Towards the modelling of combustion systems

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Background

Background

- More than 85% of the energy produced today is by combustion (it might change!)
- Primary source of propulsive systems
- Main source of pollution
- Climate change effects

Motivation

Optimization of new combustor designs towards systems with:

- Increased efficiency
- Low emissions
- Fuel flexibility

Complex physical phenomena requiring **multiphysics coupling** and **high-fidelity** numerical situations

Develop **full-engine simulations** with emphasis on the prediction of engine performance, prediction of instabilities and pollutant formation

Outline

A. Modelling approach
- Multiscale problem
- Challenges

B. Physical modelling
- Fluid mechanics
- Combustion chemistry
- Turbulence
- Tabulated chemistry

D. Computational framework

E. Practical applications
- Aeronautical combustor
- SGT5-8000H staged can combustor

MODELLING APPROACH

Modelling approach

Multiscale approach

- Solving fluid mechanics
- Solving chemistry

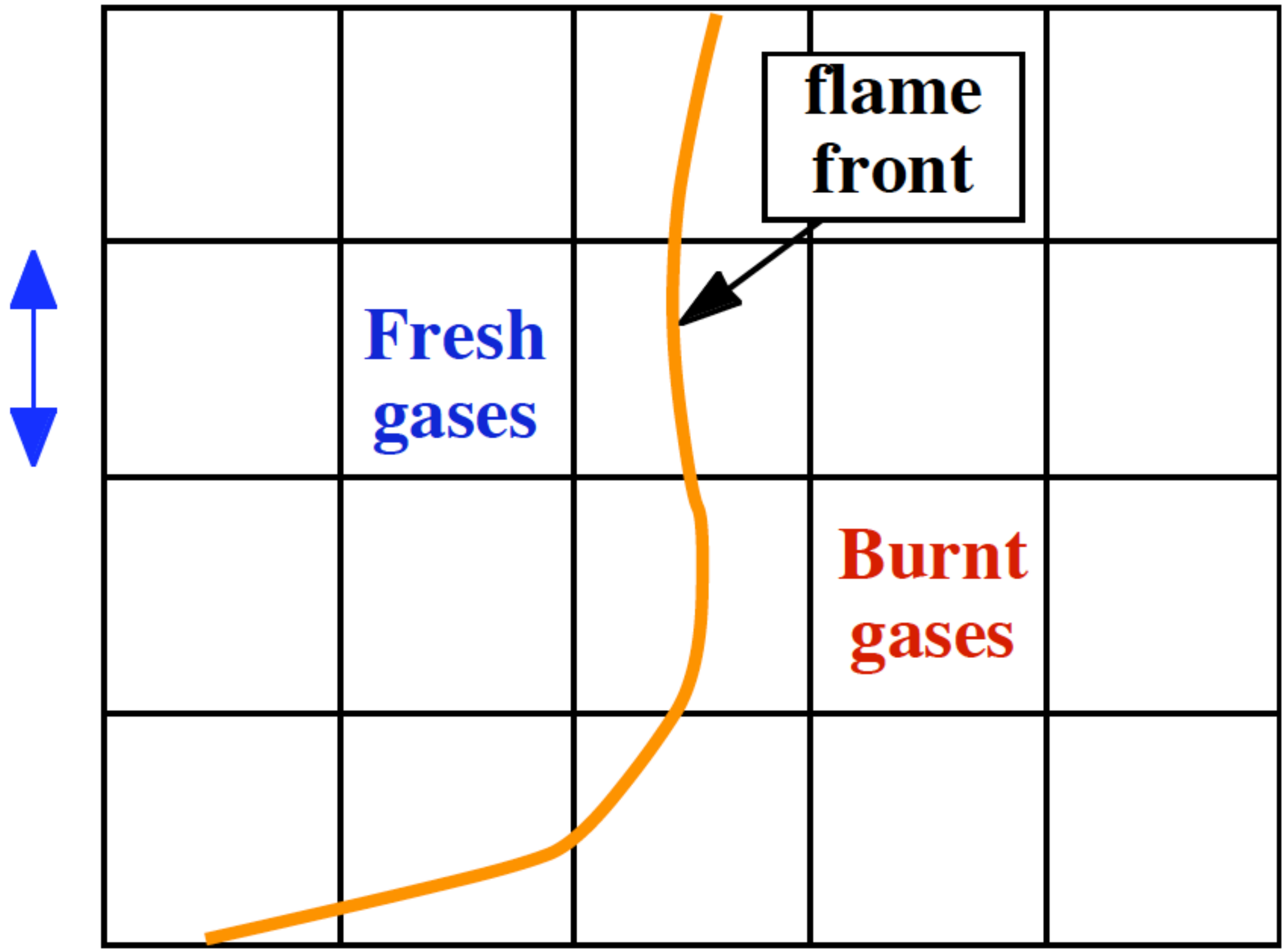
→ Fully coupled system!

