ADJOINT-BASED DESIGN OPTIMIZATION OF POLLUTANT EMISSIONS IN HEAT EXCHANGERS




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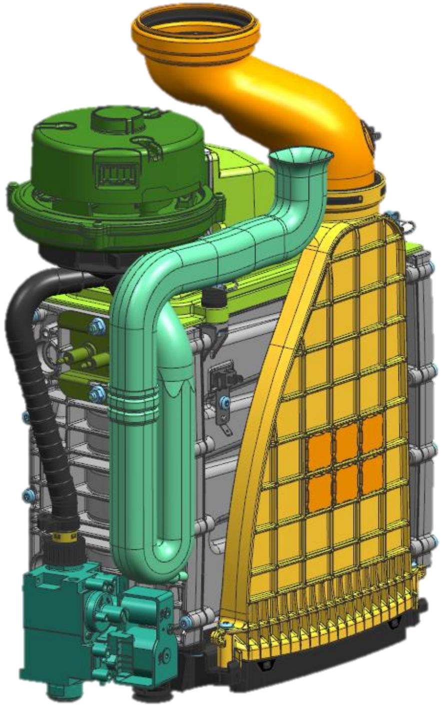
BOSCH

Motivation
Natural gas boilers for domestic heating

Wall hanging appliance


CAD model of the heat cell

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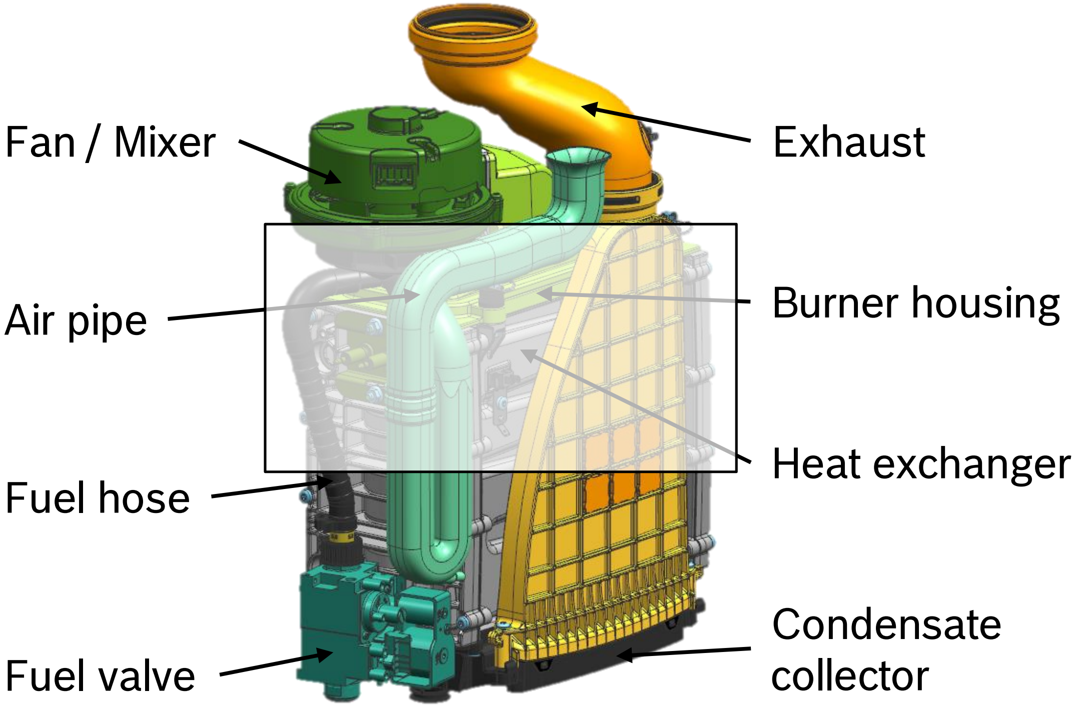
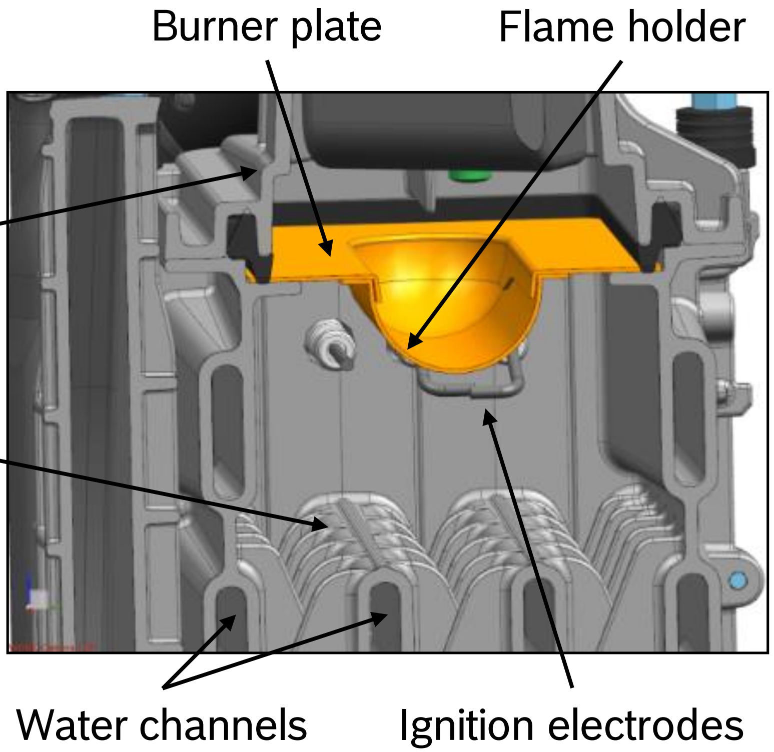
Motivation
Working principle





Combustion regime: Laminar, premixed methane gas combustion

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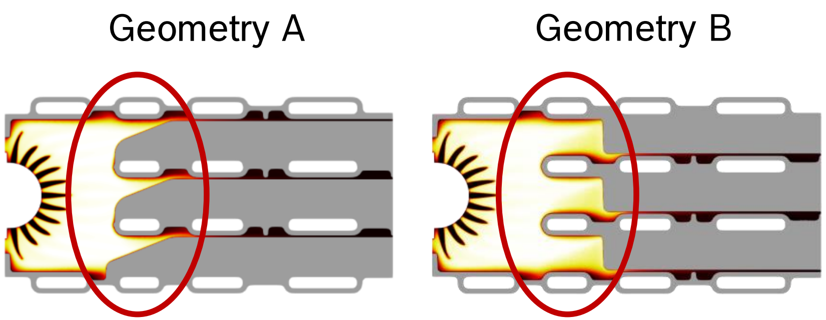
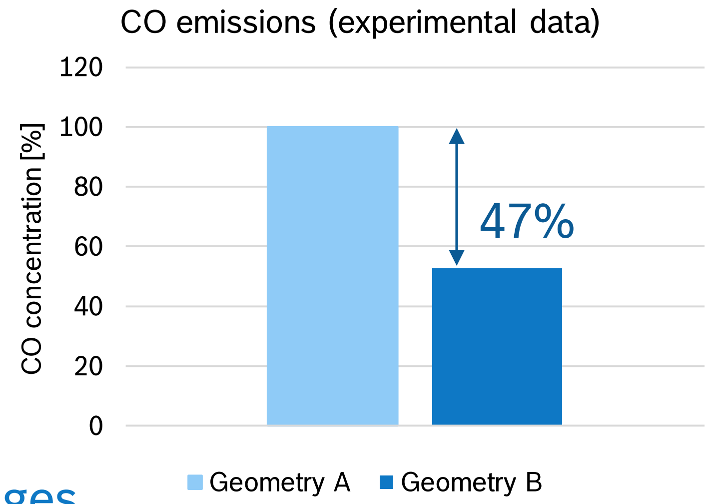
Motivation
Reduction of pollutant emissions

- During combustion harmful pollutants CO and NO_x are formed
- CO and NO_x emissions have to be reduced
- CO and NO_x emissions are strongly dependent on heat exchanger geometry
  - Emissions reduction is major driver for heat exchanger design



- CO and NO_x formation are counteracting processes
  - Difficult to reduce both CO and NO_x at the same time

- Additional constraints:
  - Thermal efficiency
  - Pressure drop
  - Manufacturing constraints like material thickness, casting process, …



Adjoint optimization is a powerful tool in overcoming these challenges

COMBUSTION MODELLING

DETAILED CHEMISTRY MODELLING
THE FLAMELET PROGRESS VARIABLE (FPV) APPROACH
WORKFLOW / TOOL CHAIN

MODEL IMPLEMENTATION IN SU2

ARCHITECTURE
CONFIGURATION
MODEL VALIDATION

APPLICATION TO ADJOINT OPTIMIZATION

CASE SETUP
GEOMETRICAL DEFORMATION CONSTRAINTS
AUTOMATED REMESHING
RESULTS

OUTLOOK

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Combustion modeling
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:

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

Expensive transport quantities:

$$\eta_{mix} = \sum_{i=1}^{n_{sp}} \frac{X_i \eta_i}{\sum_{j=1}^{n_{sp}} X_j \phi_{ij}}$$

- Mechanism used here: GRI-Mech 2.11 from UC Berkeley[1]
- It contains 49 species and 277 elementary reactions

➔ Computational costs become challenging if applied in a design cycle

[1] C.T. Bowman, R.K. Hanson, D.F. Davidson, W.C. Gardiner, Jr., V. Lissianski, G.P. Smith, D.M. Golden, M. Frenklach and M. Goldenberg, http://www.me.berkeley.edu/gri_mech/

Combustion modeling
The flamelet progress variable (FPV) approach

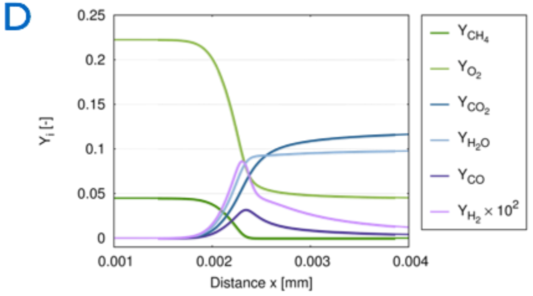
Idea: Precompute 1D flames using detailed chemistry data, parameterize chemistry, and apply lookup method instead of solving chemistry.

Lookup parameters here:

Progress variable ***C*** and enthalpy ***h***

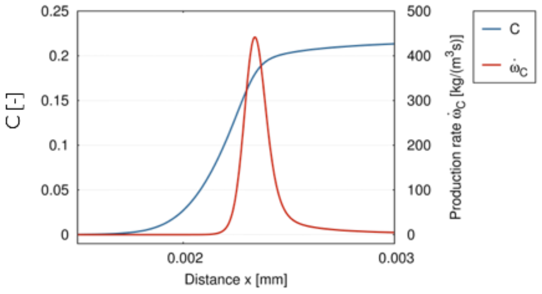
- Compute 1D simulations
- Tabulate 1D solutions as functions of progress variable C and enthalpy h
- Solve 3D transport equations for C and h using table lookups to obtain values for source terms and physical quantities

1D



$$C = Y_{CO_2} + Y_{H_2O}$$

$$\dot{\omega}_C = \dot{\omega}_{CO_2} + \dot{\omega}_{H_2O}$$



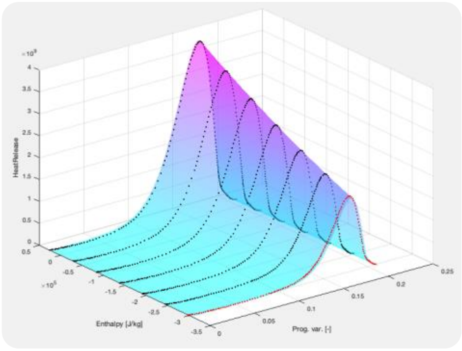
3D

$$\frac{\partial(\rho C)}{\partial t} + \vec{\nabla}\cdot(\rho\vec{v}C) - \vec{\nabla}\cdot\left(\rho\mathcal{D}_C\vec{\nabla}C\right) = \rho\dot{\omega}_C$$

$$\frac{\partial(\rho h)}{\partial t} + \vec{\nabla}\cdot(\rho\vec{v}h) - \vec{\nabla}\cdot\left(\rho\mathcal{D}_h\vec{\nabla}h\right) = \rho\dot{\omega}_h$$

C, Enthalpy (h)

$\dot{\omega}(C,h)$
$\nu(C,h)$
$\rho(C,h)$
$\mathcal{D}(C,h)$
...



