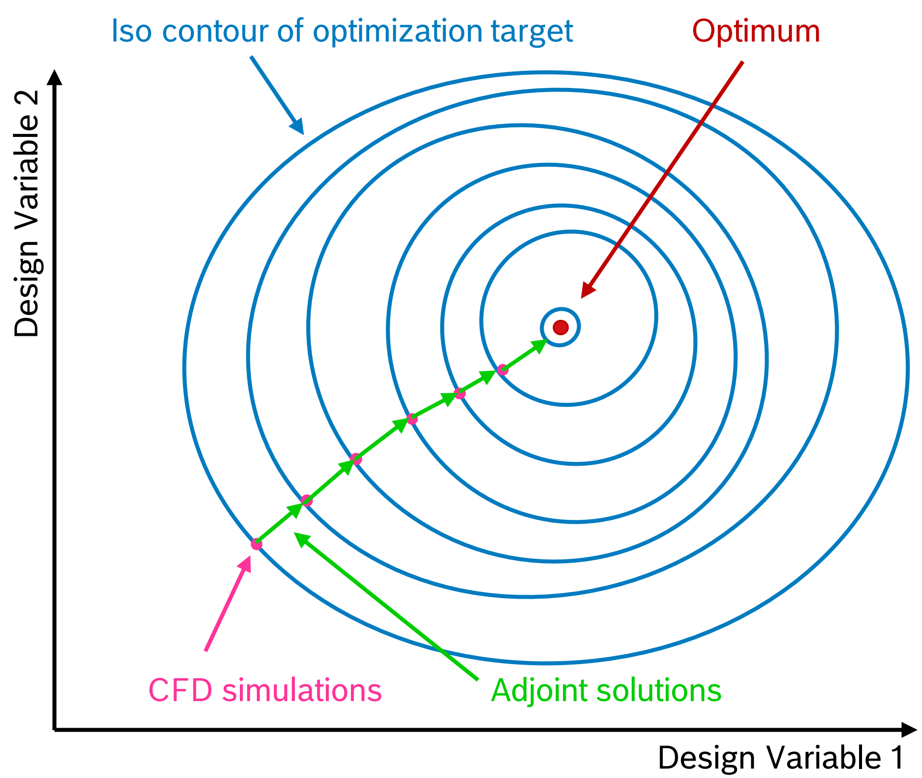
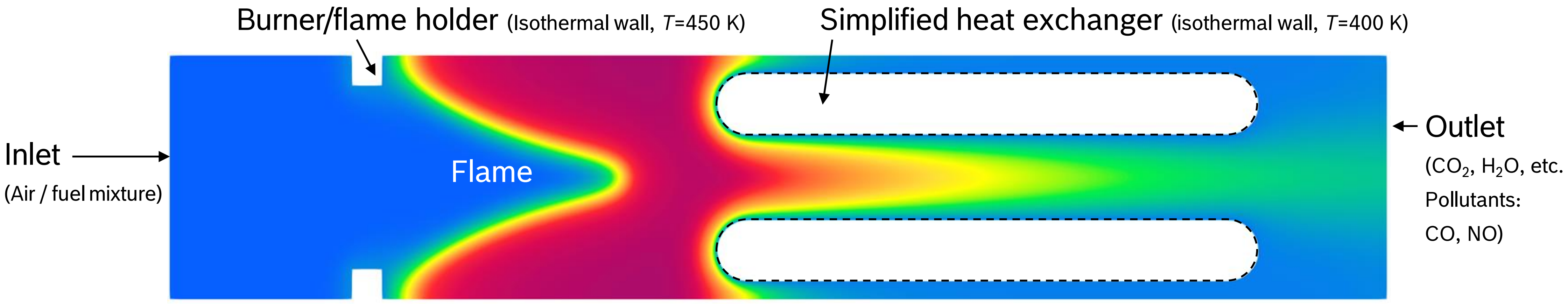
[1] DOE: Design of experiments

Adjoint design optimization
adjoint optimization



Adjoints can be used to very efficiently calculate gradients for an arbitrary number of design variables.

Adjoint design optimization
Objectives in design optimization



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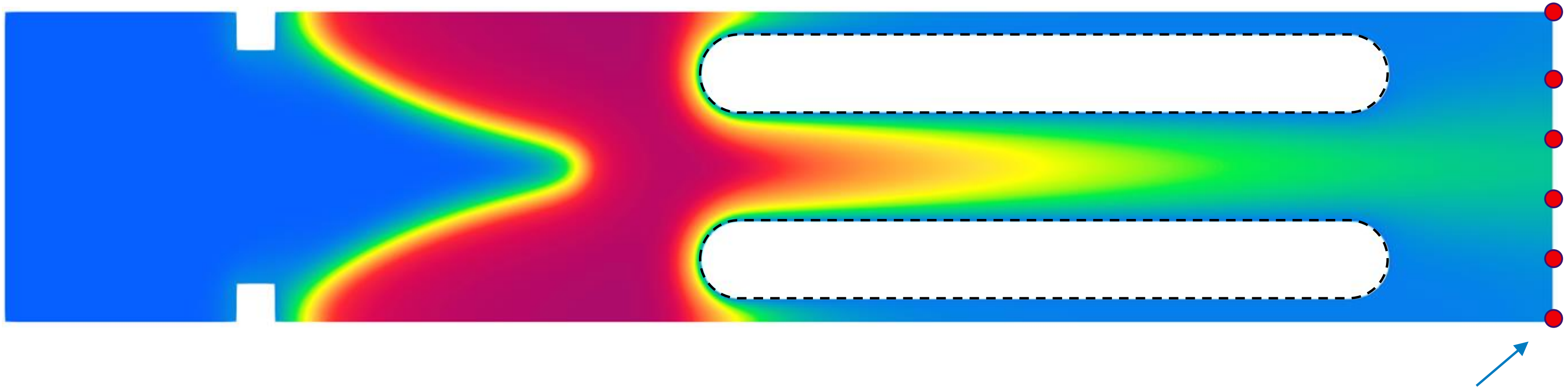
Adjoint design optimization
Objectives in design optimization



objective: minimize NO_x emissions at the outlet

objective: J

$$\min(J) = \sum Y_{NO_x}(x_{out}, y_i)$$

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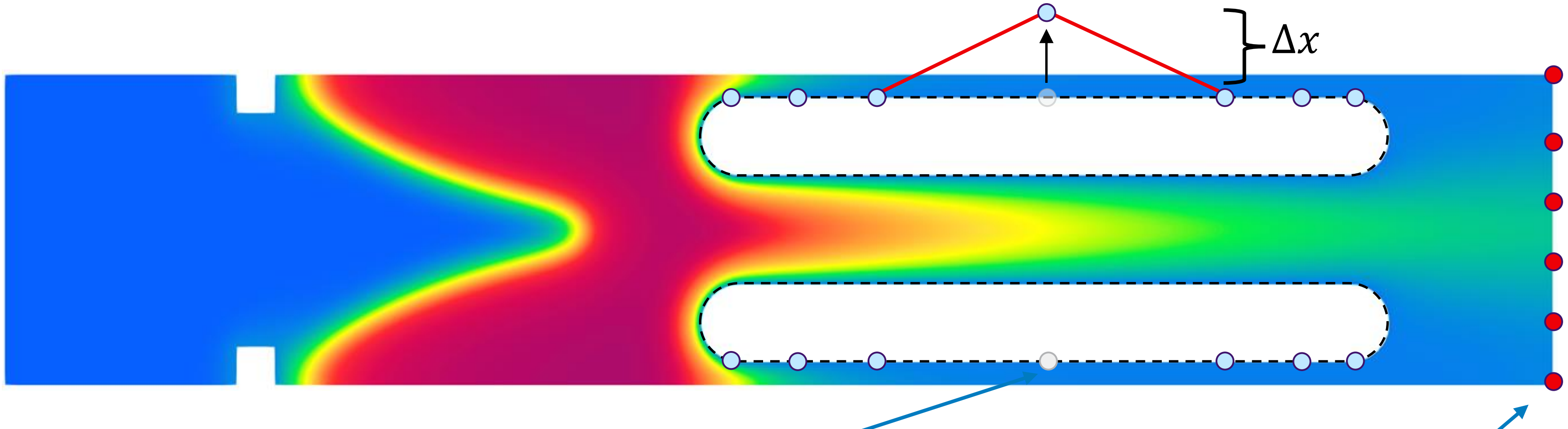
Adjoint design optimization

Objectives in design optimization

$$\frac{\partial J}{\partial x} = \begin{cases} > 0 : \text{move in opposite direction} \\ < 0 : \text{move in that direction} \end{cases}$$



control variables (design variables): surface nodes

$$\alpha = \overline{x} = (x_1, y_1, x_2, y_2, \ldots)$$

objective J: minimize NO_x emissions at the outlet

$$\min(J) = \sum Y_{NO_x}(x_{out}, y_i)$$

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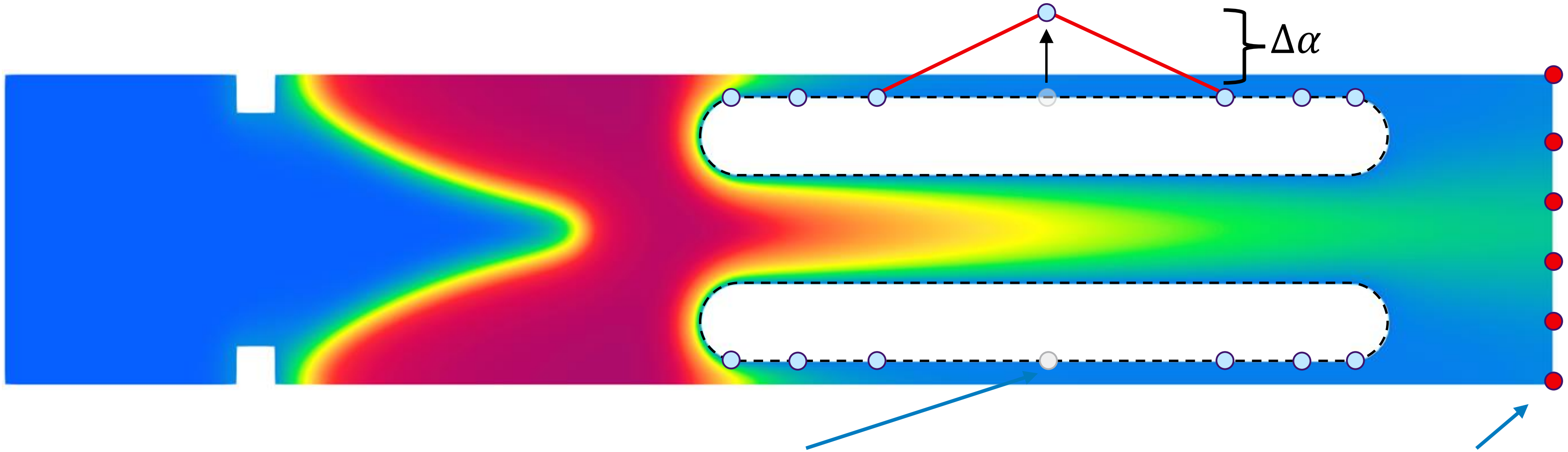
Adjoint design optimization
Objectives in design optimization

$$\frac{\partial J}{\partial \alpha} = \begin{cases} > 0 : \text{move in opposite direction} \\ < 0 : \text{move in that direction} \end{cases}$$



control variables (design variables): surface nodes

$$\alpha = (x_1, y_1, x_2, y_2, \ldots)$$

Governing equations (Navier-Stokes, RANS):

$$R(W, X, \alpha) = 0$$

objective J: minimize NO_x emissions at the outlet

$$\min(J) = \sum Y_{NO_x}(x_{out}, y_i)$$

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Adjoint design optimization

introduce Lagrange multiplier Λ and construct Lagrange function for the objective:

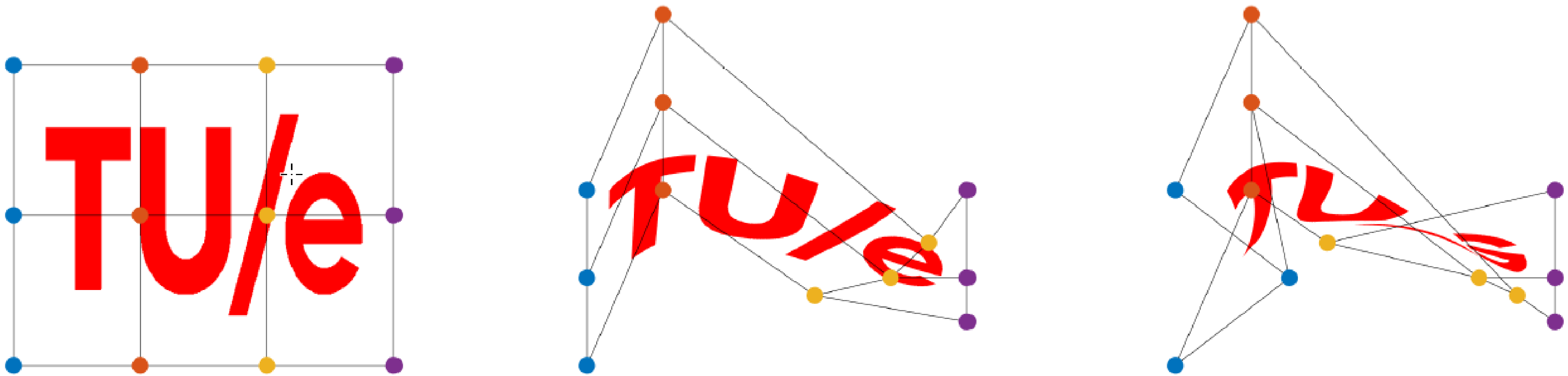
$$L = J + \Lambda^T R \quad \Longrightarrow \quad \frac{dL}{d\alpha} = \frac{d}{d\alpha}\left(J(W,X,\alpha) + \Lambda^T R(W,X,\alpha)\right)$$

$$\frac{dL}{d\alpha} = \left\{\frac{\partial J}{\partial X} + \Lambda^T \frac{\partial R}{\partial X}\right\}\frac{dX}{d\alpha} + \left\{\frac{\partial J}{\partial \alpha} + \Lambda^T \frac{\partial R}{\partial \alpha}\right\} + \left\{\frac{\partial J}{\partial W} + \Lambda^T \frac{\partial R}{\partial W}\right\}\frac{dW}{d\alpha}$$

change of Navier Stokes solution wrt. change in design variables

choose Lagrange multiplier such that $\frac{\partial J}{\partial W} + \Lambda^T \frac{\partial R}{\partial W} = 0$

Adjoint design optimization
Free Form Deformation (FFD)



FFD box with 12 nodes

logo deformed by moving the FFD nodes of the FFD box

invalid deformation

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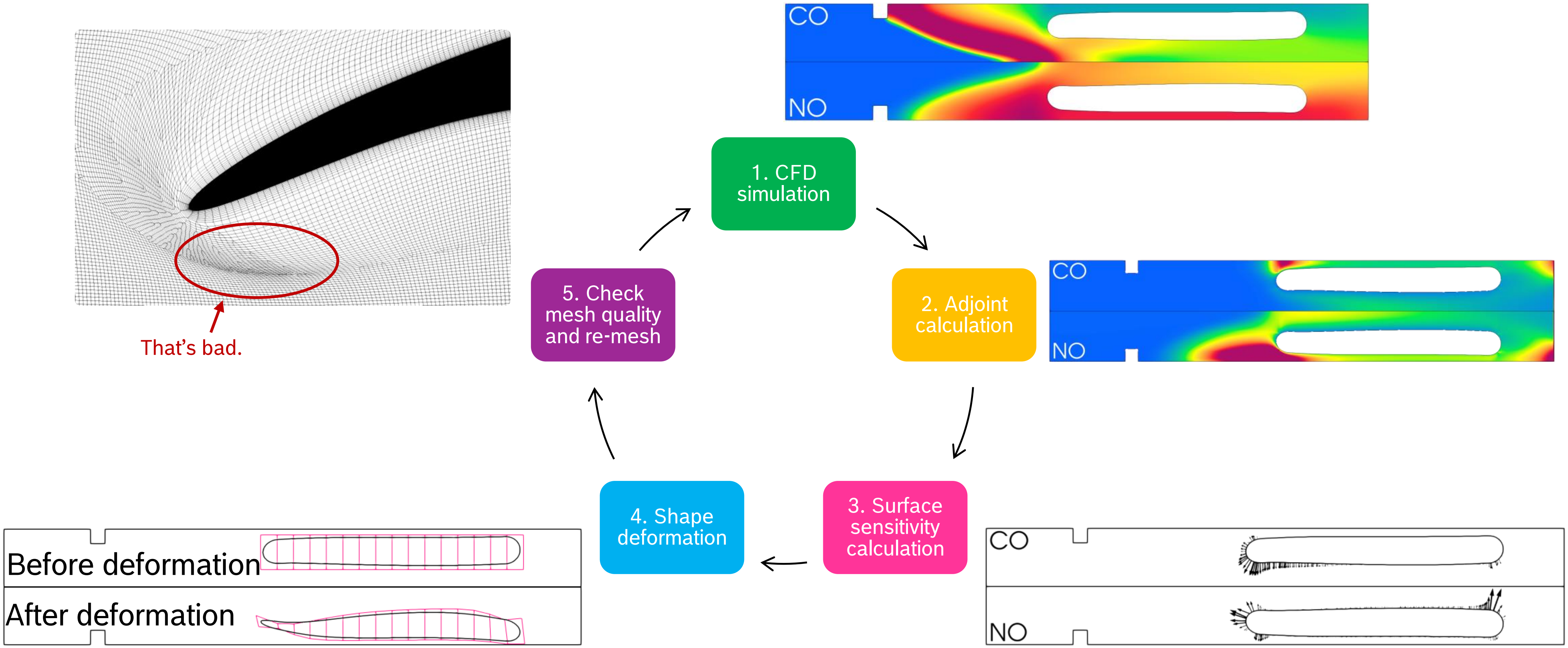
Adjoint design optimization
Optimization loop



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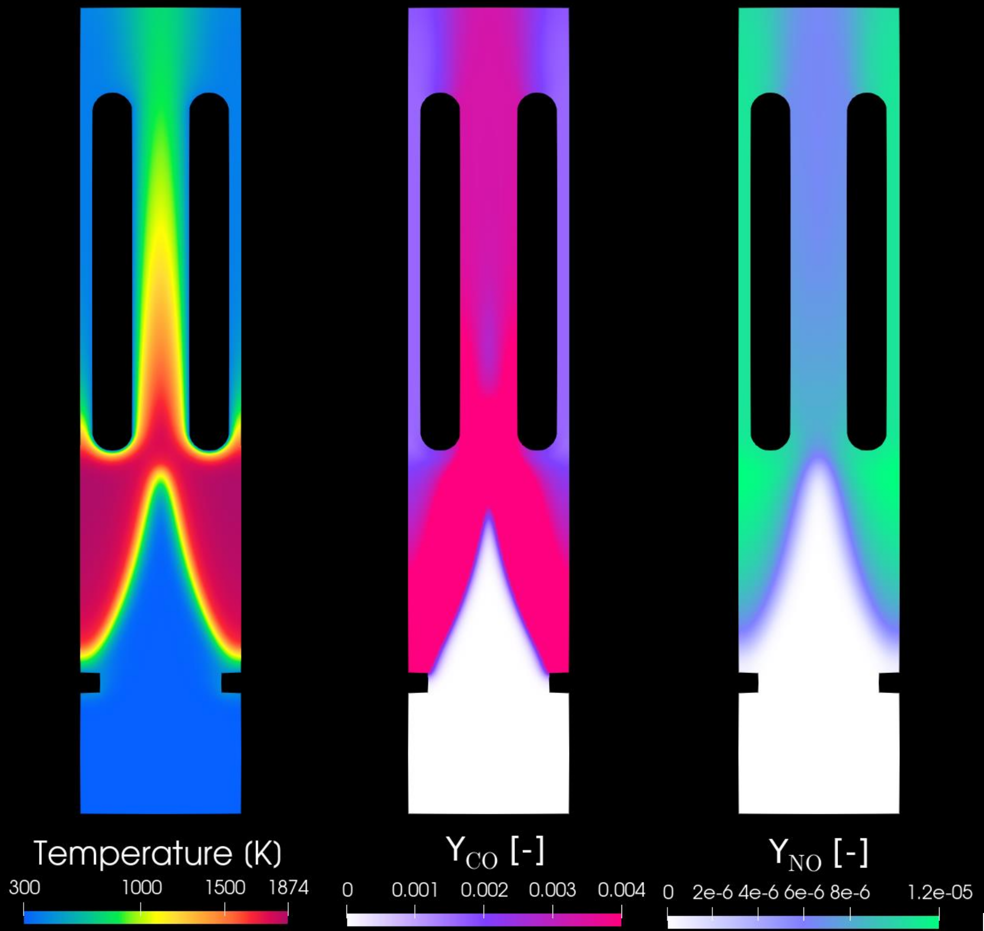
Adjoint design optimization

5 optimizations were performed with the following objective weights:

	T	Y_{CO}	Y_{NO}
1	5e-10=a	0	0
2	0	1e-4=b	0
3	0	0	1e-2=c
4	0	1e-4=b	1e-2=c
5	5e-10=a	1e-4=b	1e-2=c