- Complex geometries
- Moving/rotating parts

Modelling approach

Challenges

Combustion takes place in the flame front within the subgrid scale



PHYSICAL MODELLING

Physical modelling

Navier-Stokes equations

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_j)}{\partial x_j} = 0$$

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_j u_i)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j}$$

$$p = \rho R^0 \sum_{m=1}^{N} \frac{Y_m}{W_m} T$$

$$\frac{\partial(\rho E)}{\partial t} + \frac{\partial(\rho u_j E)}{\partial x_j} = \frac{\partial}{\partial x_j}\left(K \frac{\partial T}{\partial x_j}\right) + \frac{\partial}{\partial x_j}(\rho \sum_{m=1}^{N} h_m Y_m V_{m,j}) - \frac{\partial(p u_j)}{\partial x_j} + \frac{\partial(\tau_{ij} u_i)}{\partial x_j} + \dot{Q}^c$$

Represented by 325 reversible chemical reactions and 53 reactive species!

Number	Reaction		A	n	E	Ref.
1f	$H + O_2 \rightleftharpoons OH + O$		3.520E+16	-0.70	71.4	[1]
2f	$H_2 + O \rightleftharpoons OH + H$		5.060E+04	2.67	26.3	[1]
3f	$H_2 + OH \rightleftharpoons H_2O + H$		1.170E+09	1.30	15.2	[1]
4f	$H_2O + O \rightleftharpoons 2\ OH$		7.600E+00	3.84	53.5	[1]
5f[a]	$2\ H + M^{(1)} \rightleftharpoons H_2 + M^{(1)}$		1.300E+18	-1.00	0	[2]
6f[a]	$H + OH + M^{(2)} \rightleftharpoons H_2O + M^{(2)}$		4.000E+22	-2.00	0	[2]
7f[a]	$2\ O + M^{(3)} \rightleftharpoons O_2 + M^{(3)}$		6.170E+15	-0.50	0	[2]
8f[a]	$H + O + M^{(4)} \rightleftharpoons OH + M^{(4)}$		4.710E+18	-1.00	0	[2]
9f[a]	$O + OH + M^{(4)} \rightleftharpoons HO_2 + M^{(4)}$		8.000E+15	0.00	0	[2]
10f[a,b]	$H + O_2 + M^{(5)} \rightleftharpoons HO_2 + M^{(5)}$	k_0	5.750E+19	-1.40	0	[3, 2]
		k_∞	4.650E+12	0.44	0	
11f	$HO_2 + H \rightleftharpoons 2\ OH$		7.080E+13	0.00	1.23	[4]
12f	$HO_2 + H \rightleftharpoons H_2 + O_2$		1.660E+13	0.00	3.44	[4]
13f	$HO_2 + H \rightleftharpoons H_2O + O$		3.100E+13	0.00	7.2	[1]
14f	$HO_2 + O \rightleftharpoons OH + O_2$		2.000E+13	0.00	0	[5]
15f	$HO_2 + OH \rightleftharpoons H_2O + O_2$		2.890E+13	0.00	-2.08	[1]
16f[a,b]	$2\ OH + M^{(6)} \rightleftharpoons H_2O_2 + M^{(6)}$	k_0	2.300E+18	-0.90	-7.12	[1]
		k_∞	7.400E+13	-0.37	0	
17f	$2\ HO_2 \rightleftharpoons H_2O_2 + O_2$		3.020E+12	0.00	5.8	[1]
18f	$H_2O_2 + H \rightleftharpoons HO_2 + H_2$		2.300E+13	0.00	33.3	[6]
19f	$H_2O_2 + H \rightleftharpoons H_2O + OH$		1.000E+13	0.00	15	[7]
20f	$H_2O_2 + OH \rightleftharpoons H_2O + HO_2$		7.080E+12	0.00	6	[1]
21f	$H_2O_2 + O \rightleftharpoons HO_2 + OH$		9.630E+06	2.00	16.7	[1]
a21f[a,b]	$CO + O + M^{(11)} \rightleftharpoons CO_2 + M^{(11)}$	k_0	1.550E+24	-2.79	17.5	[6]
		k_∞	1.800E+11	0.00	9.97	
22f	$CO + OH \rightleftharpoons CO_2 + H$		4.400E+06	1.50	-3.1	[1]
23f	$CO + HO_2 \rightleftharpoons CO_2 + OH$		2.000E+13	0.00	96	[6]
24f	$CO + O_2 \rightleftharpoons CO_2 + O$		1.000E+12	0.00	200	[2]
25f[a]	$HCO + M^{(7)} \rightleftharpoons CO + H + M^{(7)}$		1.860E+17	-1.00	71.1	[8]
26f	$HCO + H \rightleftharpoons CO + H_2$		5.000E+13	0.00	0	[9]
27f	$HCO + O \rightleftharpoons CO + OH$		3.000E+13	0.00	0	[1]
28f	$HCO + O \rightleftharpoons CO_2 + H$		3.000E+13	0.00	0	[1]
29f	$HCO + OH \rightleftharpoons CO + H_2O$		3.000E+13	0.00	0	[10]
30f	$HCO + O_2 \rightleftharpoons CO + HO_2$		7.580E+12	0.00	1.72	[9]
31f	$HCO + CH_3 \rightleftharpoons CO + CH_4$		5.000E+13	0.00	0	[9]
32f[a,b]	$H + HCO + M^{(8)} \rightleftharpoons CH_2O + M^{(8)}$	k_0	1.350E+24	-2.57	1.78	[11]

Chemistry

Methane combustion

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

Turbulence

Irregularity (Random and chaotic nature of flow)