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Combustion modeling
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 $EM = \{\text{CO}, \text{NO}\}$

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

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

Stored in chemistry table — Solved using transport equation

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

Combustion modeling
Workflow / Tool chain

1. Perform 1D simulations (detailed chemistry)

- Open source solvers:
  - Cantera for steady state simulations
  - Ember for transient flame calculations

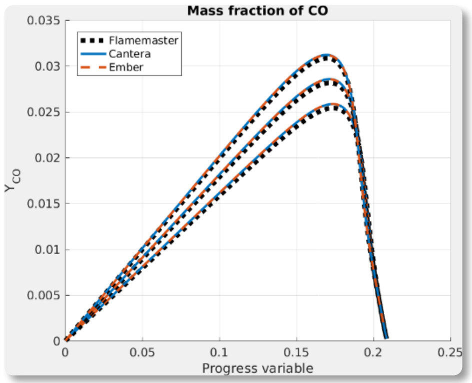
2. Tabulate 1D solutions in look-up tables

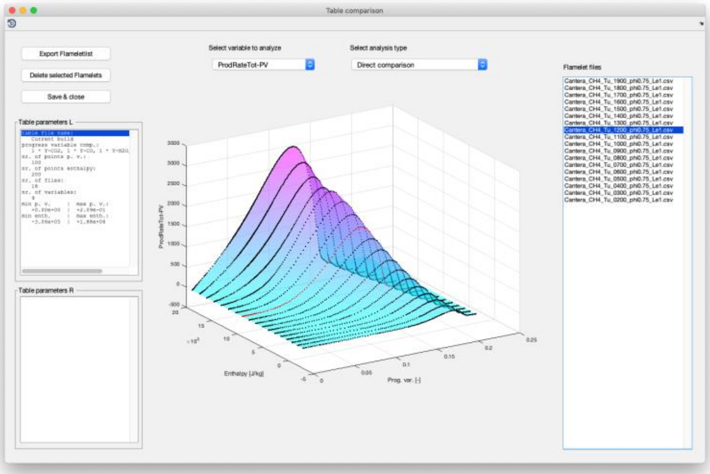
- Tabulate as *f(progress var., enthalpy)*
- In house developed tool
- Cantera, Ember, and FlameMaster[5] support

3. Solve 3D transport equations

- Just additional 4 PDEs, reaction source terms from look-up tables

Cantera[3] / Ember[4]
Chemical Kinetics • Thermodynamics • Transport Processes





SU2

[3]: www.cantera .org
[4]: https://github.com/speth/ember
[5]: https://www.itv.rwth-aachen.de/downloads/flamemaster/

COMBUSTION MODELLING

- DETAILED CHEMISTRY MODELLING
- THE FLAMELET PROGRESS VARIABLE (FPV) APPROACH
- WORKFLOW / TOOL CHAIN

MODEL IMPLEMENTATION IN SU2

- ARCHITECTURE
- CONFIGURATION
- MODEL VALIDATION

APPLICATION TO ADJOINT OPTIMIZATION

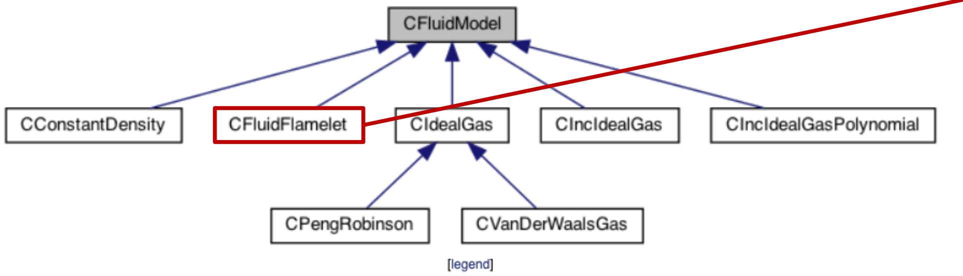
- CASE SETUP
- GEOMETRICAL DEFORMATION CONSTRAINTS
- AUTOMATED REMESHING
- RESULTS

OUTLOOK

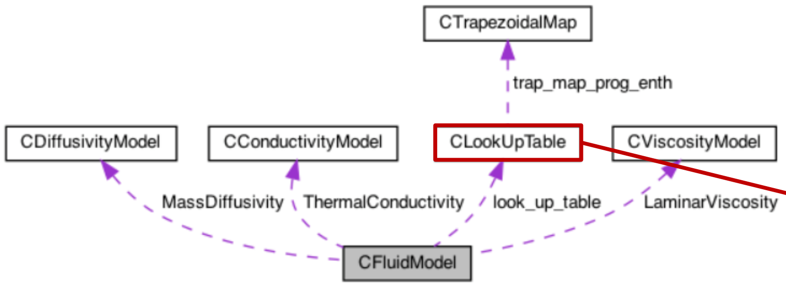
Implementation in SU2
Architecture

https://github.com/su2code/SU2/tree/feature_flamelet

Inheritance diagram for CFluidModel:



Collaboration diagram for CFluidModel:



- A dark blue arrow is used to visualize a public inheritance relation between two classes.

- A purple dashed arrow is used if a class is contained or used by another class. The arrow is labelled with the variable(s) through which the pointed class or struct is accessible.

CFluidFlamelet

Public Member Functions

	CFluidFlamelet (CConfig *config, su2double value_pressure_operating)
	~CFluidFlamelet ()
unsigned long	SetTDState_T (su2double val_temperature, su2double *val_scalars) Virtual member. More...
unsigned long	GetEnthFromTemp (su2double *enthalpy, su2double val_prog, su2double val_temp)
CLookUpTable *	GetLookUpTable ()
su2double	GetMassDiffusivity () Get fluid mass diffusivity. More...
su2double	GetThermalConductivity () Get fluid thermal conductivity. More...
su2double	GetLaminarViscosity () Get fluid dynamic viscosity. More...
pair< su2double, su2double >	GetTableLimitsEnth ()
pair< su2double, su2double >	GetTableLimitsProg ()
su2double	GetdDensitydPV ()
su2double	GetdSourcePVdPV ()
su2double	GetdDensitydEnth ()

CLookUpTable [6]

Public Member Functions

	CLookUpTable (string file_name_lut)
void	PrintTableInfo ()
unsigned long	LookUp_ProgEnth (string val_name_var, su2double *val_var, su2double val_prog, su2double val_enth)
unsigned long	LookUp_ProgEnth (vector< string > &val_names_var, vector< su2double * > &val_vars, su2double val_prog, su2double val_enth)
pair< su2double, su2double >	GetTableLimitsEnth ()
pair< su2double, su2double >	GetTableLimitsProg ()

[6]: A. Rubino, M. Pini, M. Kosec, S. Vitale, and P. Colonna, Journal of Computational Science 28 (2018) 70-77.

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Implementation in SU2
Configuration

https://github.com/su2code/SU2/tree/feature_flamelet

- Implemented in incompressible solver [7]
- Arbitrary number of scalar transport equations $(h, C, Y_1, Y_2, \ldots, Y_N)$
  - config.cfg: `SCALAR_NAMES= (Enthalpy, ProgVar, Y-CO, Y-NO)`
  - Total enthalpy and progress variable must always be the first and second transported variable
- Handling of source terms:

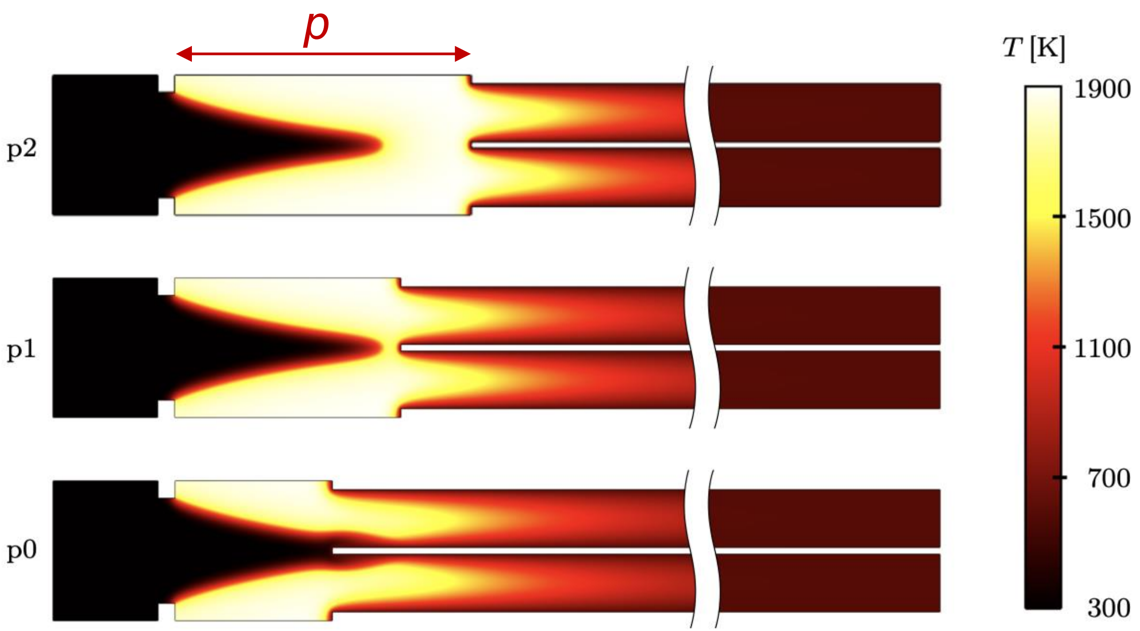
  src enth. | src p.v. | src Y-CO | src Y-NO

  - config.cfg: `SCALAR_SOURCETERM_NAMES=(NULL, NULL, S-PV, NULL, Spos-CO, Sneg-CO, Spos-NO, Sneg-NO)`
  - Names of source terms must correspond to names in the lookup table
  - Names can be NULL for no source term: reduces to transport of passive scalar
- Non-transported lookup variables (looked up for visualization)
  - config.cfg: `LOOKUP_NAMES=(Src-PV, MolarWeightMixture, Y-CO-TABLE)`
- Lookup table: ASCII file with unstructured data
  - config.cfg: `FILENAME_LUT = chemtable.drg`

[7]: T.D. Economon, AIAA Journal 58:2 (2020) 757-769.

Implementation in SU2
Model validation

Test case for validation / verification



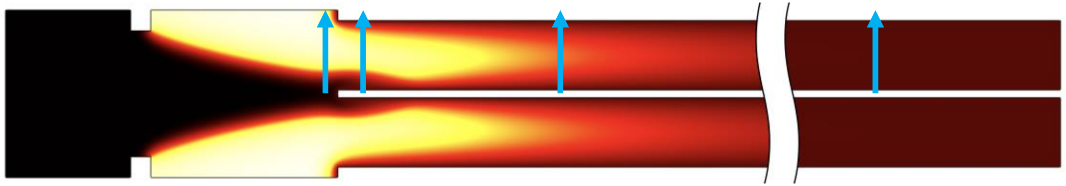
Investigated operating points

	$p = 4.5\,\mathrm{mm}$	$p = 6.5\,\mathrm{mm}$	$p = 8.5\,\mathrm{mm}$
Adiabatic wall	p0.adia	p1.adia	p2.adia
$T_{\mathrm{wall}} = 1800\,\mathrm{K}$	p0.1800	p1.1800	p2.1800
$T_{\mathrm{wall}} = 1500\,\mathrm{K}$	p0.1500	p1.1500	p2.1500
$T_{\mathrm{wall}} = 1200\,\mathrm{K}$	p0.1200	p1.1200	p2.1200
$T_{\mathrm{wall}} = 900\,\mathrm{K}$	p0.0900	p1.0900	p2.0900
$T_{\mathrm{wall}} = 600\,\mathrm{K}$	p0.0600	p1.0600	p2.0600
$T_{\mathrm{wall}} = 300\,\mathrm{K}$	p0.0300	p1.0300	p2.0300