Baseline



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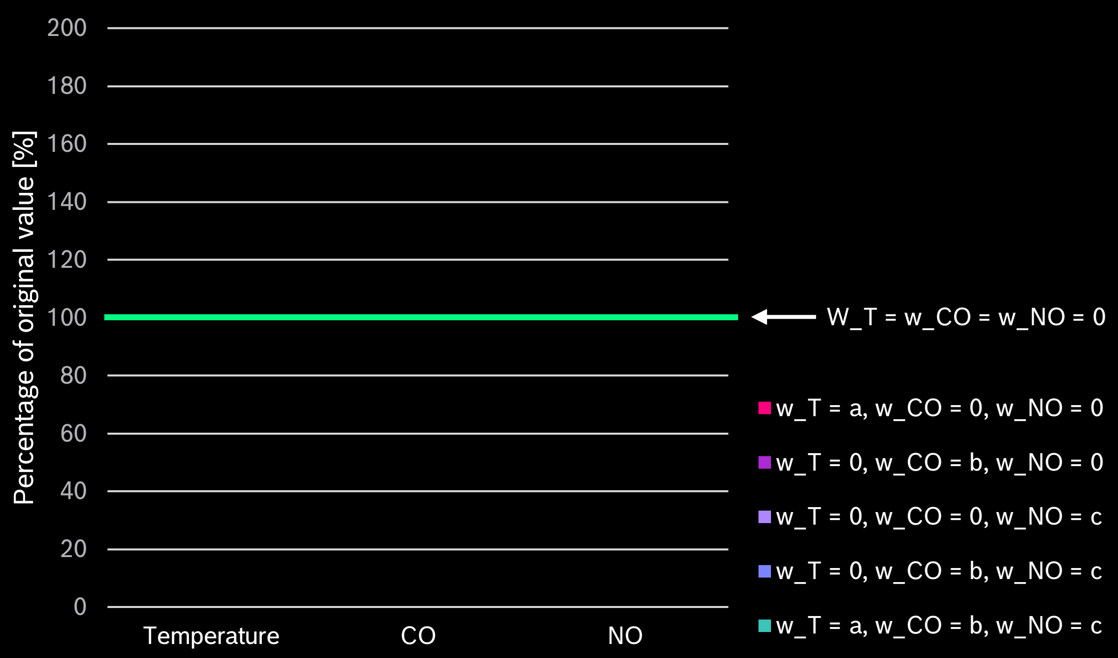
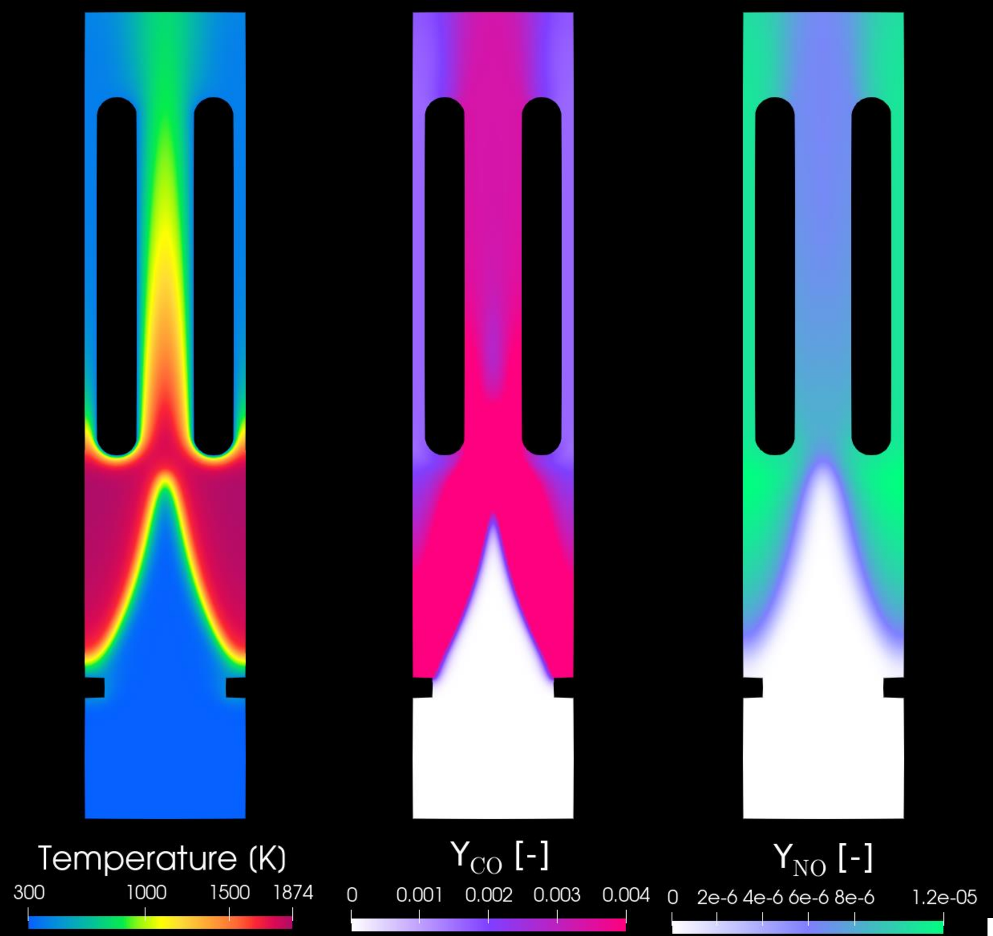
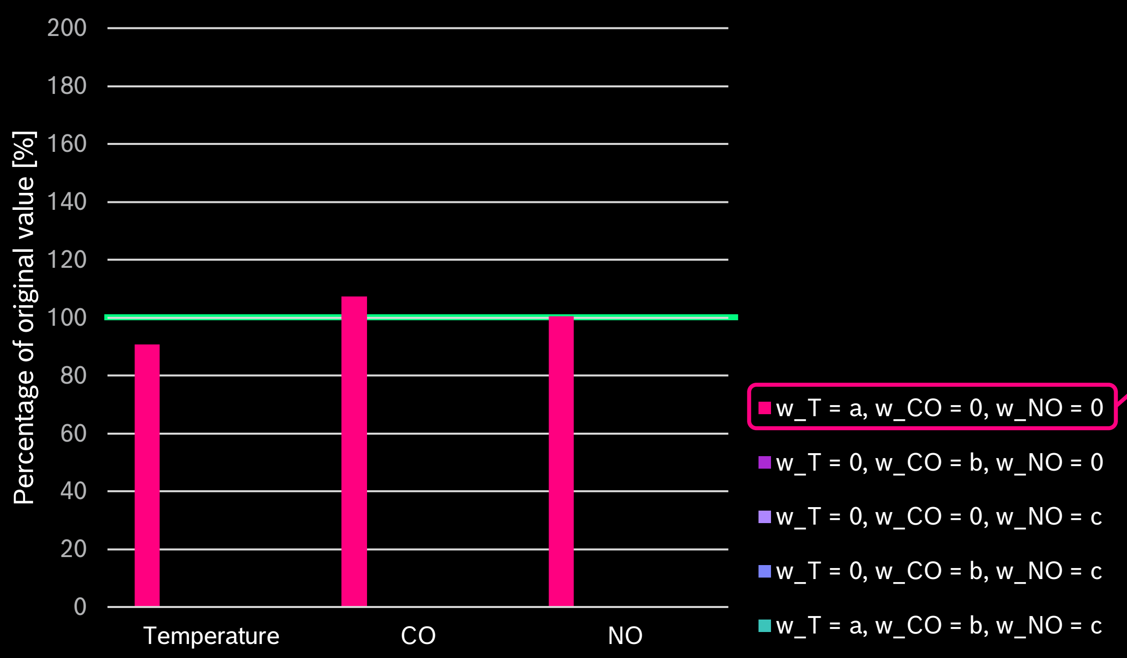
Adjoint design optimization