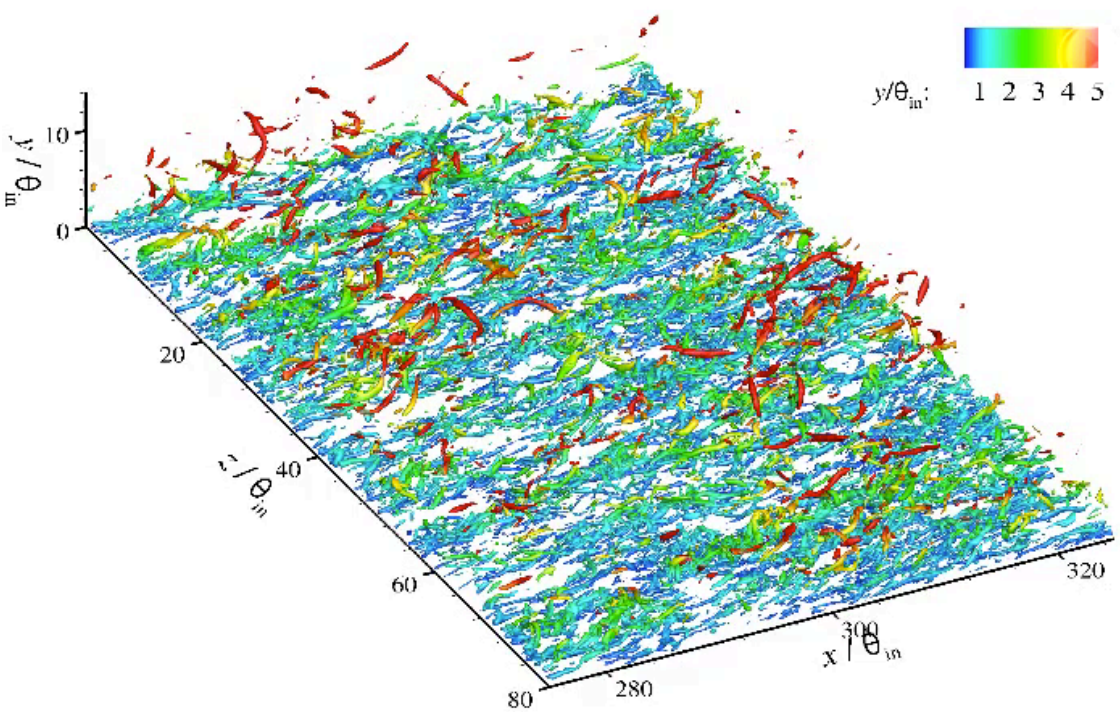
Increased exchange of momentum (Diffusivity - spreading rate of jets, boundary layers etc.)