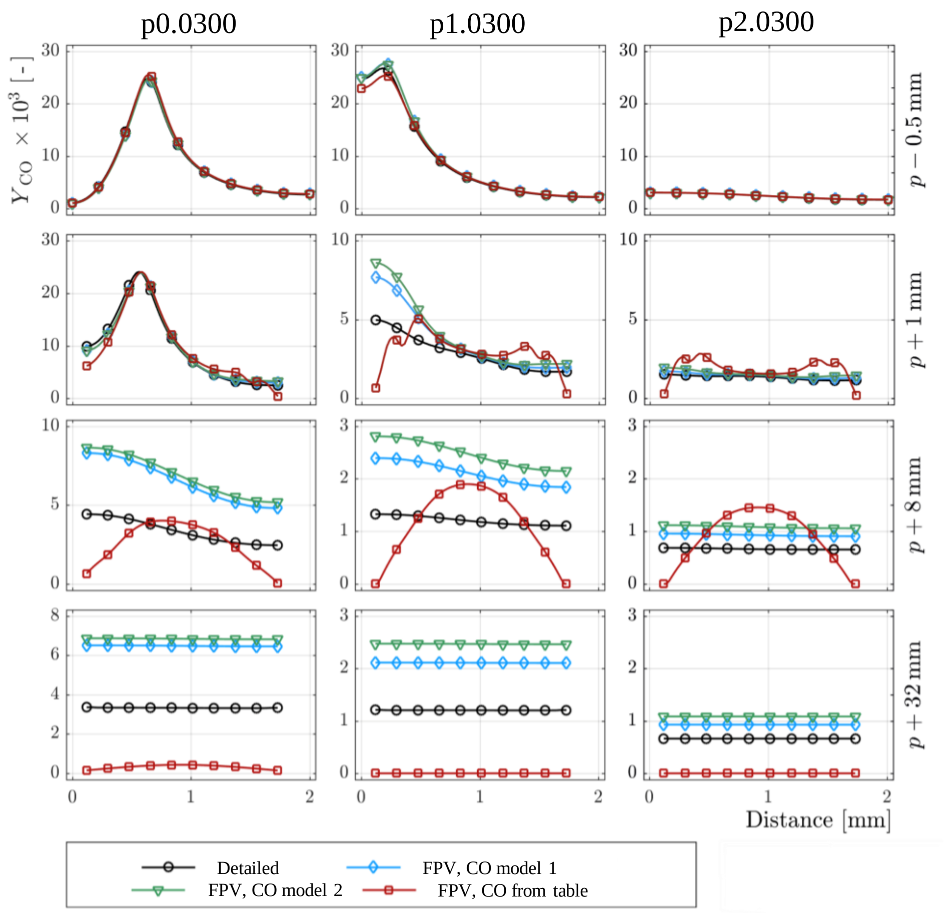
Validation data generated with detailed chemistry CFD code CIAO [8]

[8]: Institute for Technical Combustion of the RWTH Aachen University, www.itv.rwth-aachen.de

Implementation in SU2
Model validation



Blue arrows: plot lines in figure on the left



- 3 models with different computational costs investigated
- Table look-up (red) is not physically correct
- Model 1 (blue) shows best agreement but expensive
- Model 2 (green) shows best accuracy/cost trade-off

Model used in this work

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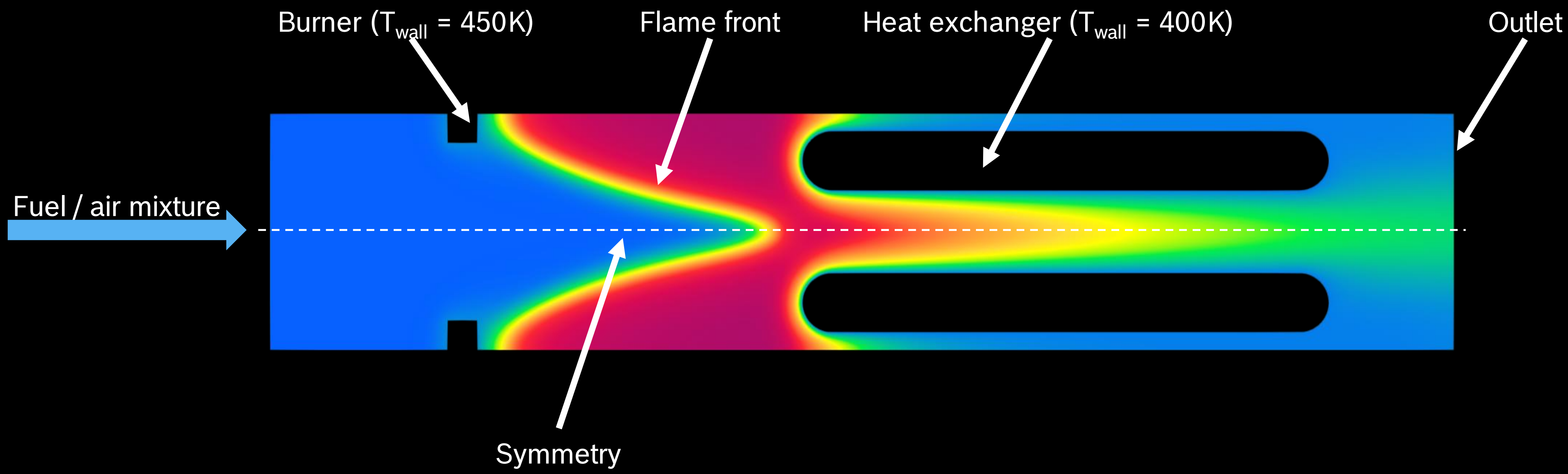
OUTLOOK

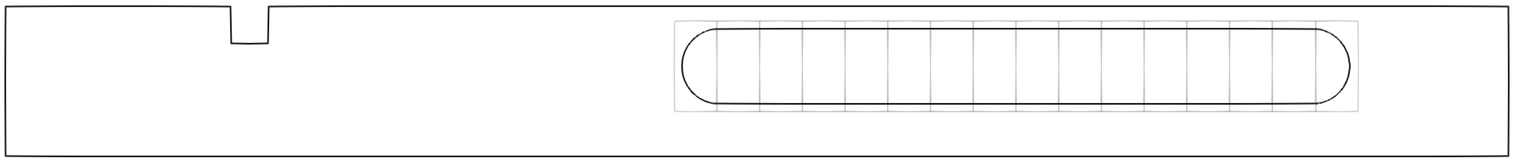
Application to Optimization
Case setup



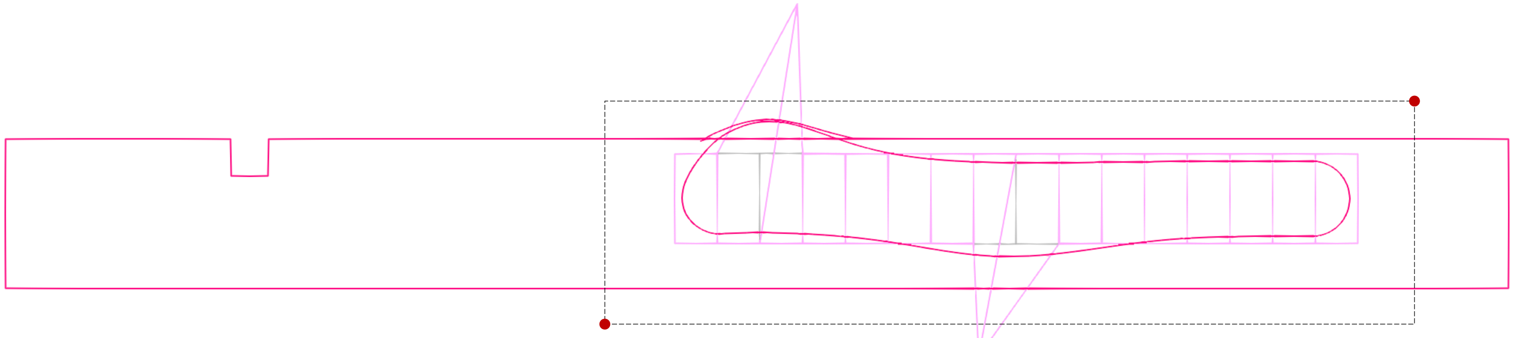
Goal: Shape optimization of heat exchanger geometry to reduce Y_{CO}, Y_{NO}, & Temperature

Application to Optimization
Geometrical deformation constraints

Original geometry and FFD box

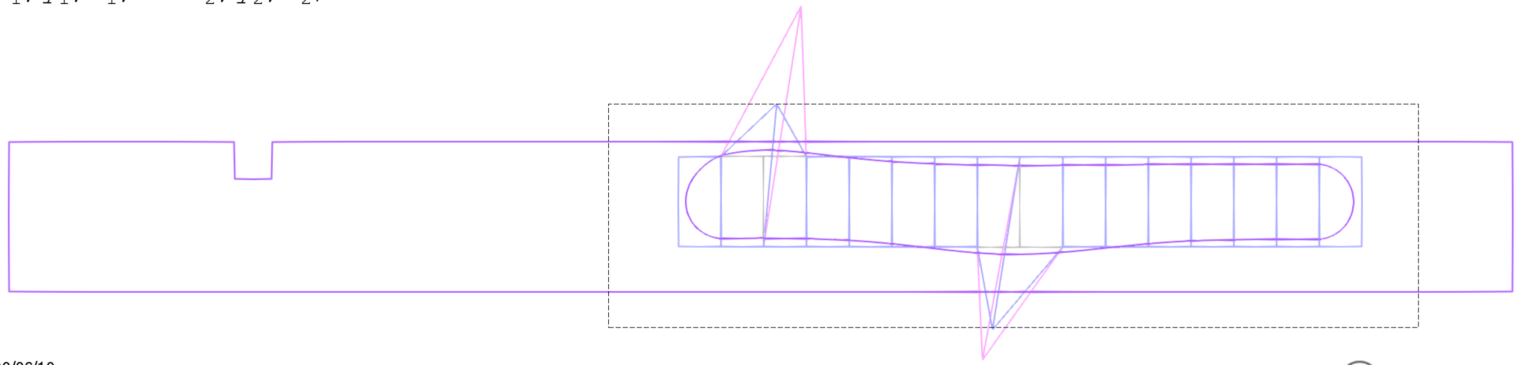


Deformed geometry and FFD box without constraints



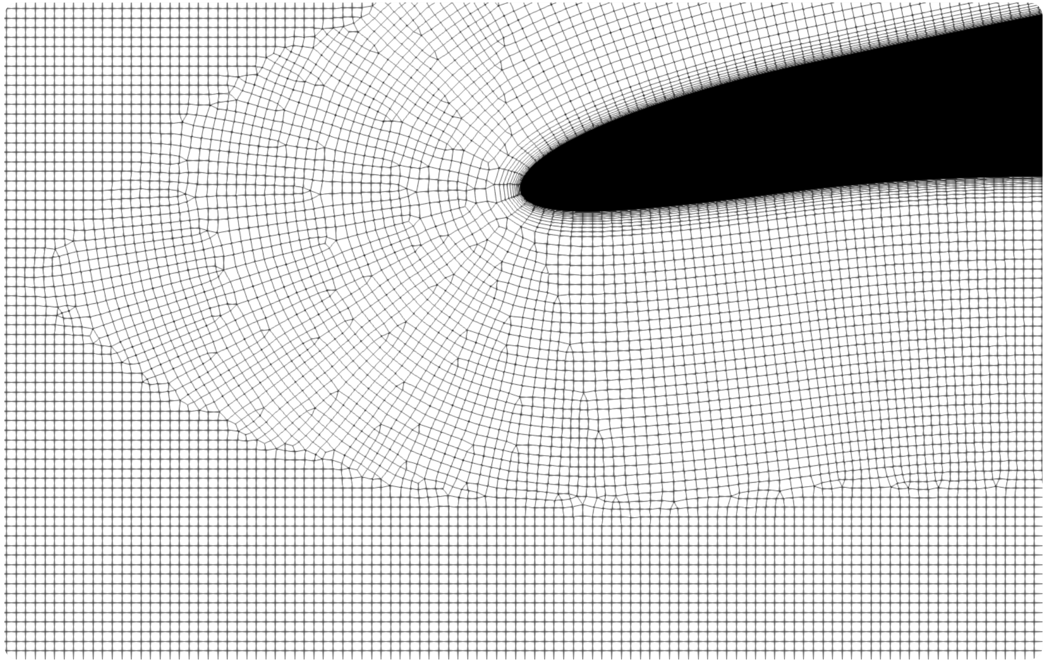
config.cfg: `FFD_BOUNDS = (<FFD BOX ID>,  x1,y1,z1,  x2,y2,z2)`