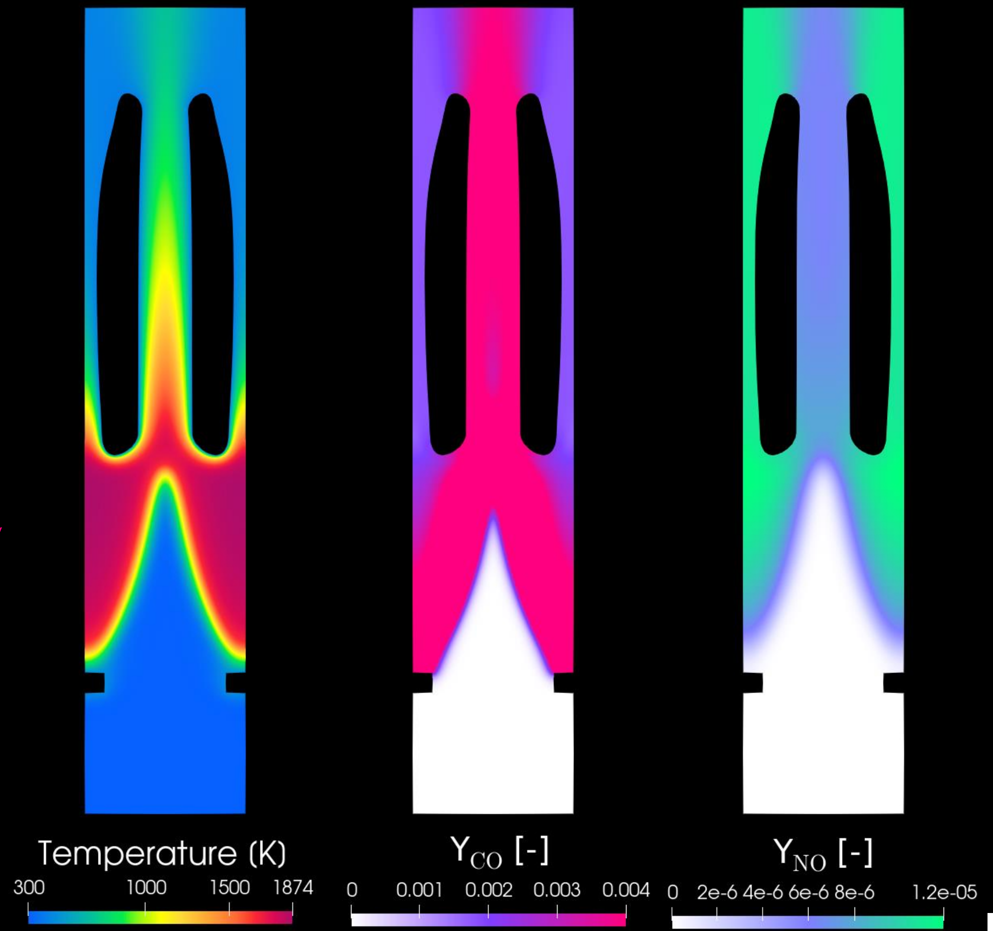
Baseline



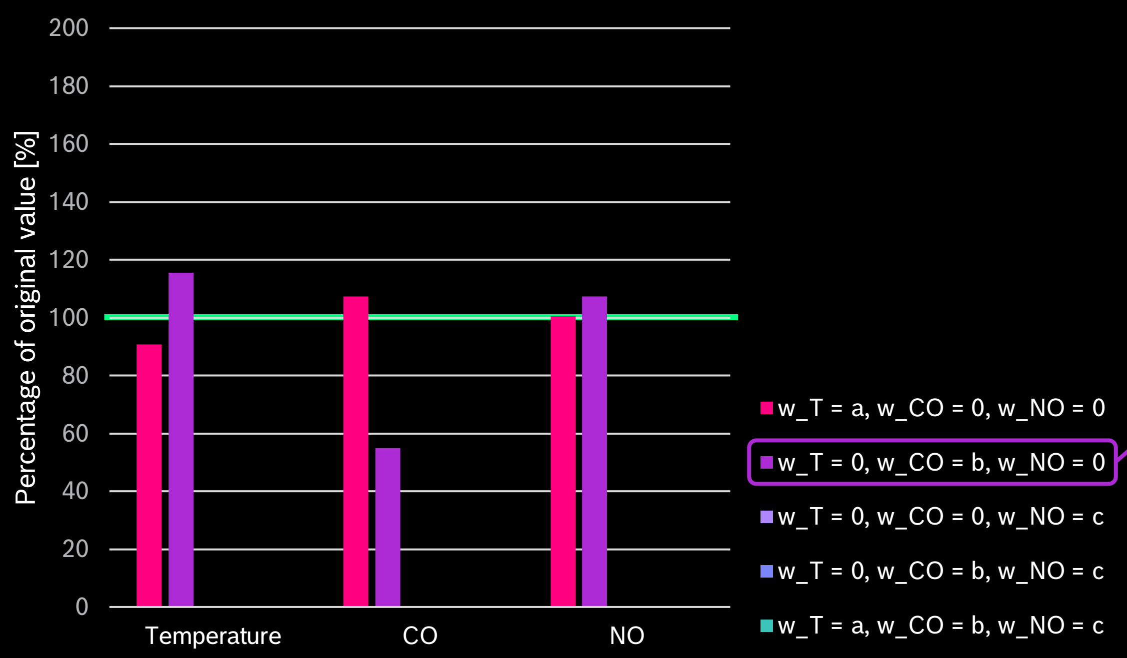
Adjoint design optimization



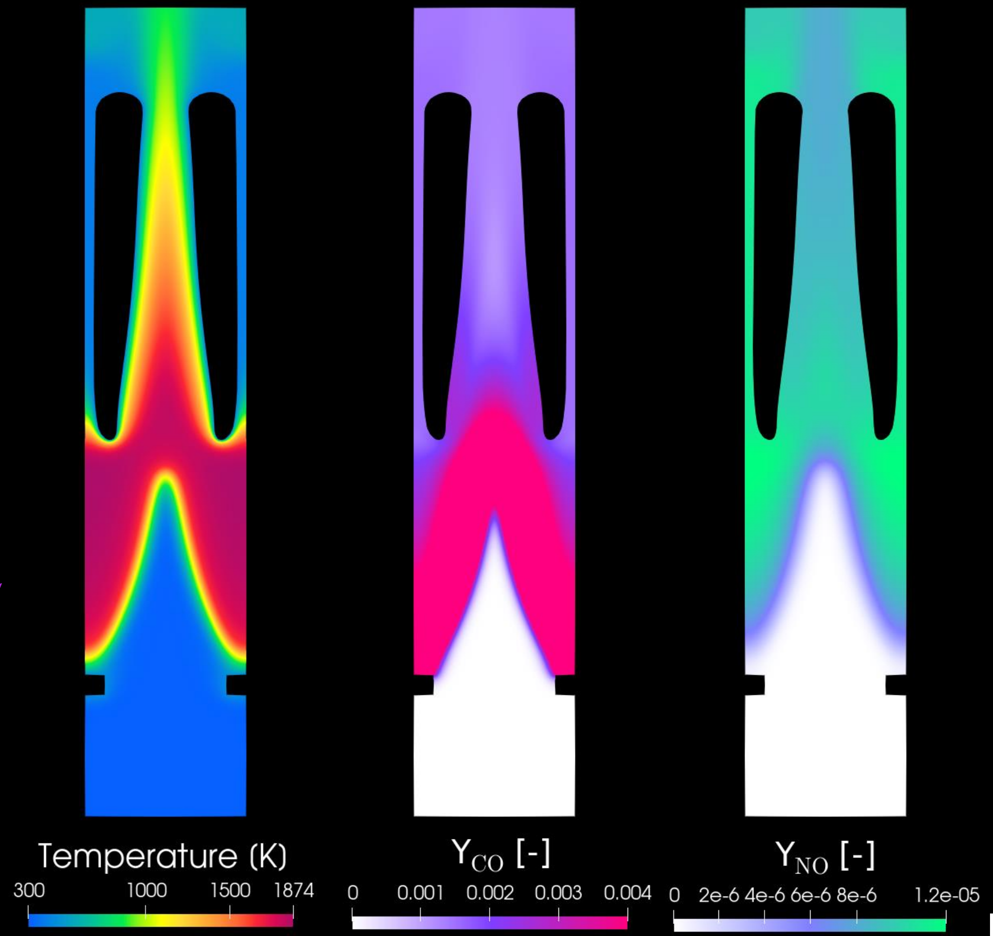
Optimize Temperature only



Adjoint design optimization



Optimize Y_{CO} only



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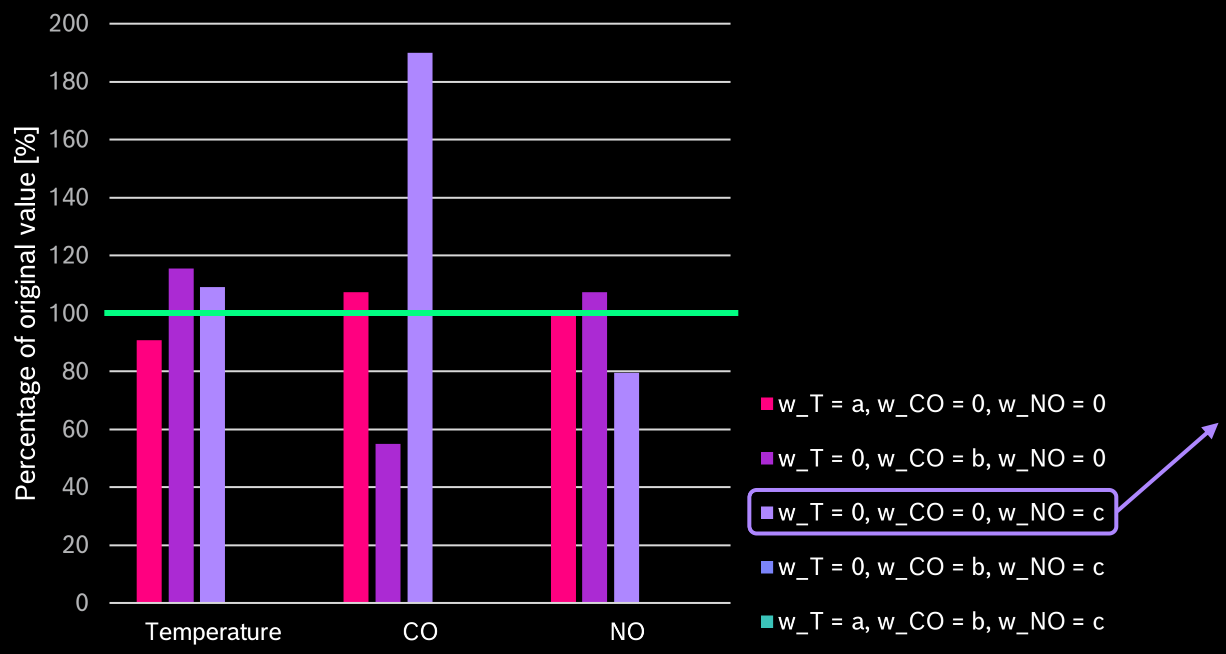
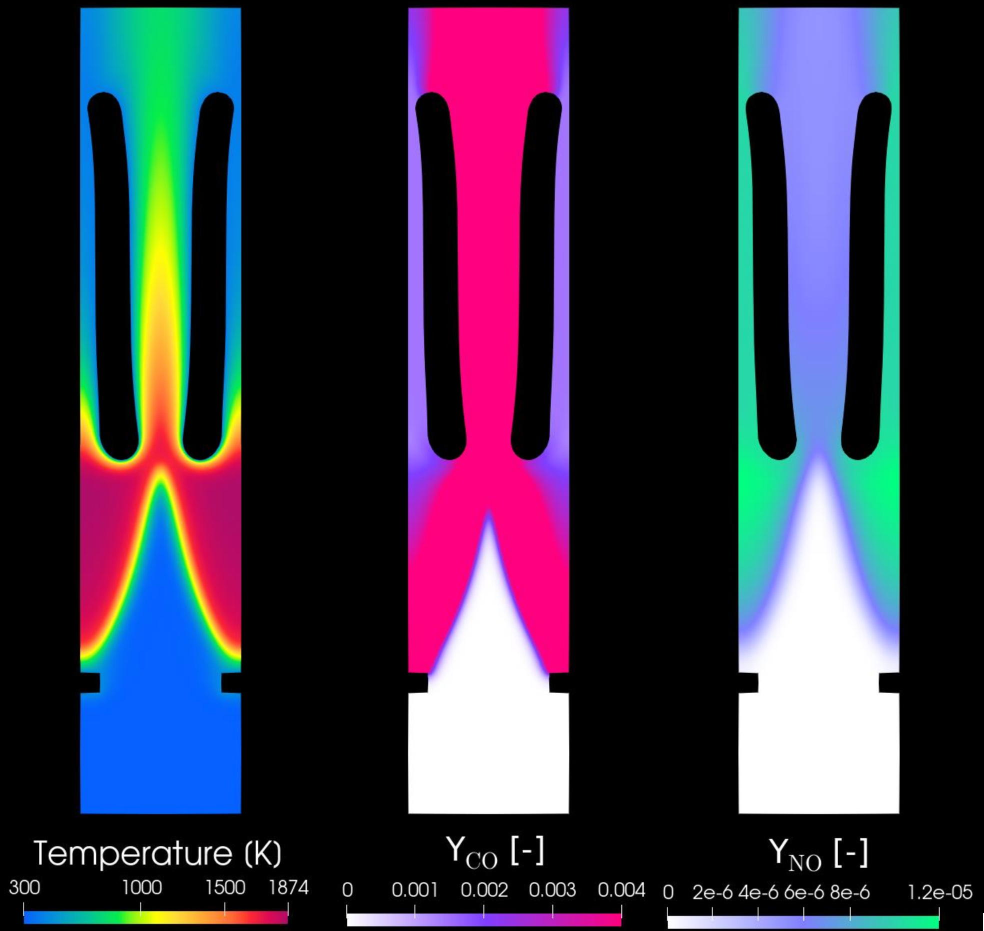
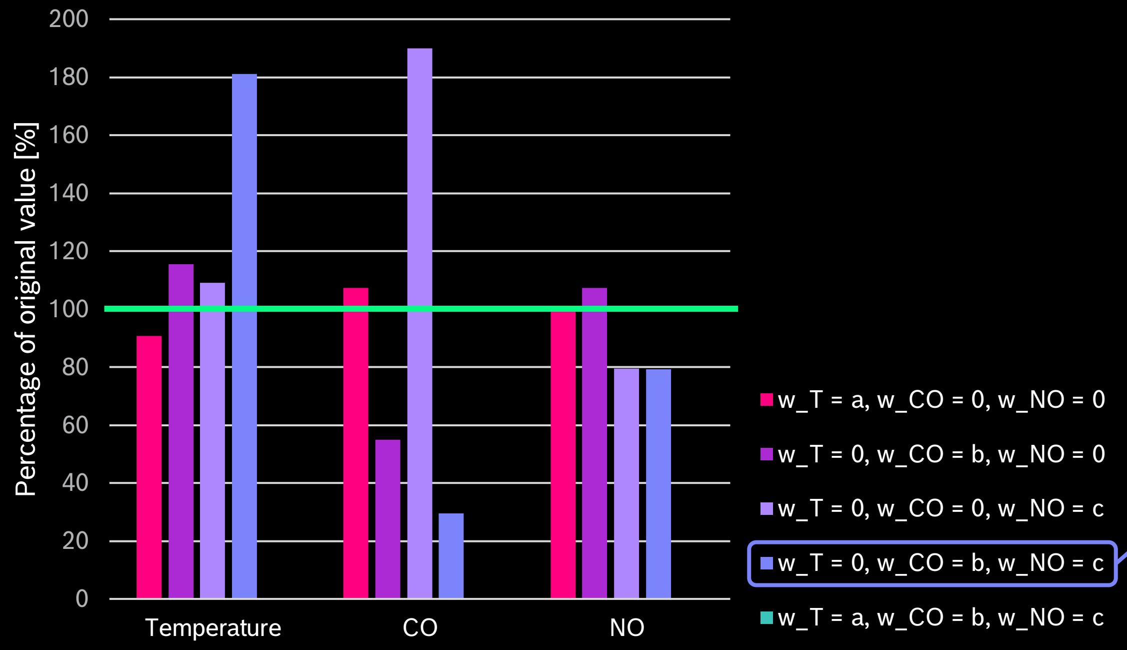
Application to Optimization