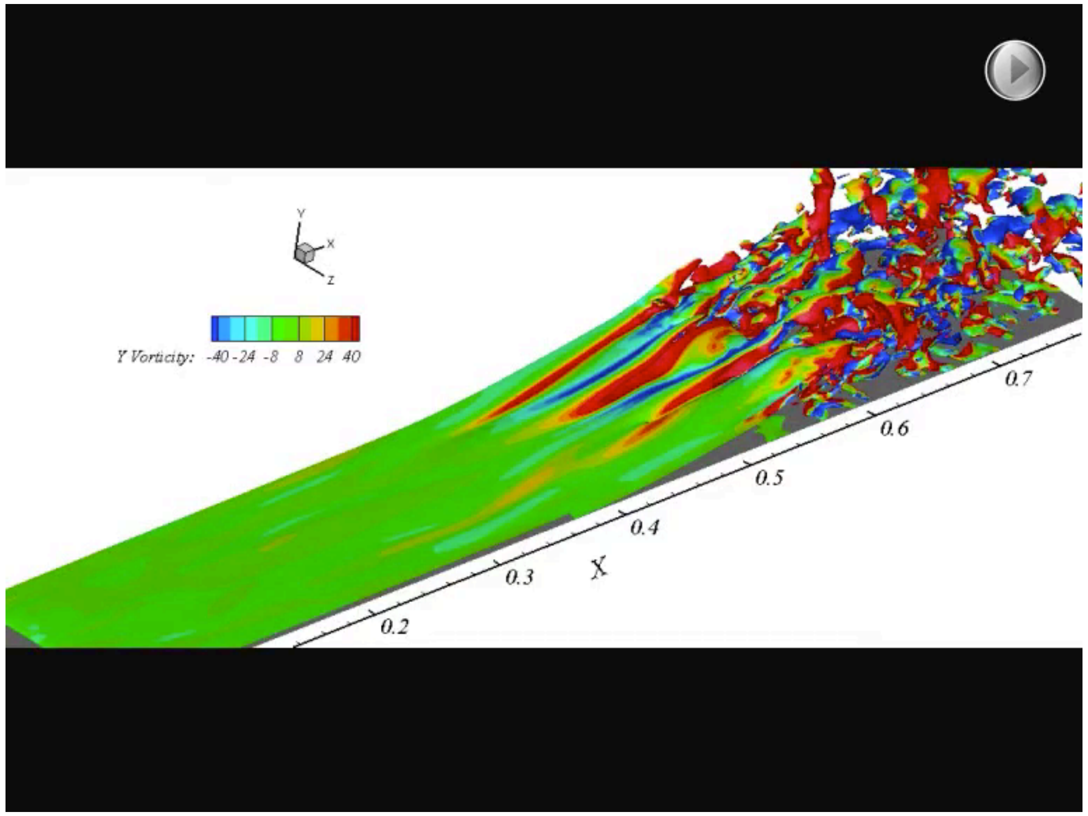
Large Reynolds numbers

Dissipation of kinetic energy to internal energy

Wide range of time and length scales

Almost all practical flows are turbulent.





Challenges in turbulent combustion

- Large number of reacting species

➡ Solving additional transport equations

- Large number of chemical reactions
- Multi-scale problem: large spatial and temporal length scales (slow/fast reactions and species)
- Strong non-linearities in the source terms
- Turbulence/chemistry interactions