Deformed geometry and FFD box with constraints

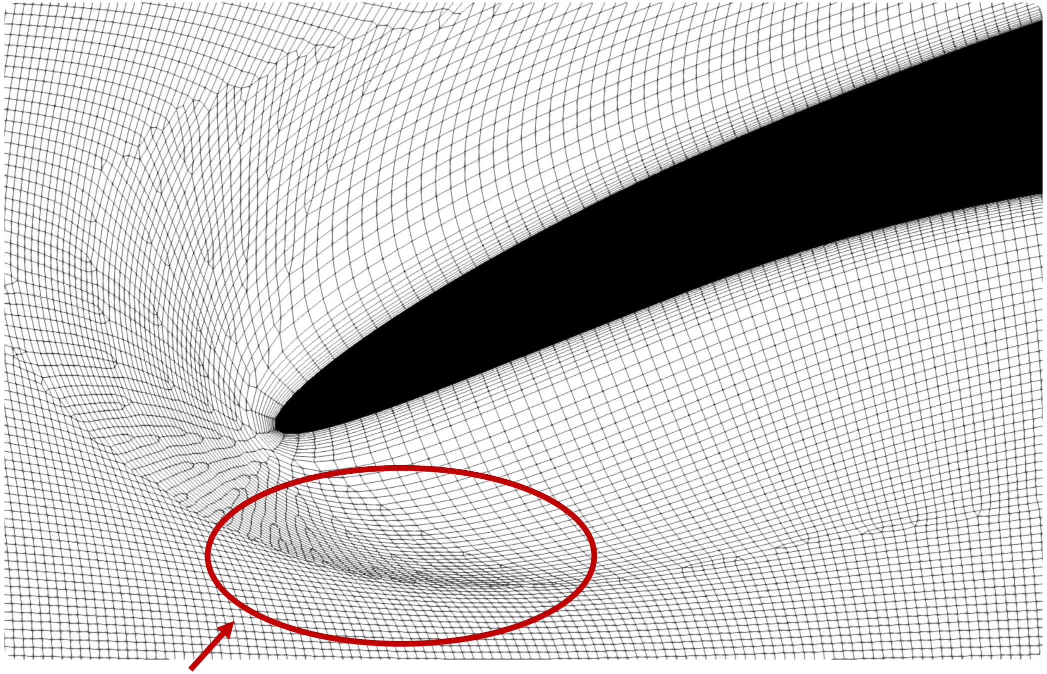


Application to Optimization
Large mesh deformation may result in low mesh quality

Before deformation



After deformation



That's bad.

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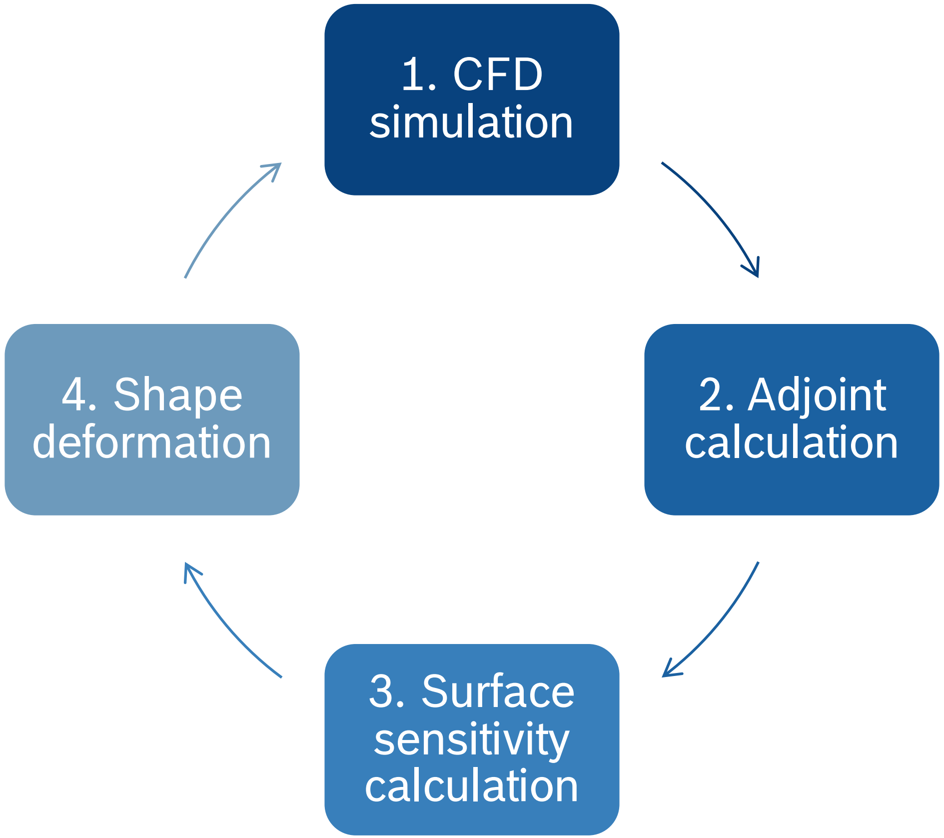
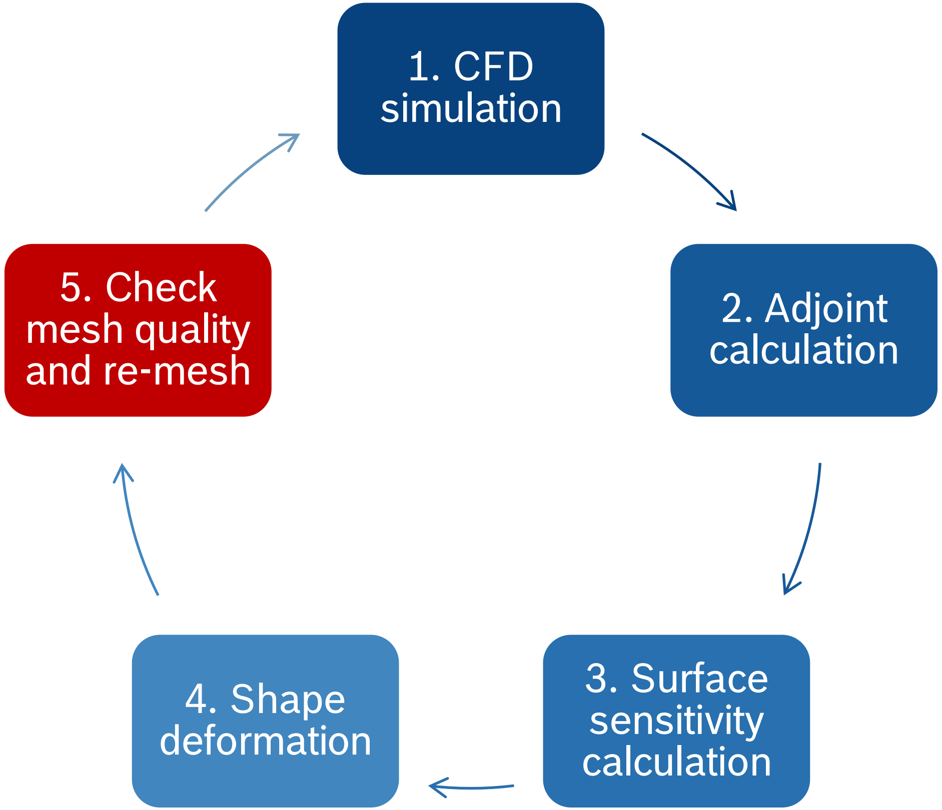
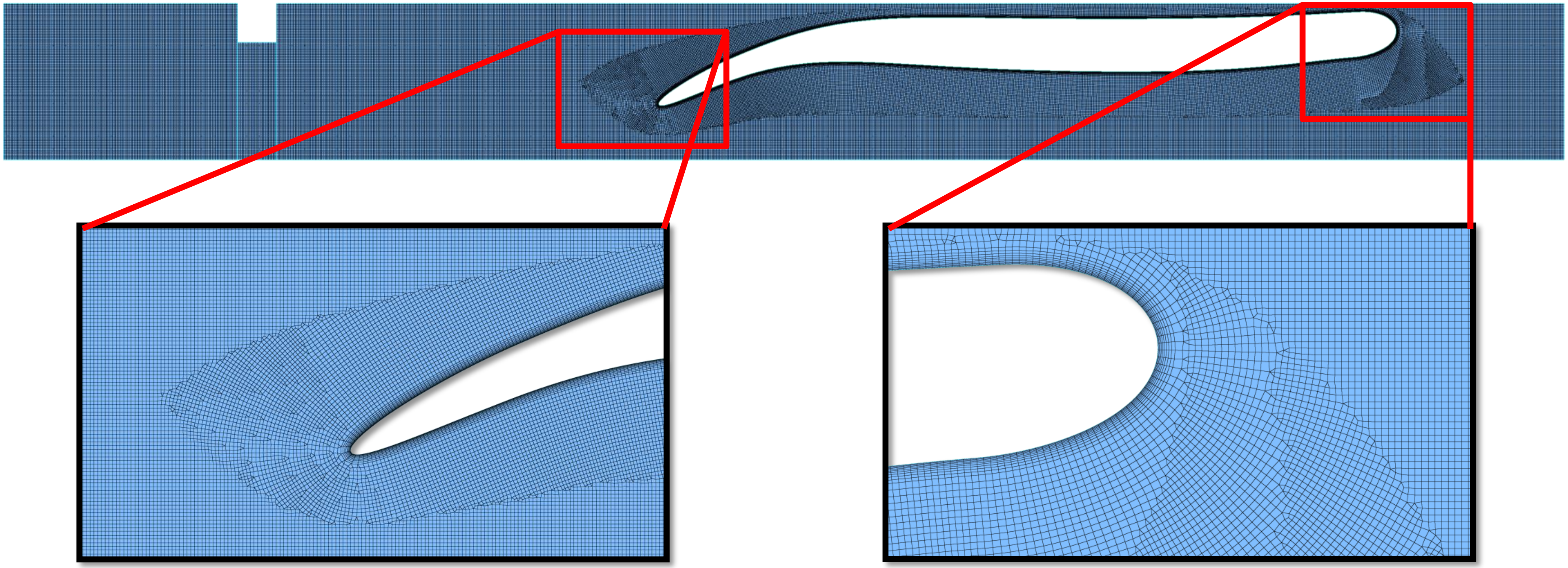
Application to Optimization
Solution: Automated Remeshing