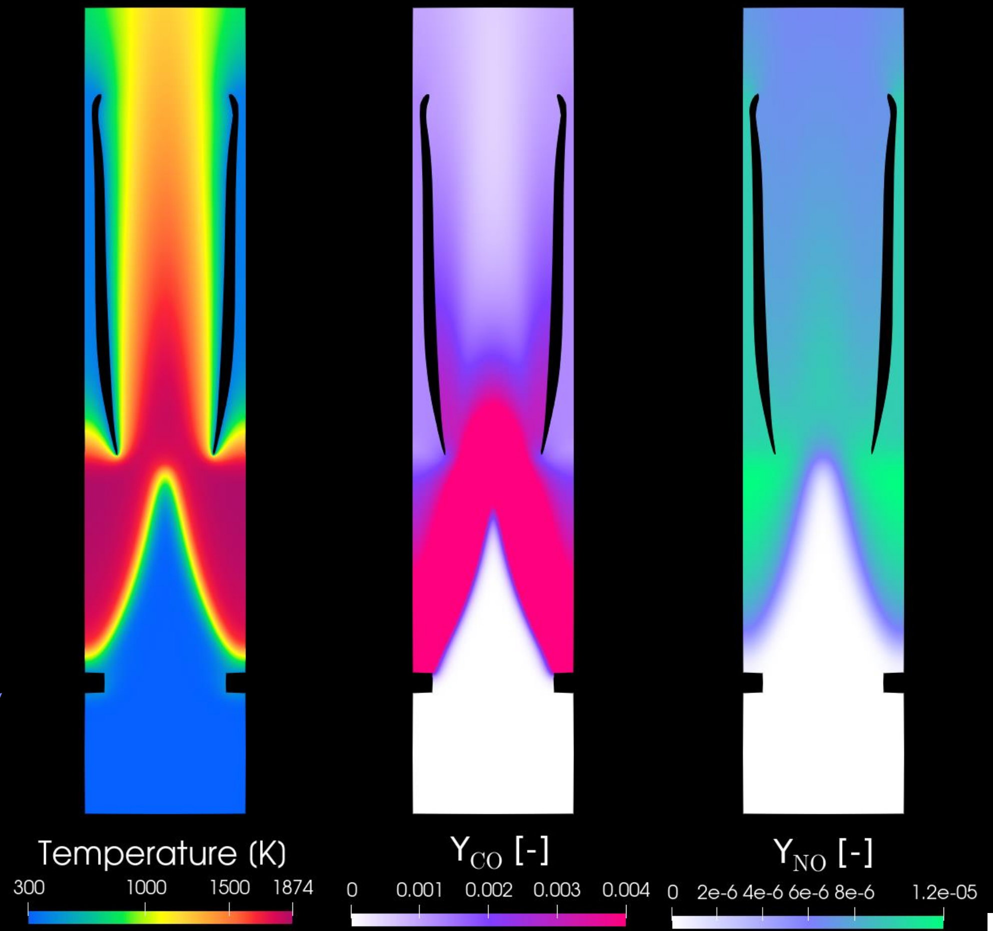
Optimize Y_{NO} only



Adjoint design optimization



Optimize Y_{CO} & Y_{NO}



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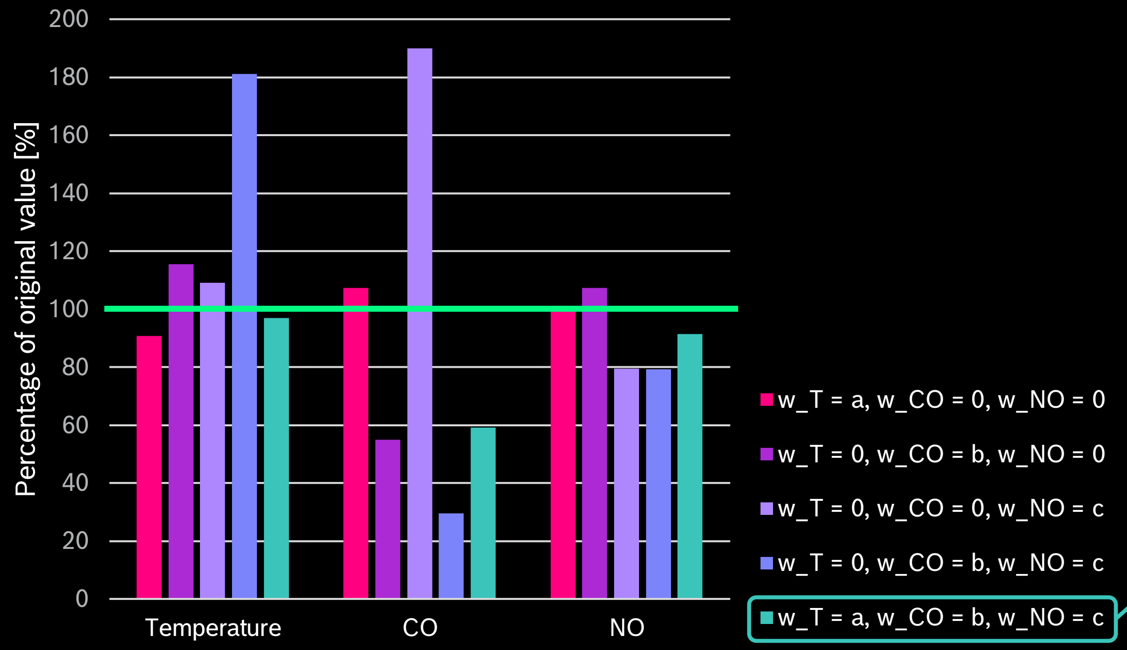
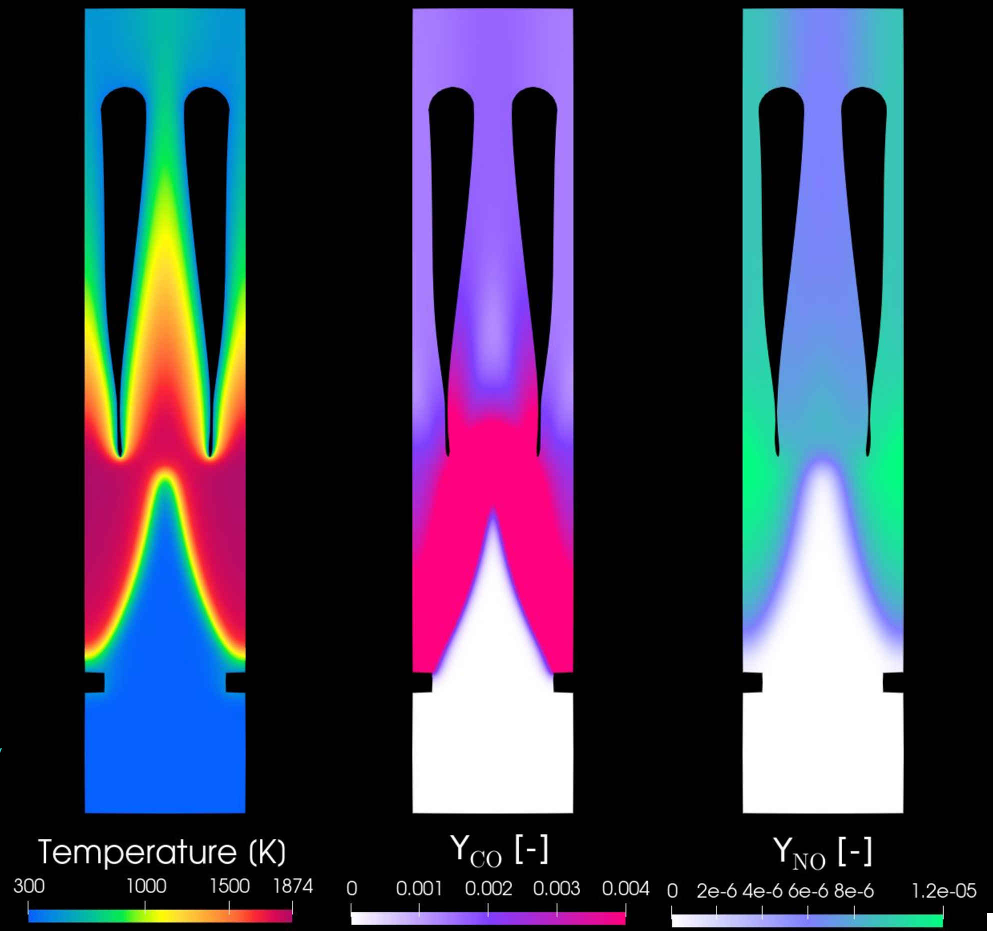
Adjoint design optimization