➡ Stiff system

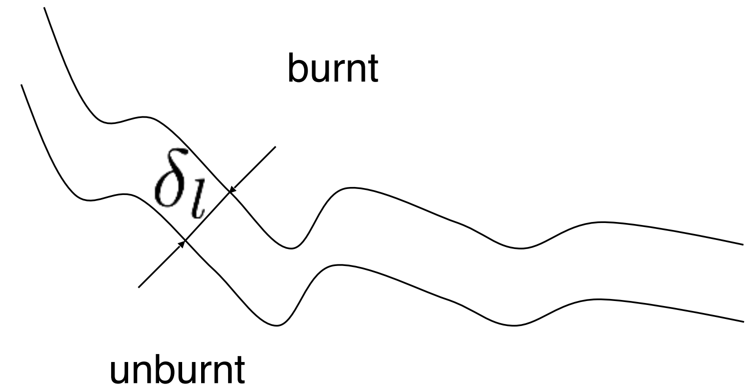
Approaches for chemical kinetics

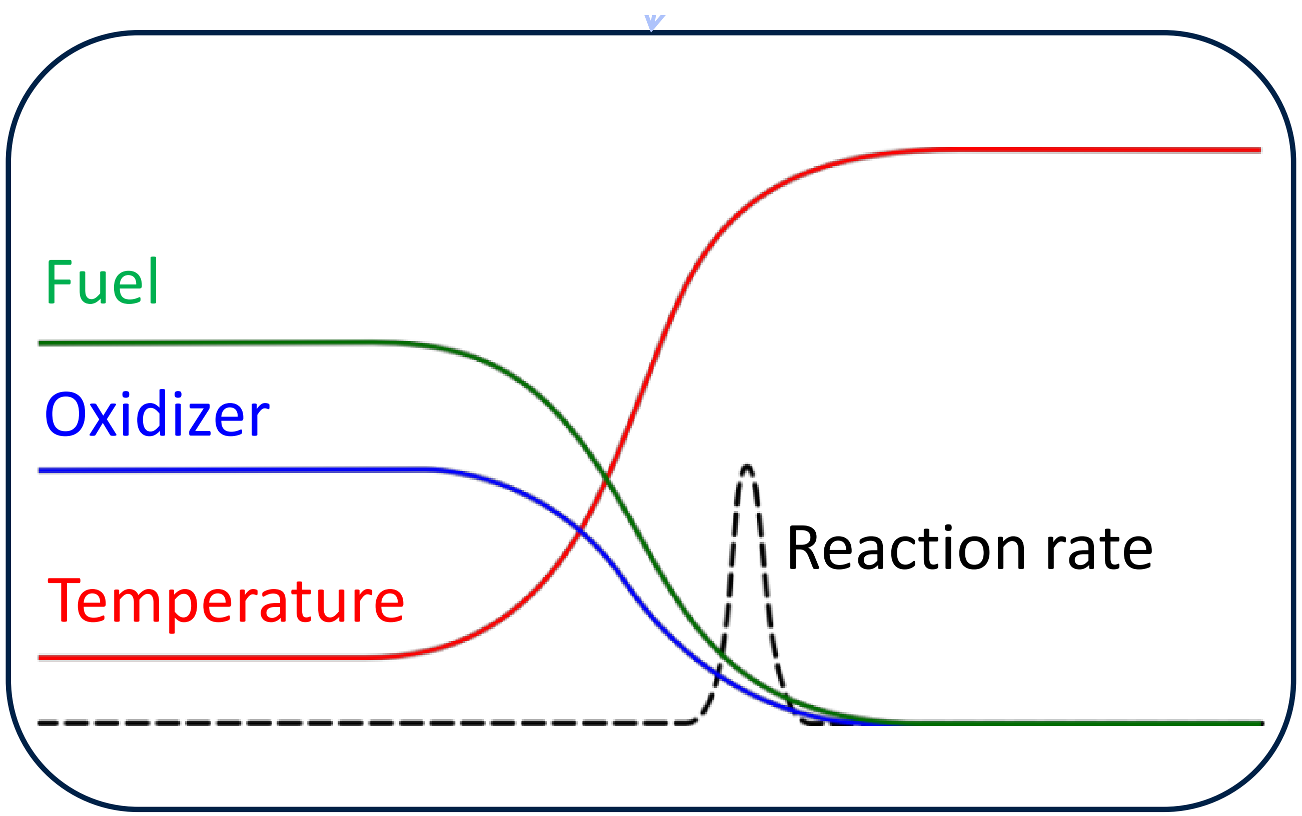
- Infinitely fast chemistry
- Solve the full system
- Reduced chemical schemes
- Chemistry tabulation

Approaches for chemical kinetics

Chemistry tabulation

- Assume 3D flame can be defined by a composition of 1D flames ("flamelets")
- Define a controlling variable that defines the unburnt mixture and the burnt mixture: RPV
- Tabulate all properties depending on that variable ("manifold")