Application to Optimization
Solution: Automated Remeshing

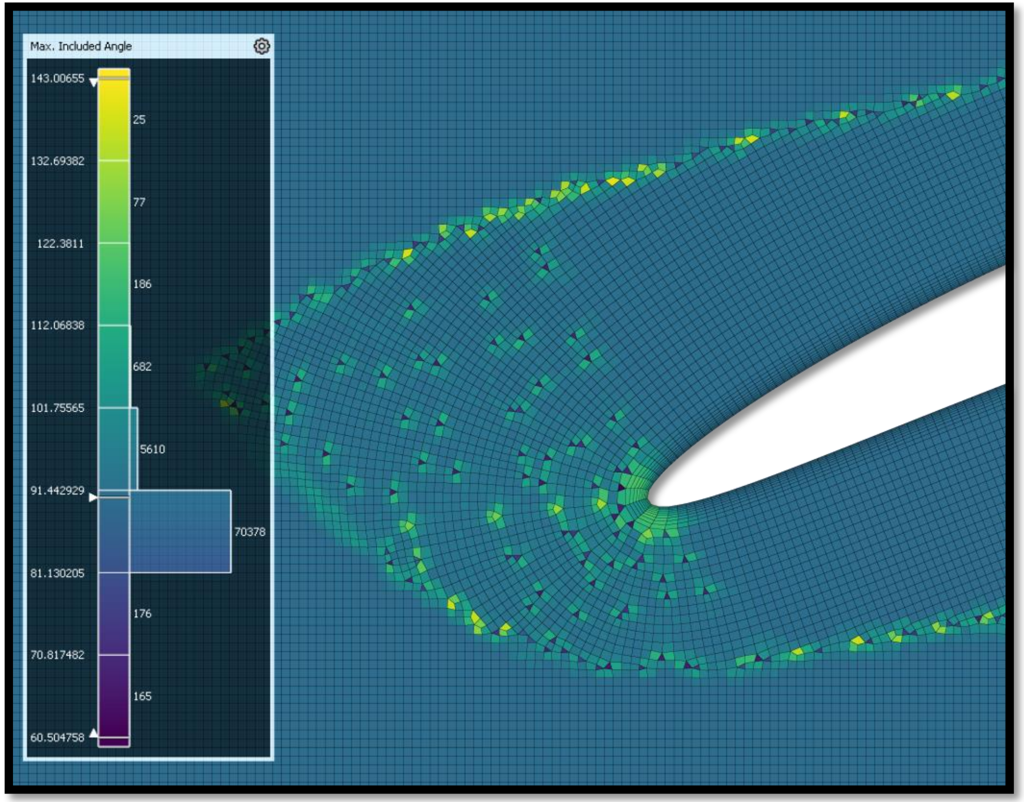


Application to Optimization
Baseline Grid

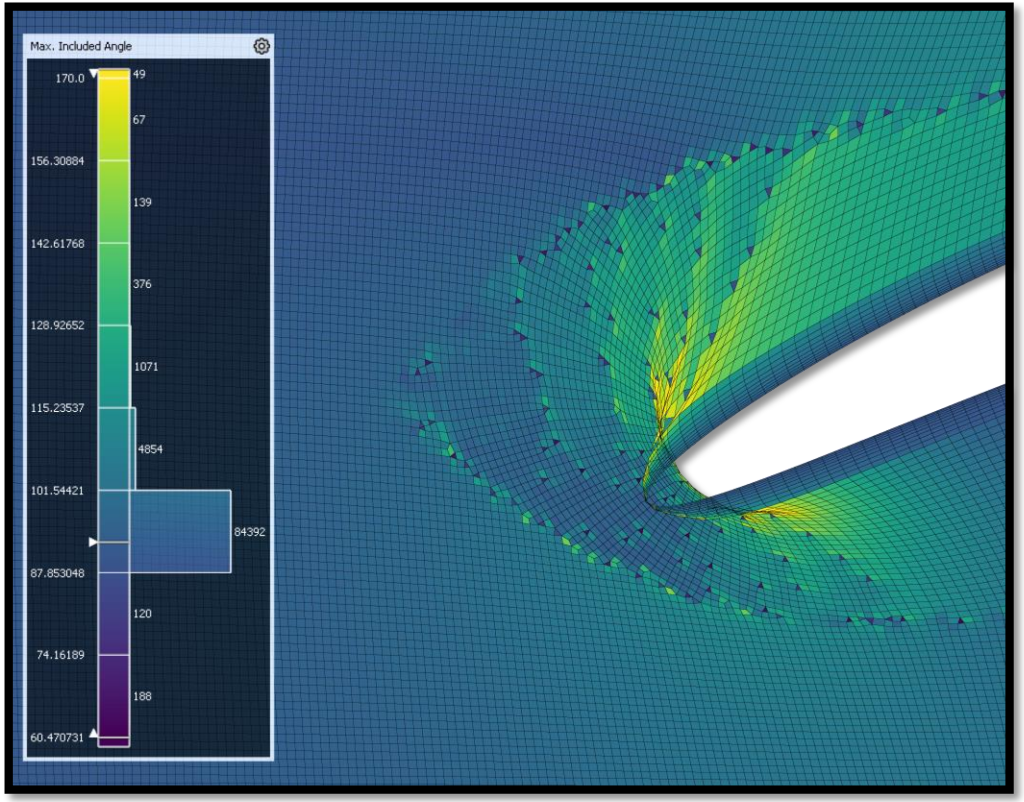


Hybrid quad-dominant grid generated using Pointwise

Application to Optimization
Grid Quality Investigation



Max. Angle < 170 deg.



Max. Angle > 170 deg.

Application to Optimization
Automatic Remeshing

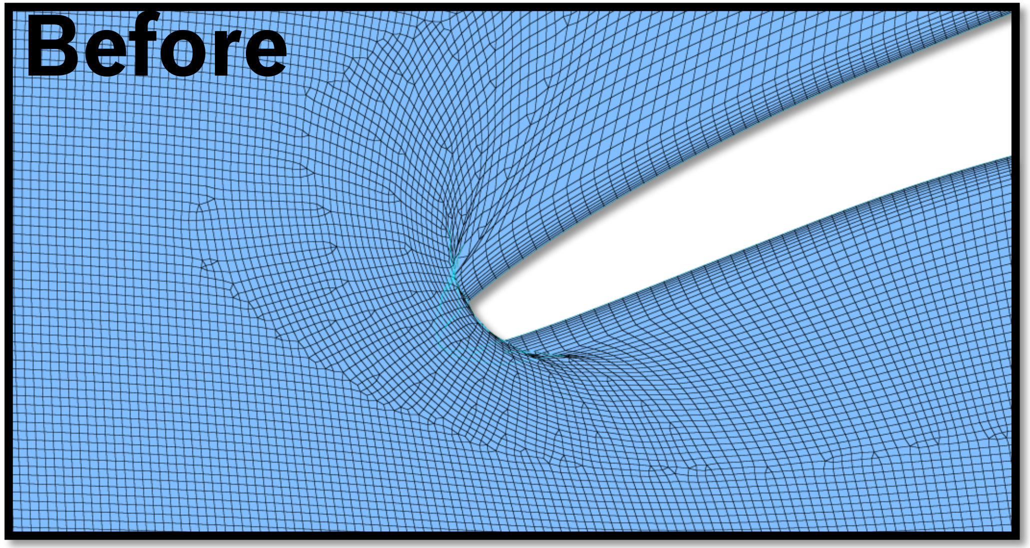
```
package require PWI_Glyph

# User parameters
set filename "mesh_03_deformed_neg_vol_updated"
set quality 170
set interiorEdgeName "wall_probe"
set probeSpacing 2e-5

# Procedure to remove entities from a list
proc lremove {listVariable value} {
    set idx [lsearch -exact $listVariable $value]
    return [lreplace $listVariable $idx $idx]
}

# Load the defaults
set cwd [file dirname [info script]]
pw::Application load "$cwd/Defaults.pw"

# Import the SU2 grid file
set importMode [pw::Application begin GridImport]
    $importMode initialize -strict -type SU2 "$cwd/$filename.su2"
    $importMode setAttribute GridImportConditionData true
    $importMode read
    $importMode convert
$importMode end

set domains [pw::Grid getAll -type pw::Domain]
set connectors [pw::Grid getAll -type pw::Connector]

# Examine grid quality
set examine [pw::Examine create DomainMaximumAngle]
    $examine addEntity $domains
    $examine examine
    set max [$examine getMaximum]

puts "Max. Angle = $max deg."

if {$max > $quality} {
    puts "Quality lower than re-meshing threshold."
    puts "Begin re-meshing operation."
} else {
    puts "Quality higher than re-meshing threshold."
    puts "Exiting."
    exit
}
```

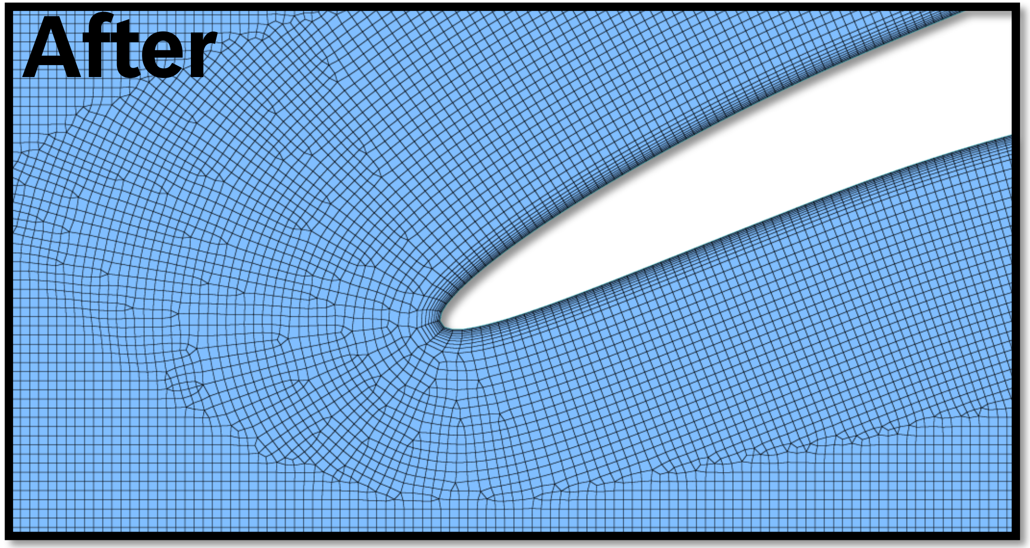
config.cfg:

```
ENABLE_REMESHING = YES
```

Provide files:

```
pointwise_defaults.pw
pointwise_remesh.glf
```



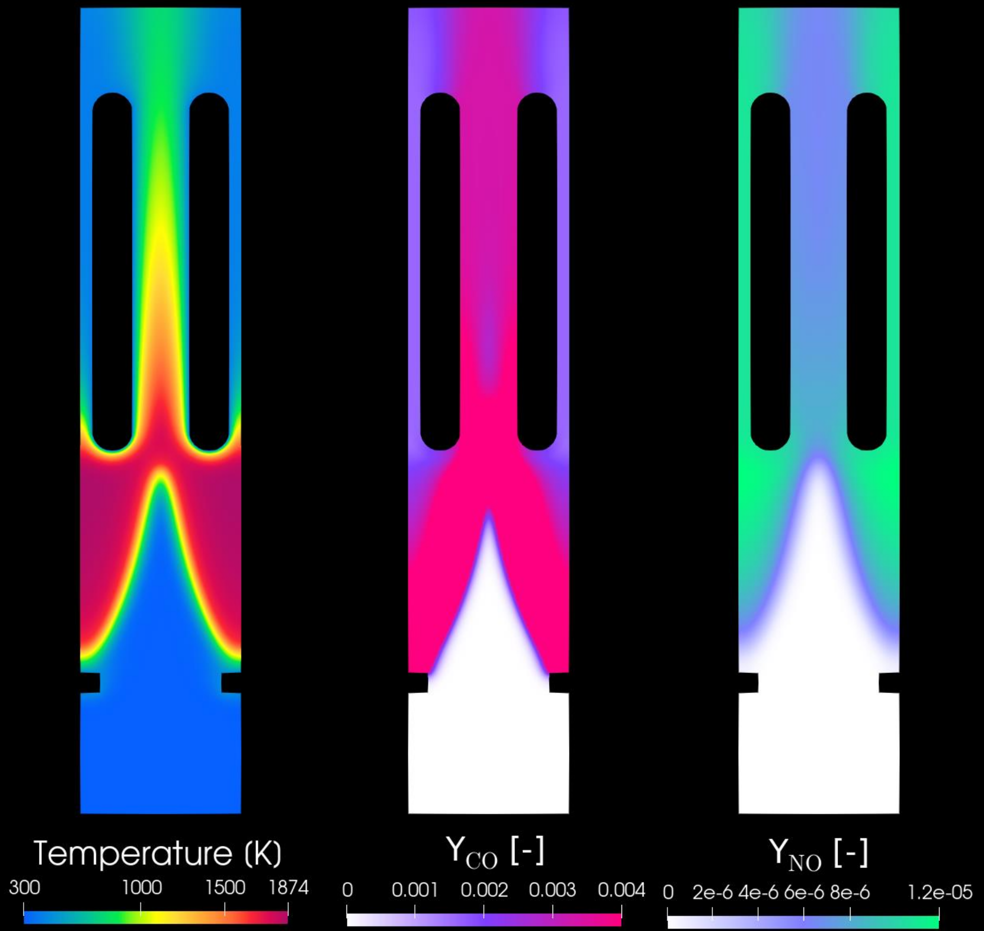


Application to Optimization
Results

5 optimizations were performed with the following objective weights:

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

Baseline



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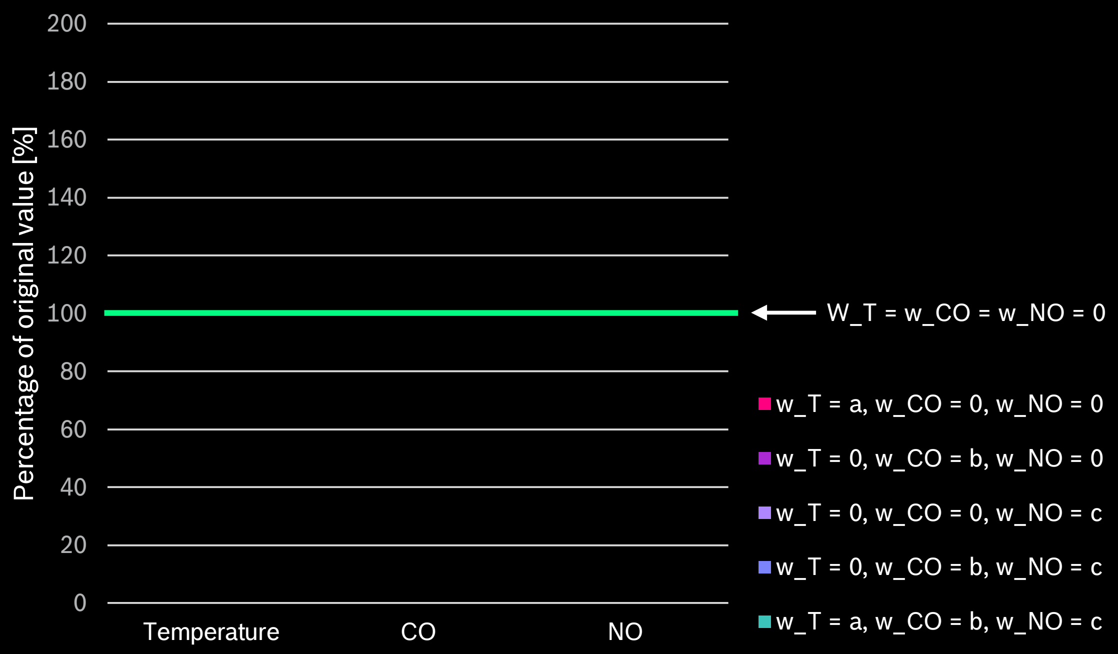
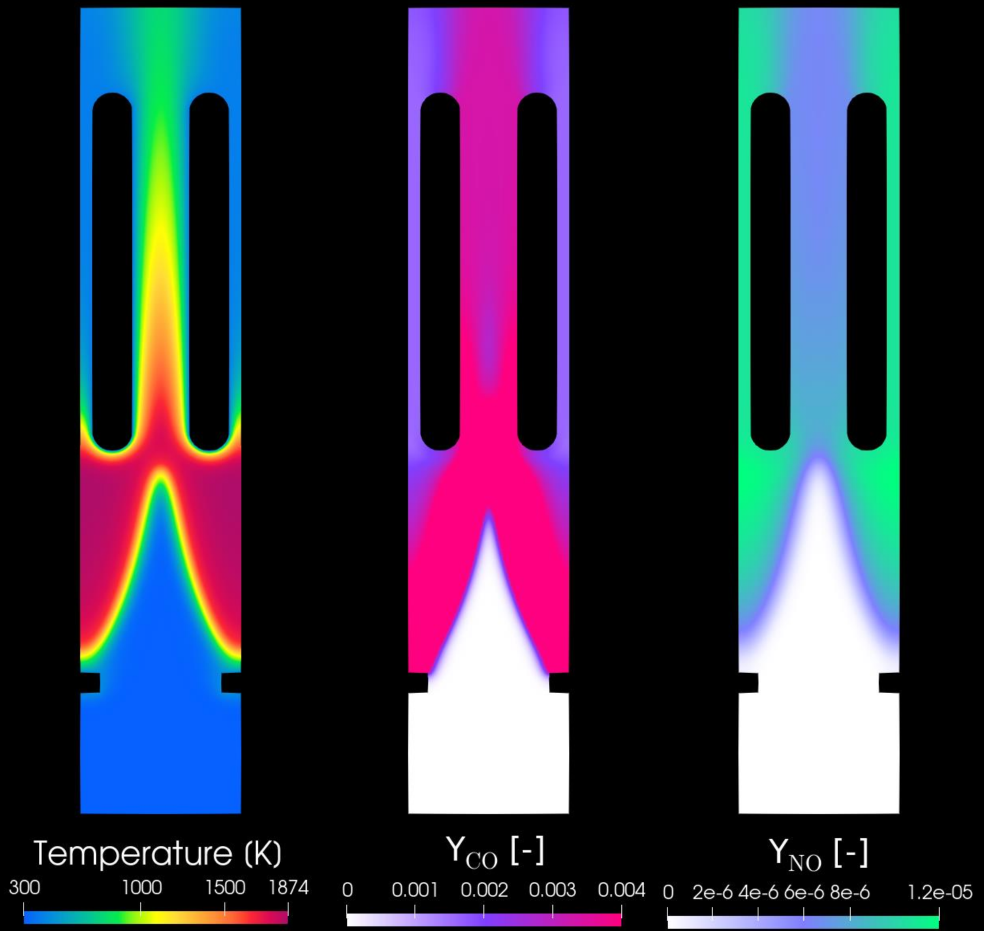
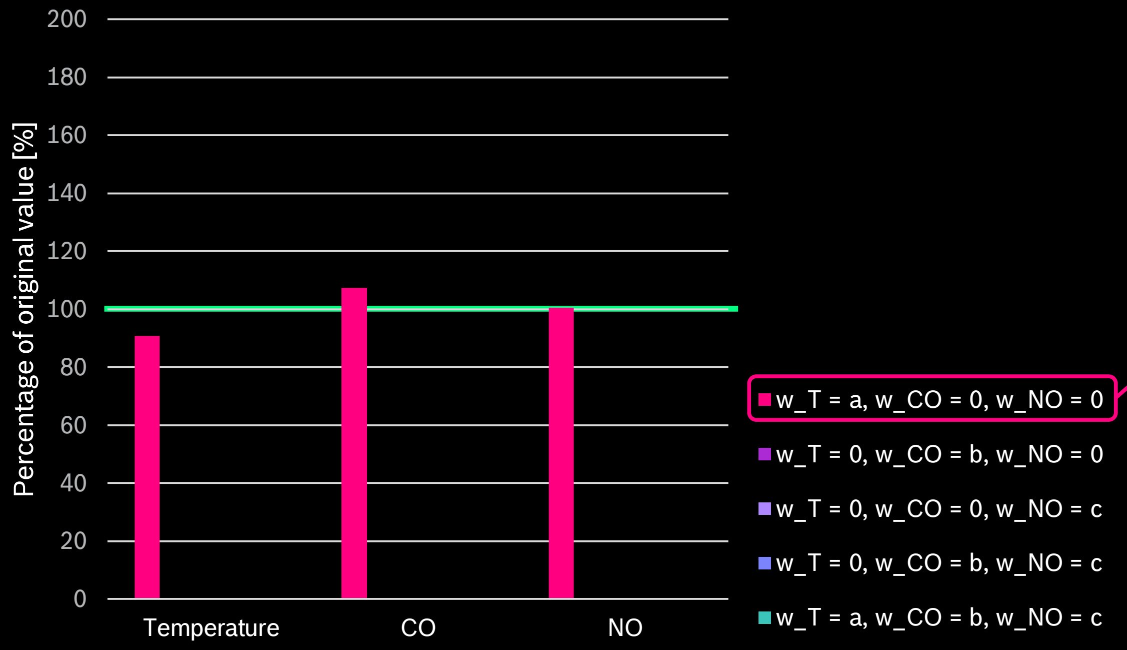
Application to Optimization
Results



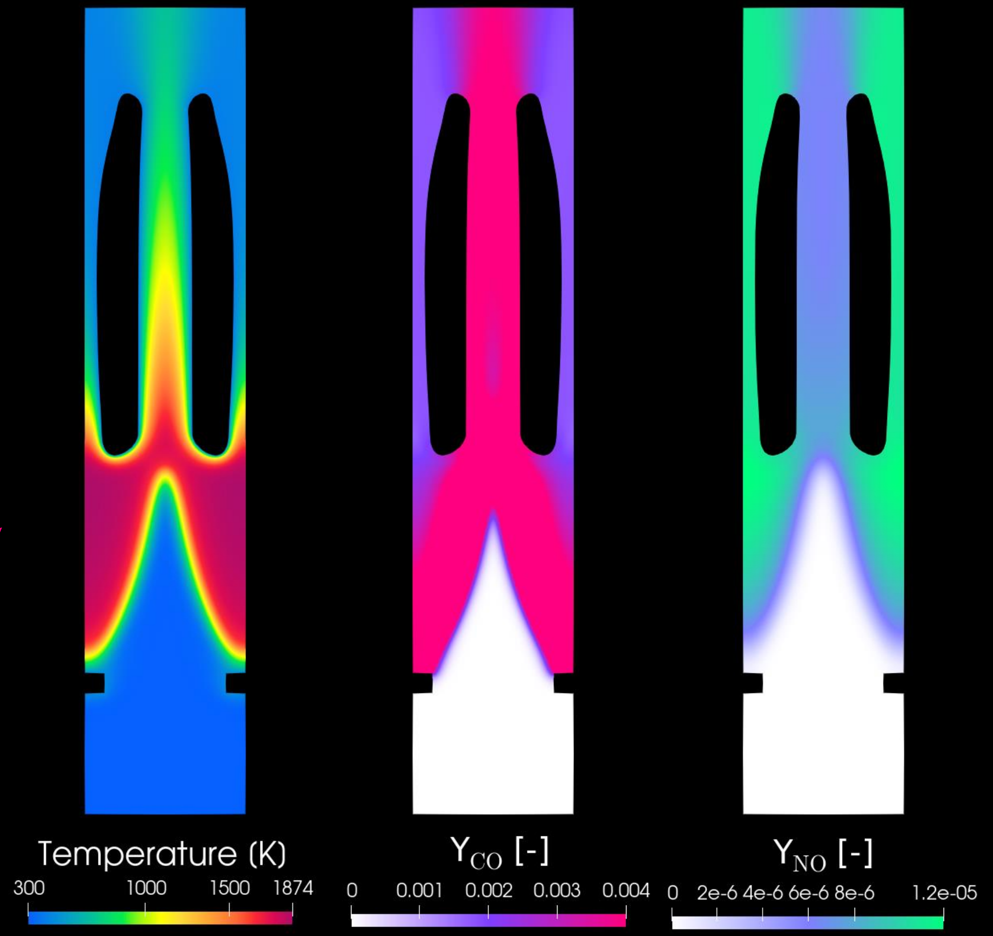
Baseline



Application to Optimization
Results



Optimize Temperature only



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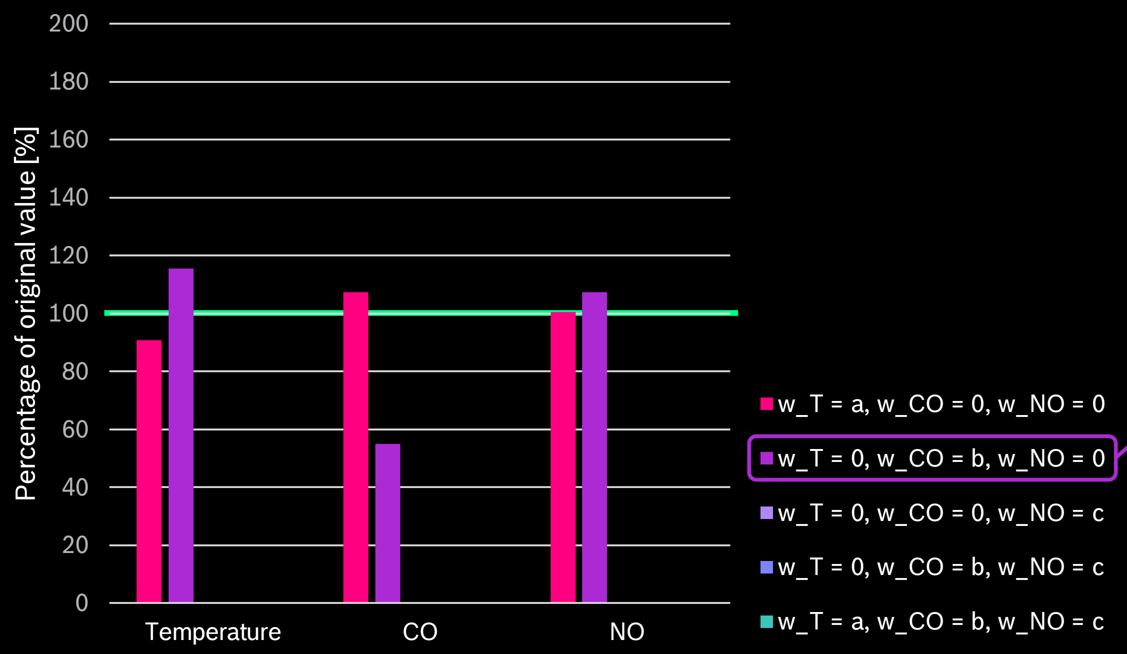
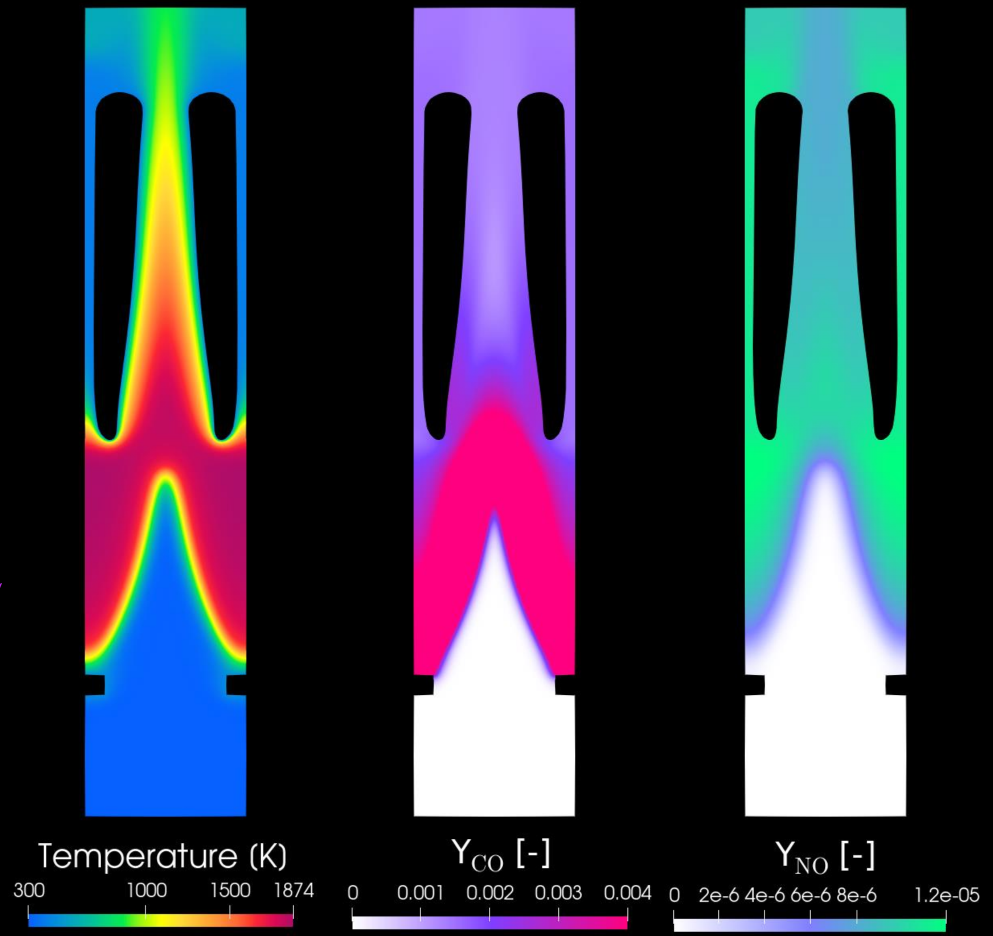
Application to Optimization
Results