Optimize Y_{CO}, Y_{NO}, and Temperature



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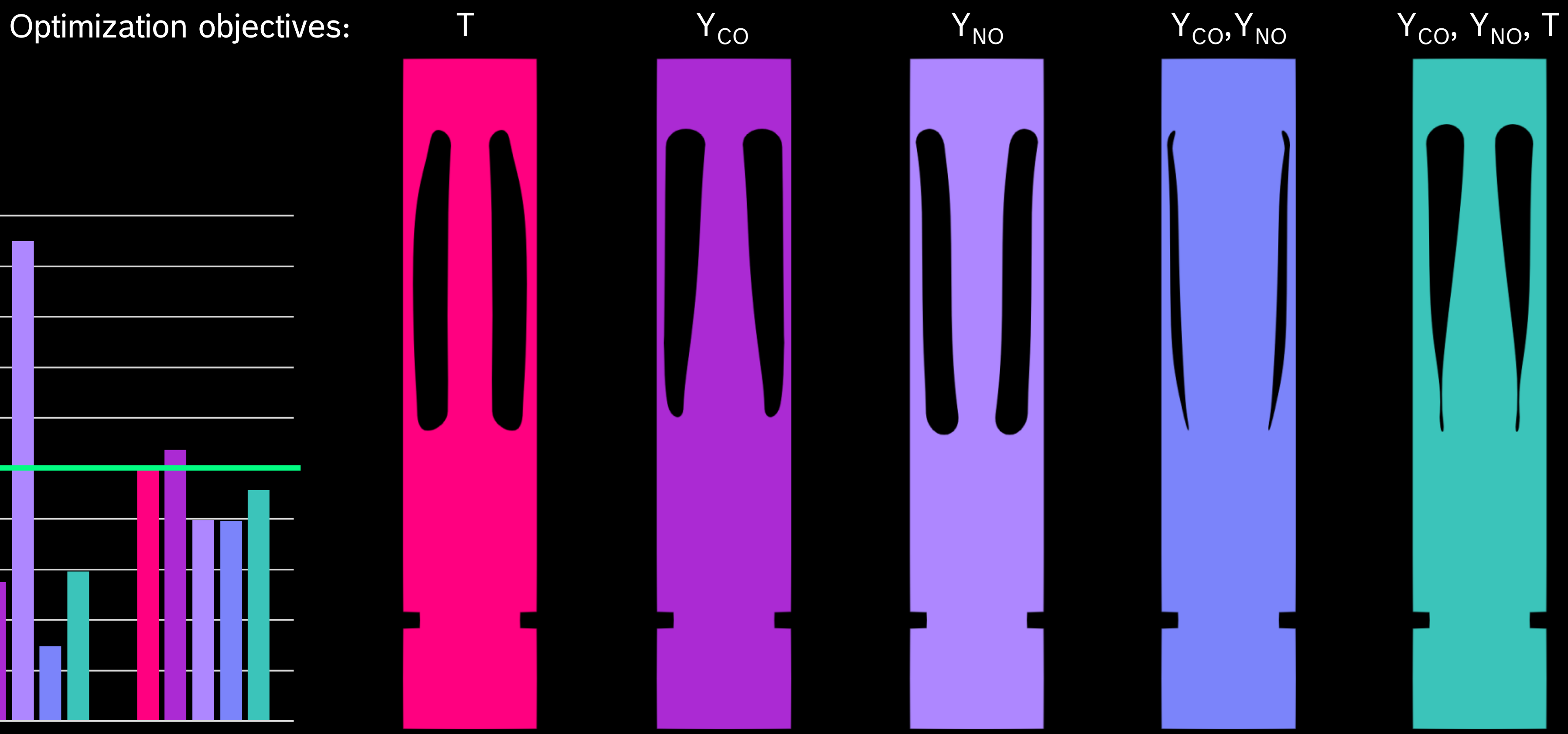
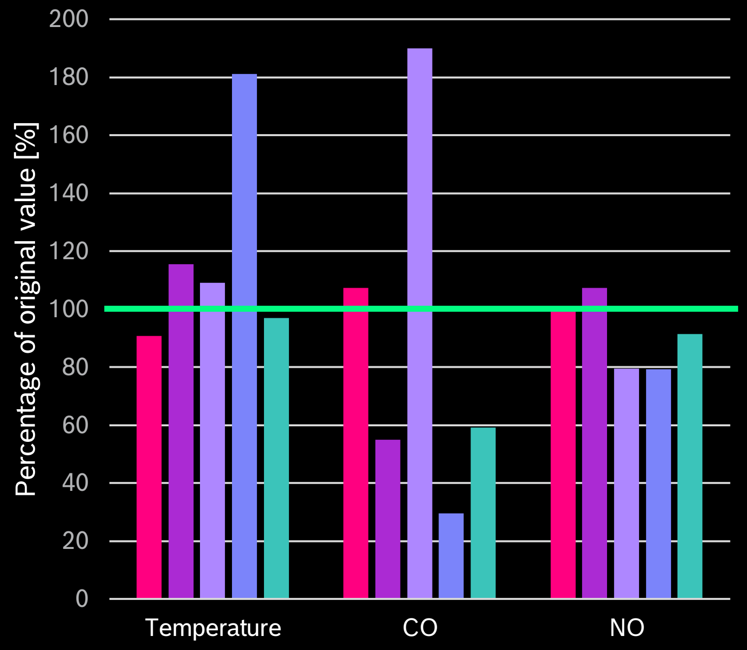
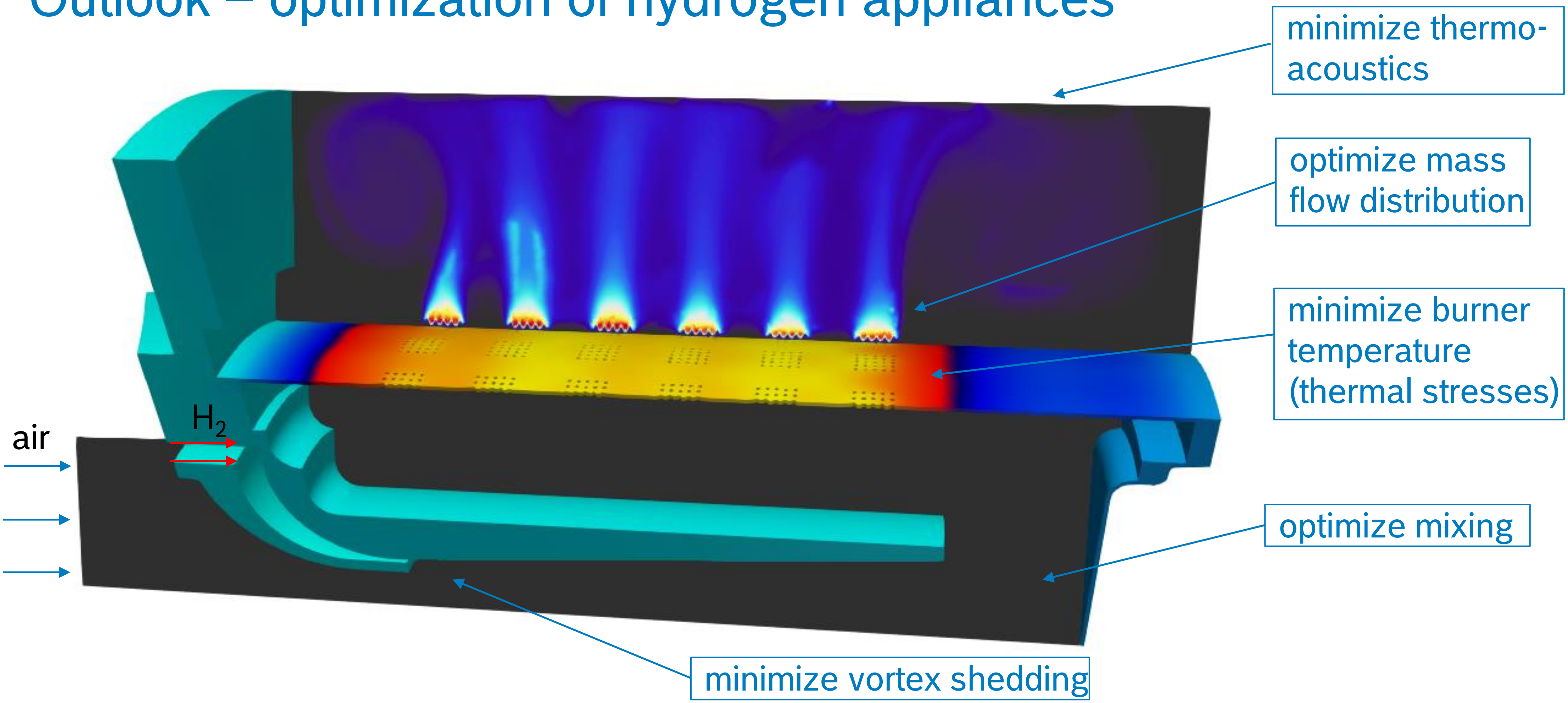
Adjoint design optimization





Adjoint design optimization
Outlook – optimization of hydrogen appliances



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THANK YOU!