We obtain the following relation:

$c = 0$ Unreacted mixture

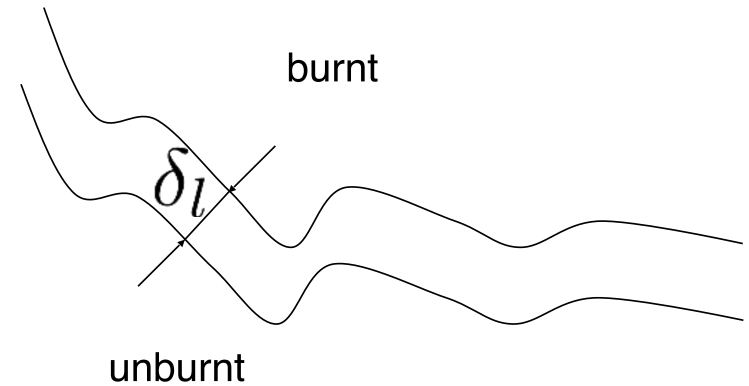
$c = 1$ Fully reacted mixture (equilibrium)

Physical modelling

Approaches for chemical kinetics

Chemistry tabulation

$\widetilde{f}$	$\widetilde{f''^2}$	$\widetilde{c}$	$\widetilde{c''^2}$	$\widetilde{i}$
0	0	0	0	0
0	0	0	0	0.1
0	0	0	0	0.2
0	0	...	...	...
0	0	0	0	1.0
0	0	0	0.1	0
0	0	0	0.1	0.1
0	0	0	0.1	0.2
0	0	...	...	...
0	0	0	0.1	1.0
0	0	0.1	0	0
0	0	0.1	0	0.1
0	0	0.1	0	0.2
0	0	0.1	0	...