Optimize Y_{CO} only



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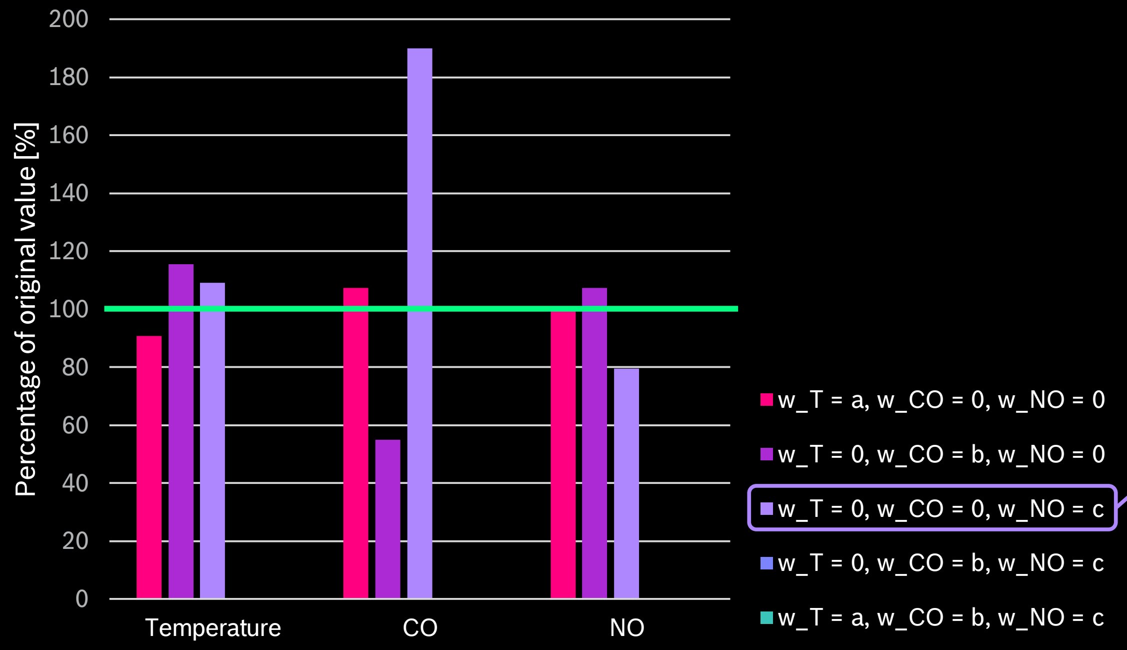
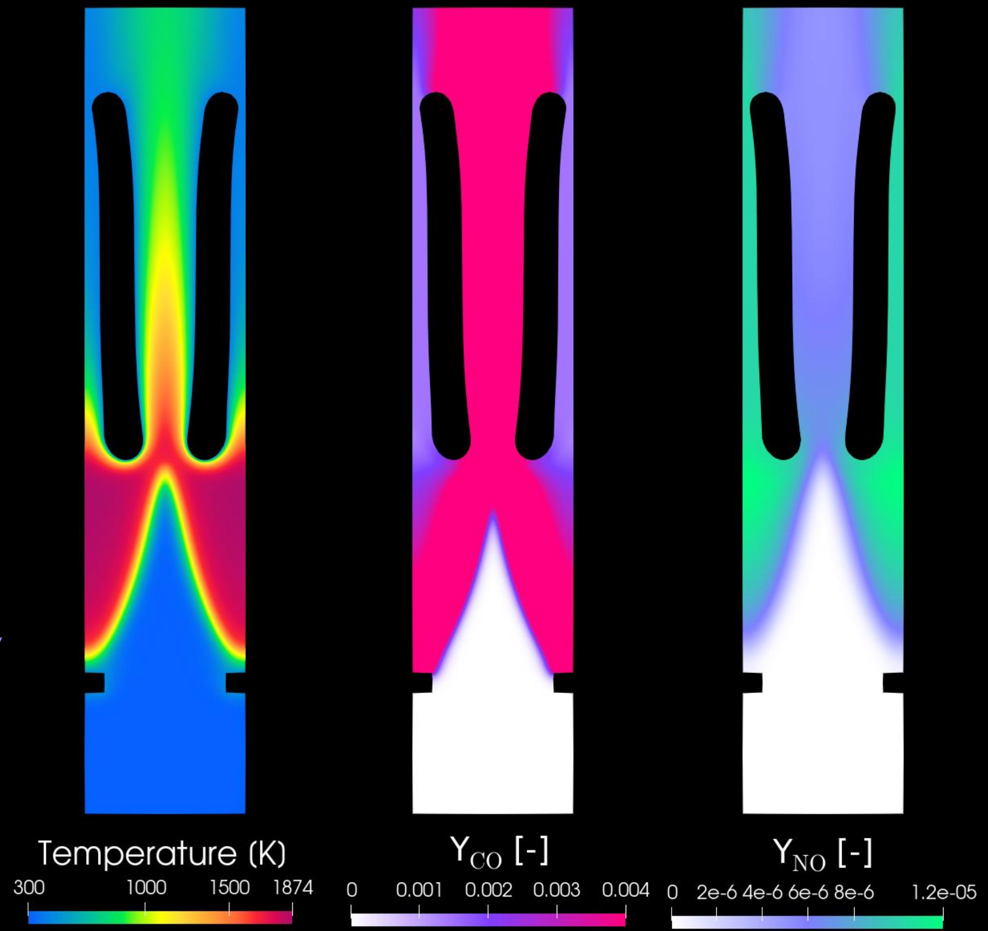
BOSCH