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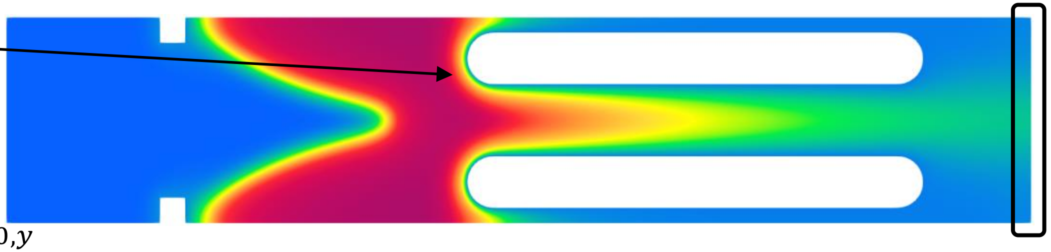
Adjoint-based design optimization for combustion applications
The adjoint approach: Forward simulation (CFD)

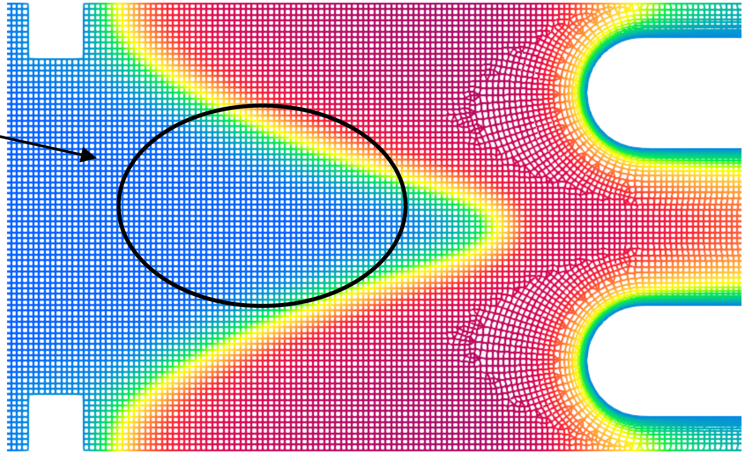
Forward simulation (primal)

- 500 surface points
- Deformation in 2D
- ➔ 1000 design variables

$p_{1,x}, \dots, p_{500,x}, p_{1,y}, \dots p_{500,y}$



Solve $u, v, p, h, c, Y_{\mathrm{NO_x}}$ on every grid point



~170'000 points × 6 variables
= ~1M degrees of freedom

Calculate 1 optimization target ($\overline{Y_{\mathrm{NO_x}}}$)

- *1000 primal solutions are needed to calculate the gradient of $\overline{Y_{\mathrm{NO_x}}}$ with respect to the design variables (DVs).*
- *We are interested in the effect of 1000 DVs on 1 target and throw away 1M variables needed for the computation.*

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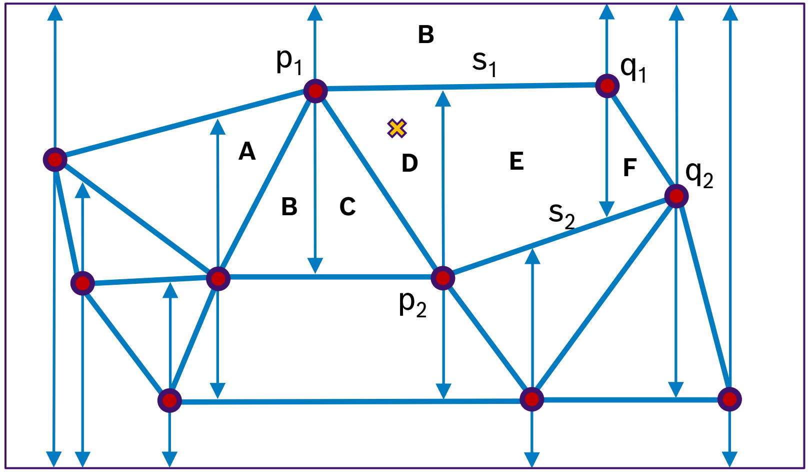
Adjoint-based design optimization for combustion applications

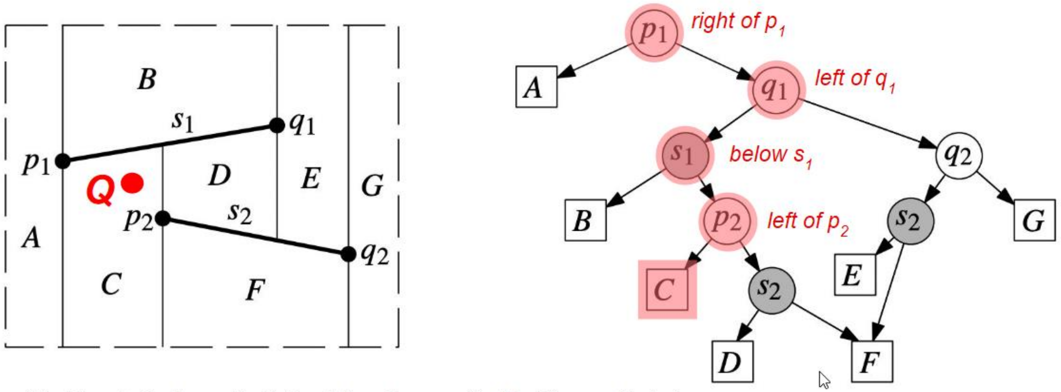
trapezoidal map – data structure

- Data storage: Directed Acyclic Graph

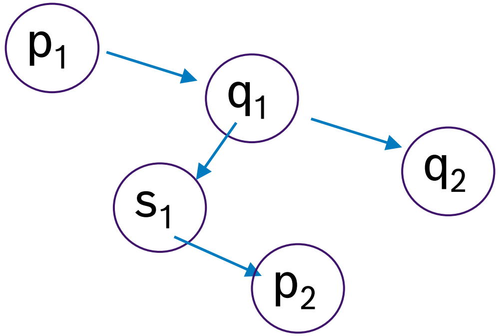


Directed Acyclic Graph (DAG)

- Intermediate notes are vertices (vertical lines) and line segments
- The leaves are the trapezoidal regions (map back to original polygons)



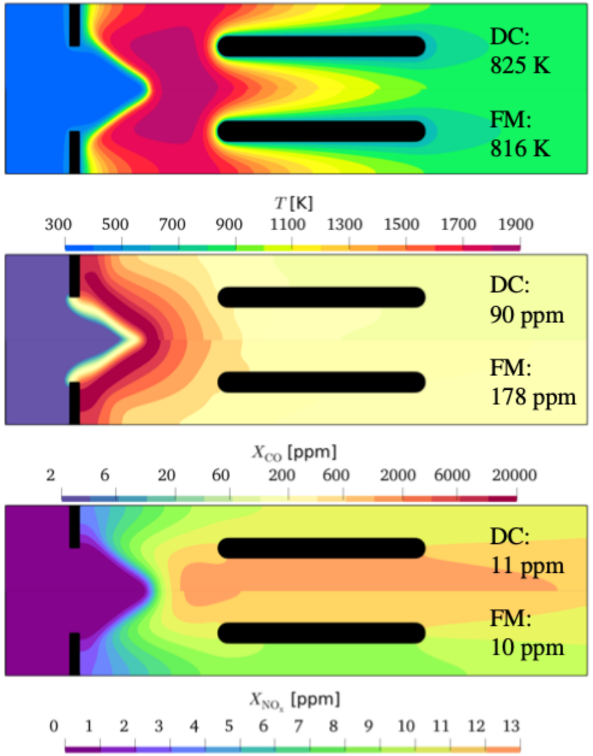
Computational Geometry Algorithms and Applications, de Berg, Cheong, van Kreveld and Overmars, Chapter 6



Adjoint-based design optimization for combustion applications

Methane/Air test optimization

Model validation[1]:

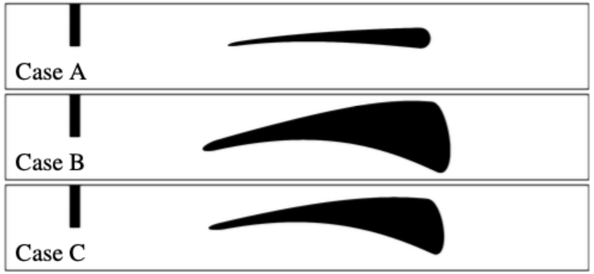


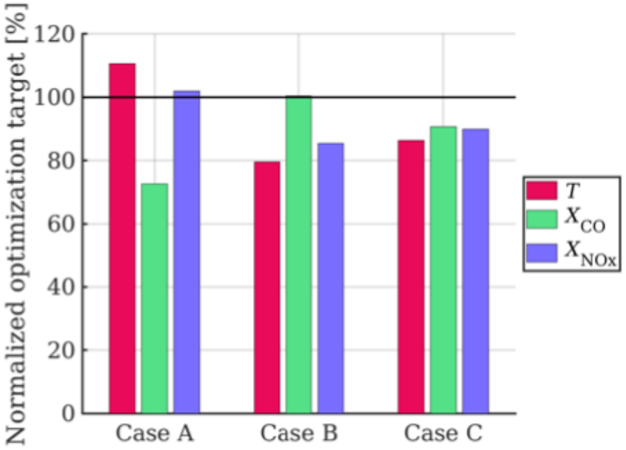
Multi-objective optimization:

- Reduction of temperature T
- Reduction of pollutant emissions X_{CO} and X_{NOx}
- Remeshing using Pointwise in case of no convergenc
- Adjoint: Discrete Adjoint using CoDiPack
- Driver: FADO[2] framework

Case	Weight T	Weight X_{CO}	Weight X_{NOx}
A	1/2	4/3	1
B	1	2/3	1
C	1	1	1

Results:





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[1]: DC: Detailed Chemistry; FM: Flamelet model
[2]: https://github.com/pcarruscag/FADO