$$\lambda, c_p, \mu, \dot{S}_c, MW_{mix}$$

We use these variables in the CFD code

CFI turbulent combustion model

$$\bar{\rho}\frac{\partial\tilde{c}}{\partial t} + \bar{\rho}\tilde{\boldsymbol{u}}\cdot\nabla\tilde{c} = \nabla\cdot\left[\left(D + D_t\right)\nabla\tilde{c}\right] + \tilde{S}_c$$

$$\bar{\rho}\frac{\partial\tilde{f}}{\partial t} + \bar{\rho}\tilde{\boldsymbol{u}}_i\cdot\nabla\tilde{f} = \nabla\cdot\left[\left(D + D_t\right)\nabla\tilde{f}\right]$$

$$\bar{\rho}\frac{\partial\widetilde{c"^2}}{\partial t} + \bar{\rho}\tilde{\boldsymbol{u}}\cdot\nabla\widetilde{c"^2} = \nabla\cdot\left[\left(D + D_t\right)\nabla\widetilde{c"^2}\right] + 2\left(\widetilde{S_c\,c} - \tilde{S}_c\,\tilde{c}\right) + \overline{P}_k + \overline{D}_k$$

$$\bar{\rho}\frac{\partial\widetilde{f''^2})}{\partial t} + \bar{\rho}u_i\cdot\nabla\widetilde{f''^2} = \nabla\cdot\left[\left(D + D_t\right)\nabla\widetilde{f''^2}\right] + \bar{P}_k + \bar{D}_k$$

RPV

$$\overline{P}_k = 2\overline{\rho}\frac{\nu_t}{Sc_t}\left|\nabla\tilde{c}\right|^2$$

$$\overline{D}_k = -2\overline{\rho}\frac{\nu_t}{\Delta^2 Sc_t}\widetilde{c"^2}$$

Domingo et al. (2005)

MF

$$\overline{P}_k = 2\overline{\rho}\frac{\nu_t}{Sc_t}\left|\nabla\tilde{f}\right|$$

$$\overline{D}_k = -2\overline{\rho}\frac{\nu_t}{\Delta^2}\widetilde{f"^2}$$

Domingo et al. (2008)

COMPUTATIONAL FRAMEWORK

Computational framework

Alya is in the **PRACE benchmark suite**

respective user communities, as well the coverage of scientific a
a final list of 12 codes to form the initial version of UEABS, whi

Particle Physics:	QCD
Classical MD:	NAMD, GROMACS
Quantum MD:	Quantum Espresso, CP2K, GPAW
CFD:	Code_Saturne, ALYA
Earth Sciences:	NEMO, SPECFEM3D
Plasma Physics:	GENE
Astrophysics:	GADGET

PRACE

Available online at www.prace-ri.eu

Partnership for Advanced Computing in Europe

Selection of a Unified European Application Benchmark Suite

J. Mark Bull[a]*, Andrew Emerson[b]

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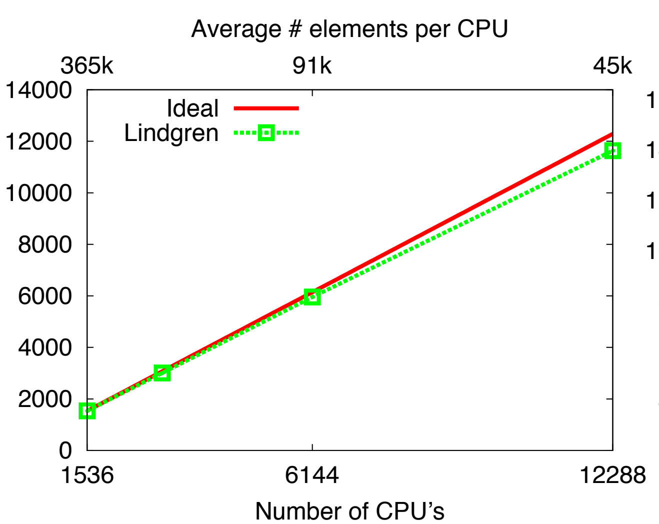
[b]CINECA, via Magnanelli 6/3, 40033 Casalecchio di Reno, Bologna, Italy.