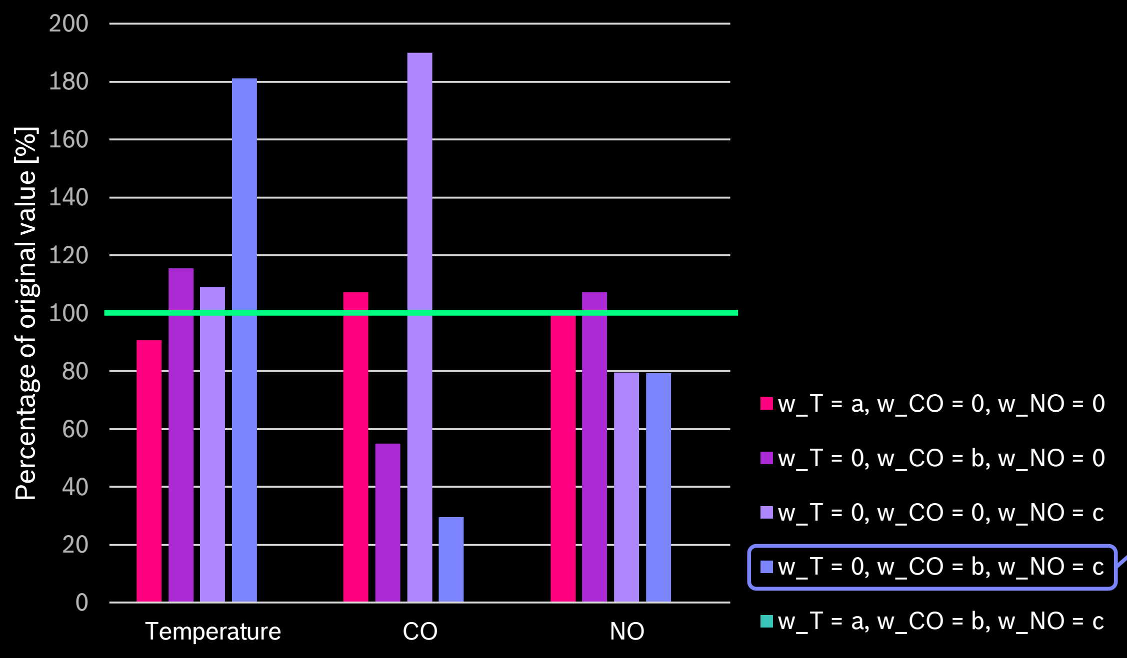
Application to Optimization
Results

Optimize Y_{NO} only

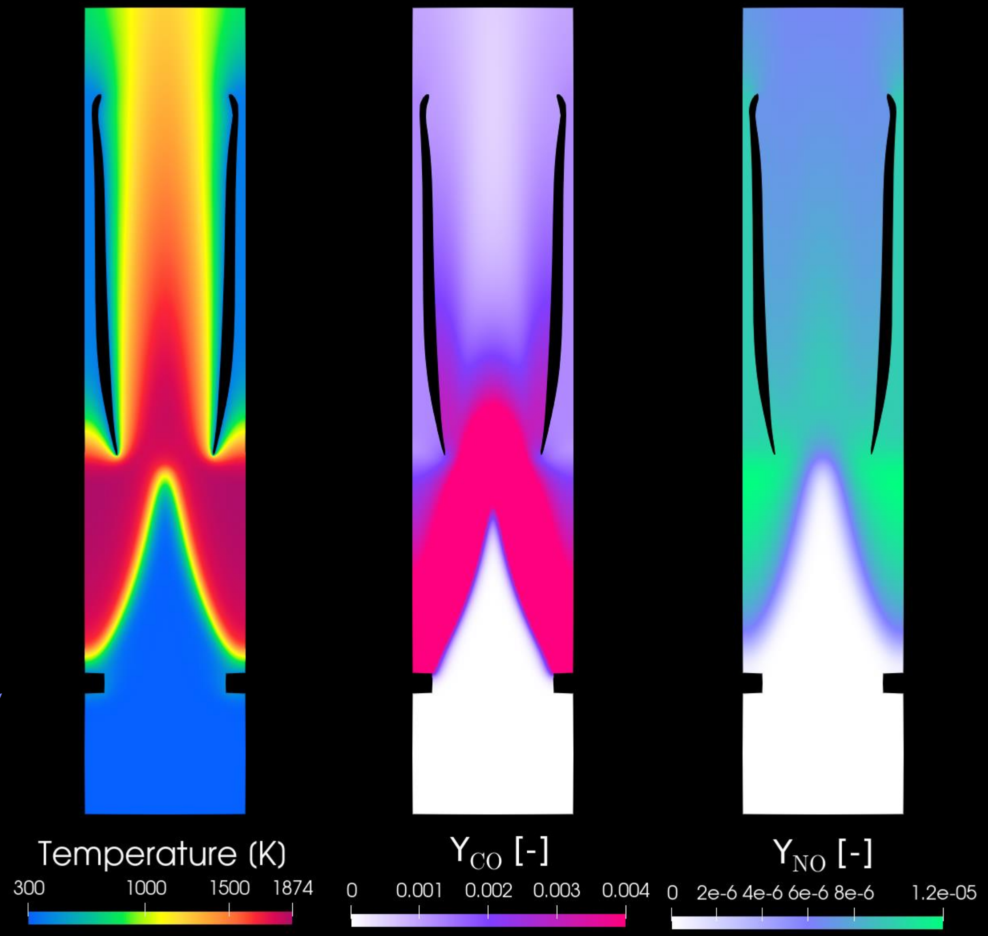




Application to Optimization
Results



Optimize Y_{CO} & Y_{NO}



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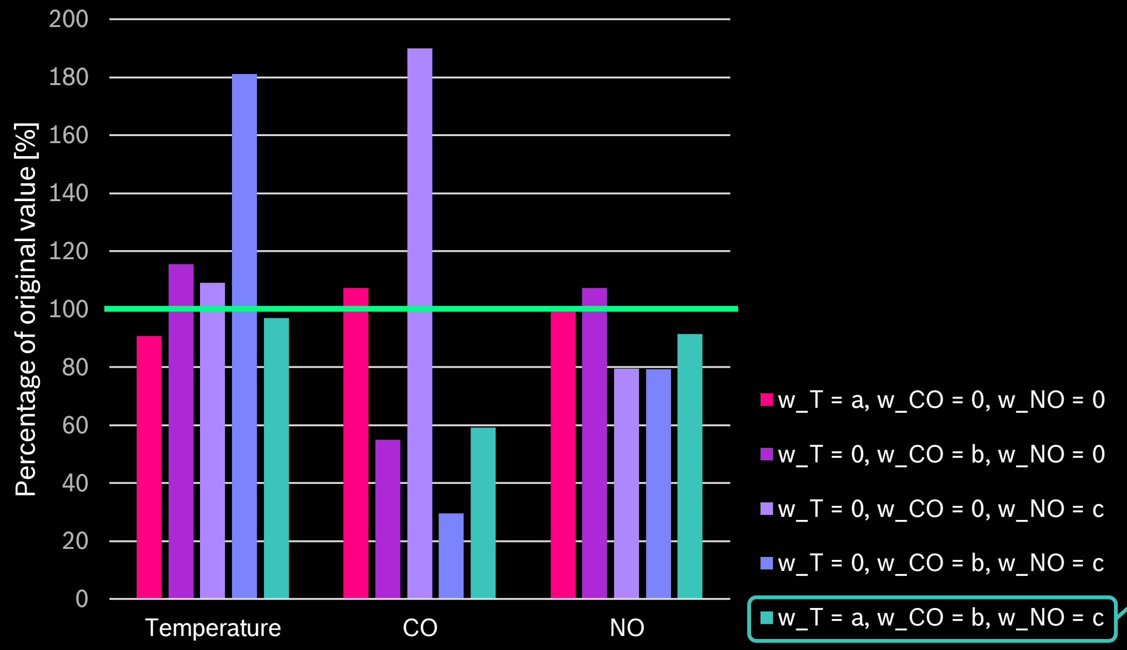
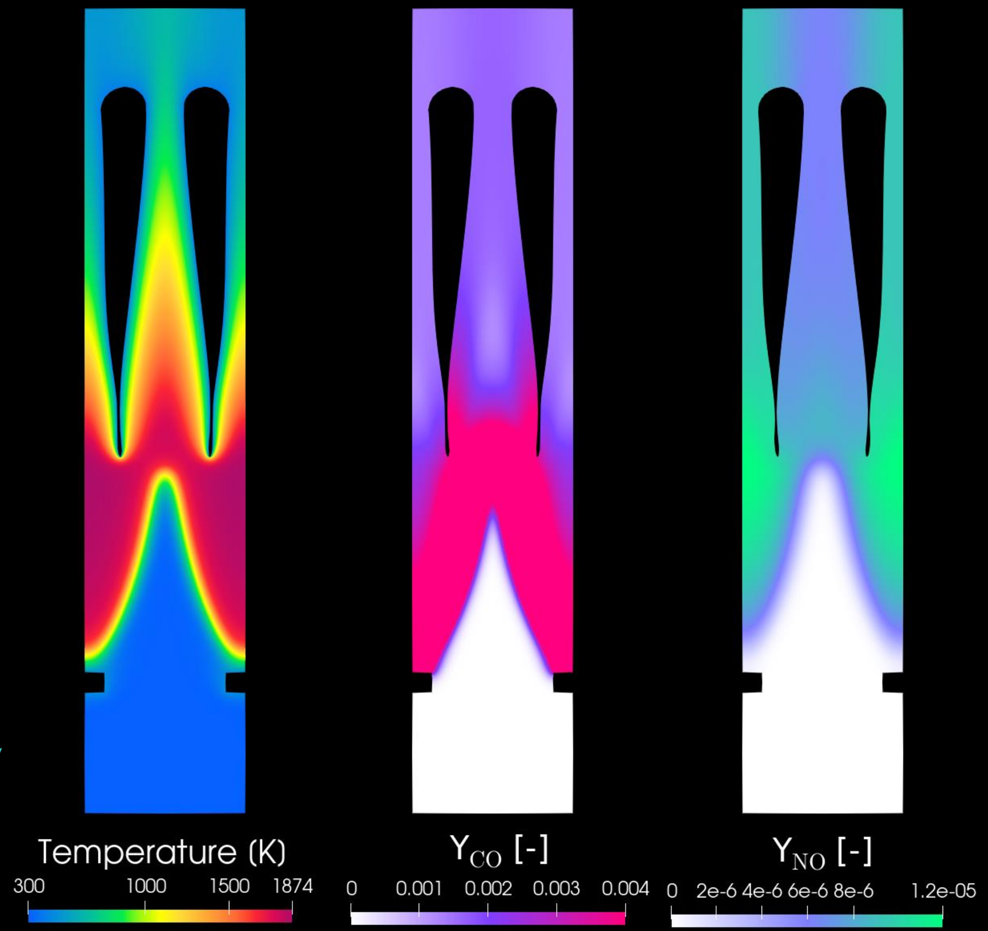
Application to Optimization
Results



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



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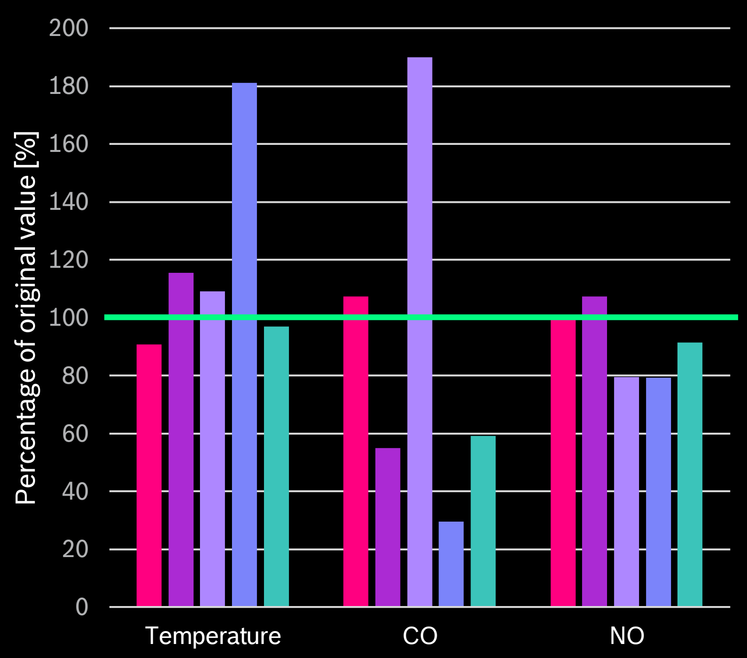
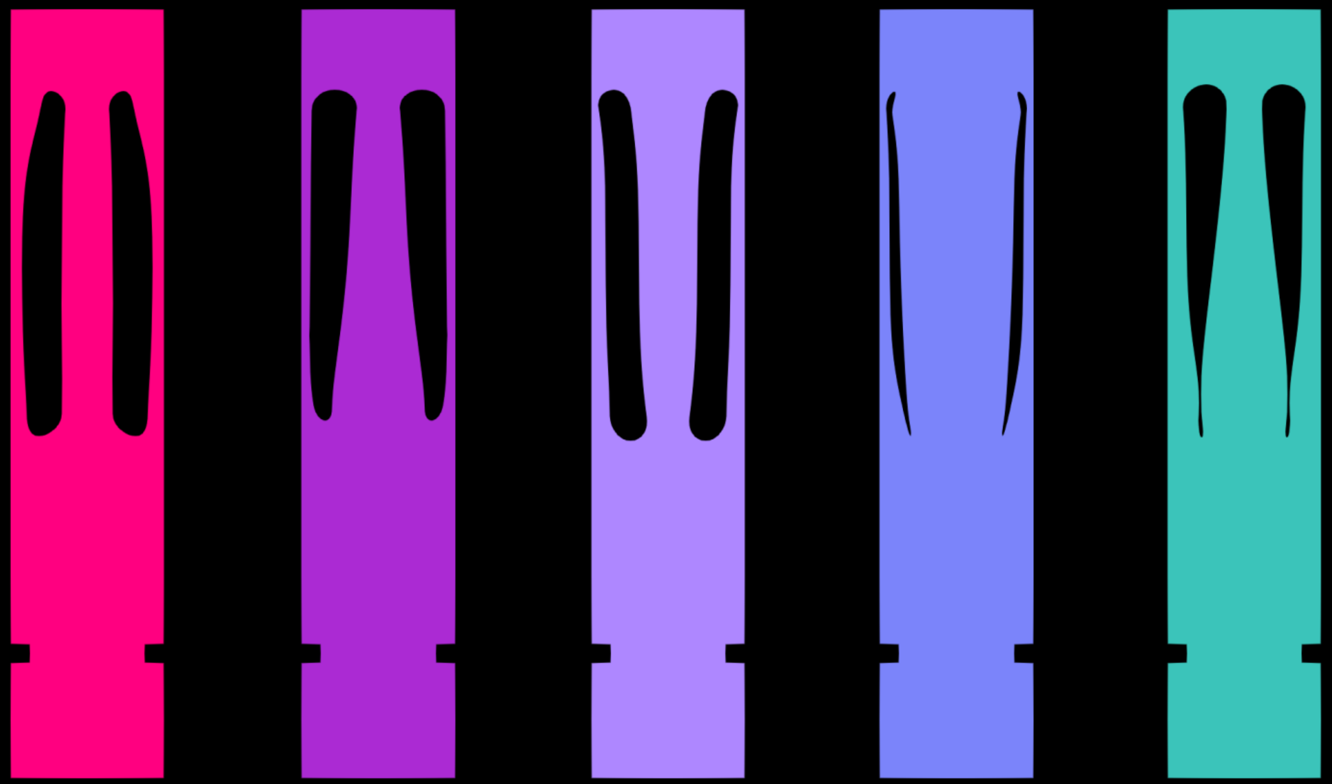
Application to Optimization
Results

Optimization objectives: T Y_{CO} Y_{NO} Y_{CO}, Y_{NO} Y_{CO}, Y_{NO}, T





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COMBUSTION MODELLING

DETAILED CHEMISTRY MODELLING
THE FLAMELET PROGRESS VARIABLE (FPV) APPROACH
WORKFLOW / TOOL CHAIN

MODEL IMPLEMENTATION IN SU2

ARCHITECTURE
CONFIGURATION
MODEL VALIDATION

APPLICATION TO ADJOINT OPTIMIZATION

CASE SETUP
GEOMETRICAL DEFORMATION CONSTRAINTS
AUTOMATED REMESHING
RESULTS

OUTLOOK

BOSCH

OUTLOOK

Implementation of more sophisticated geometrical constraints

Application to more realistic 3D heat exchanger geometry

Inclusion of conjugate heat transfer model

Hydrogen combustion ➔ partially premixed flames, 3D lookup tables

THANK YOU