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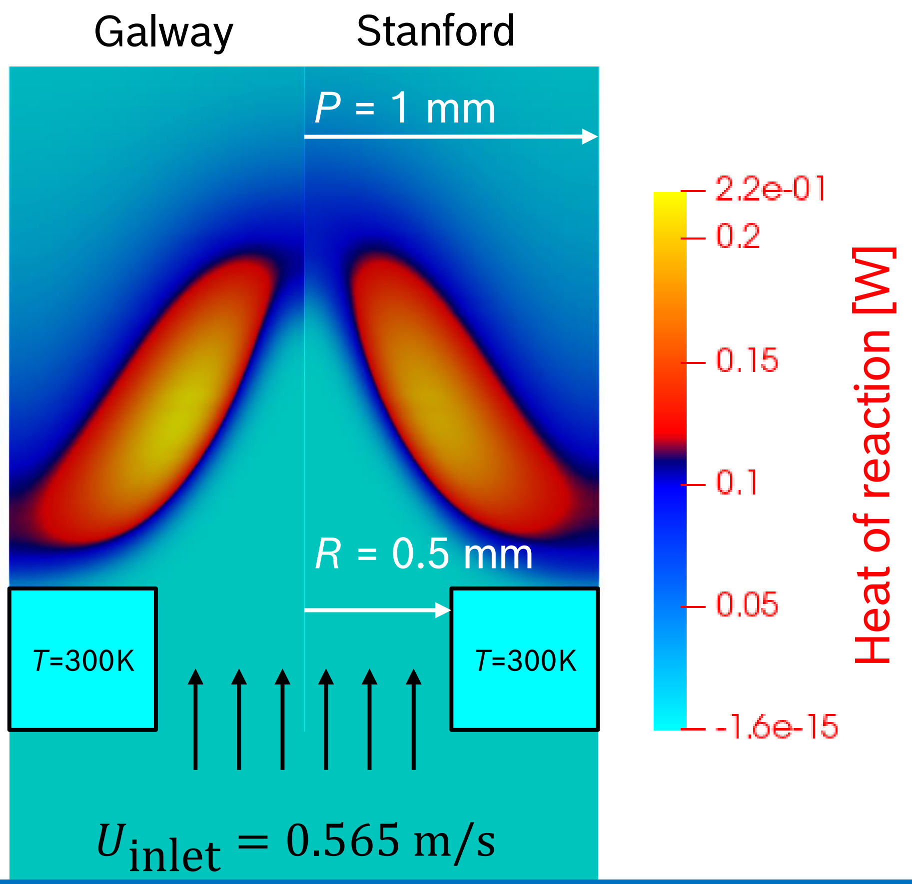
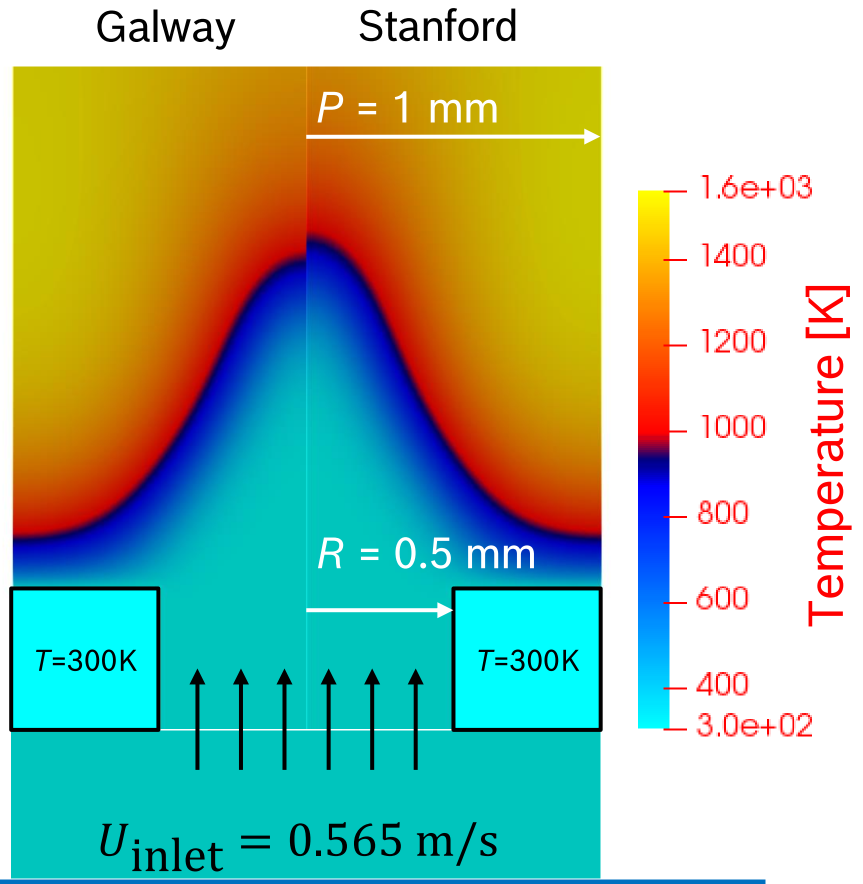
Hydrogen vs. methane
2D planar H_2-air simulations at ϕ=0.5 (Fluent v19.2)

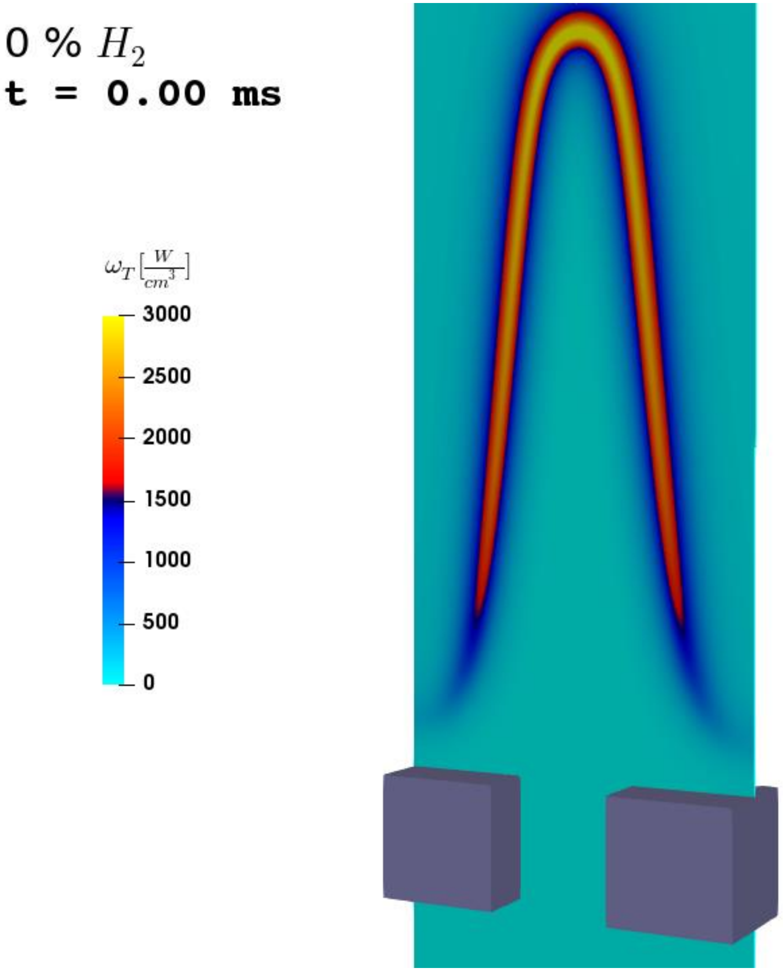


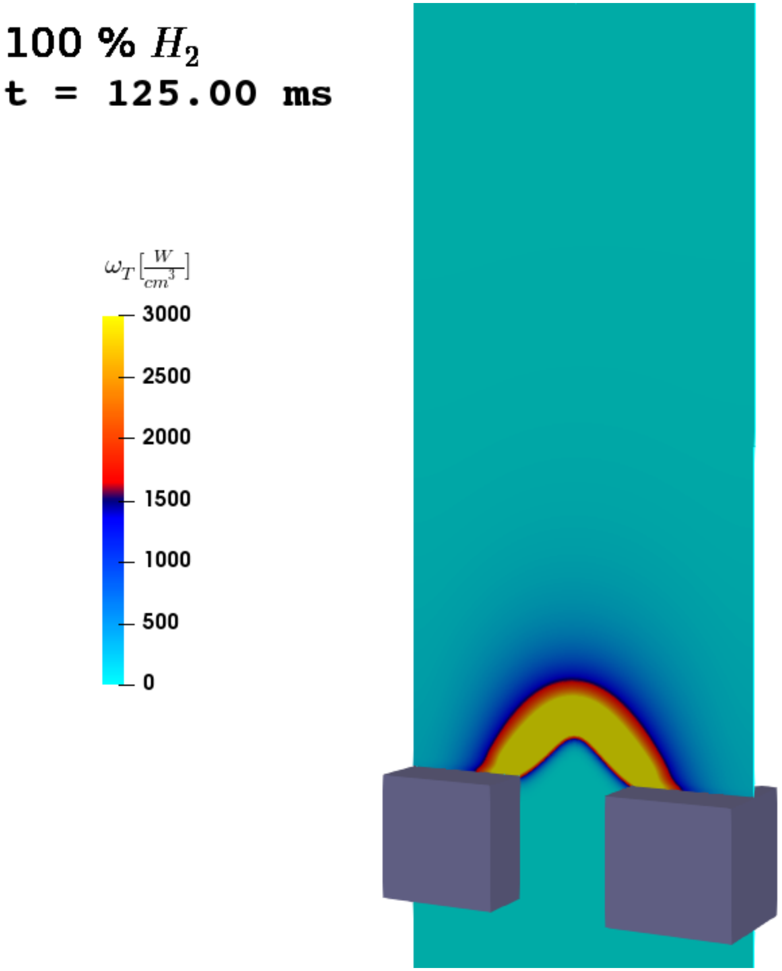


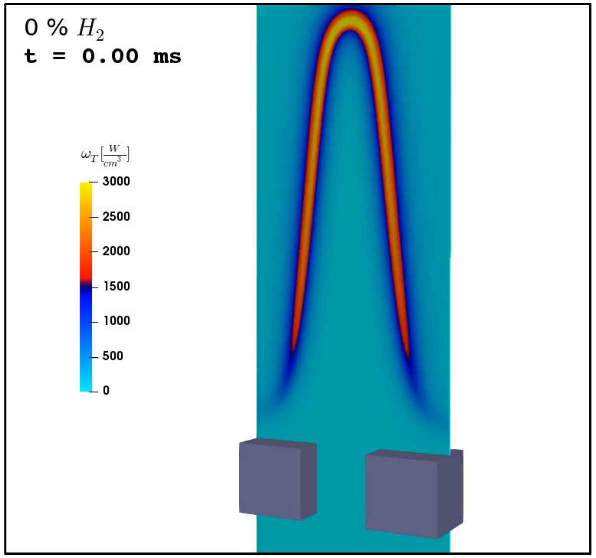
2D simulations show small differences in flame length, heat release rate and temperature

➔ Cheaper mechanism (Stanford) is sufficient for this study

Hydrogen vs. methane
From natural gas to hydrogen







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Hy4Heat

phi=0.80

100% hydrogen
hydrogen ready
hydrogen blend
hybrid

CH_4	O_2	CH_4	H_2	
100%	0.2226	0.0447	0.0	
80%	0.2229	0.04215	0.00132	x
60%	0.2233	0.03848	0.00321	x
40%	0.2240	0.03276	0.00615	x
20%	0.2251	0.02264	0.01134	x
10%	0.2265	0.01318	0.01481	
0%	0.2277	0.0	0.02290	

phi	O_2	CH_4	H_2	SL	2*SL
1.0	0.2264	0	0.02847	2.17	4.34
0.8	0.2277	0	0.02290	1.63	3.26
0.6	0.2290	0	0.01728	0.93	1.86
0.5	0.2297	0	0.0144		
0.4	0.2303	0	0.01158	0.25	0.5

Hy4Heat

3D conjugate heat transfer – burner temperature (steel)

phi=0.8			
v=1.63	T=790.04		
v=	T=		

Hy4Heat
conjugate heat transfer – burner temperature (steel)

phi=0.4			
v=0.4	T=		
v=0.5	T=786.16		

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Hydrogen vs. methane
from natural gas to hydrogen

here a movie of the 2D planar flame, showing the hydrogen concentration and the time, and 2D contours of the H2 concentration, temperature, heat release rate, h2o concentration(?)

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