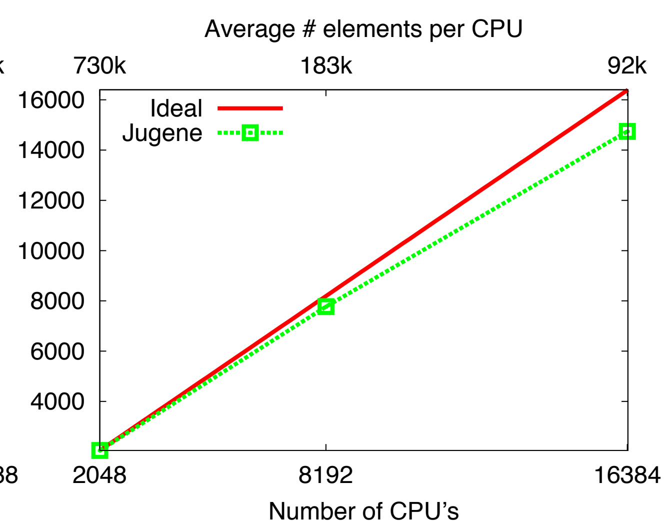
Lindgren - Cray XE6
Sweden

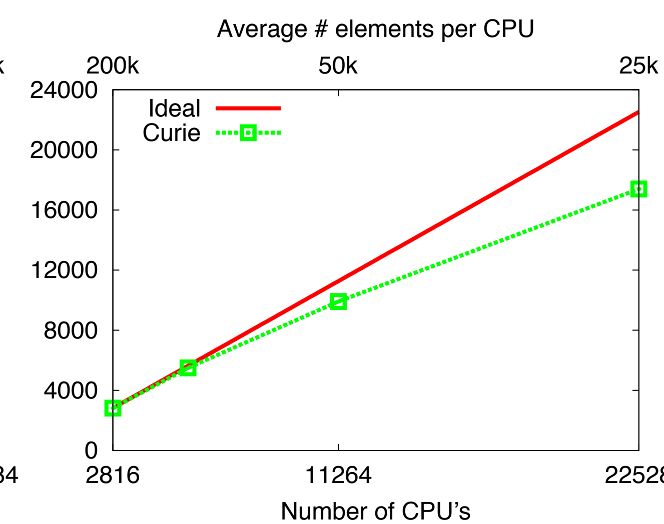
Jugene - Blue Gene/P
Germany

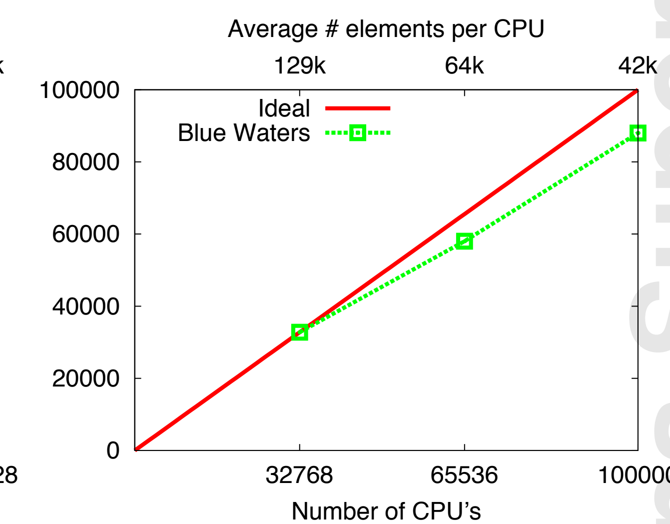
Curie - BullX
France

Blue Waters - Cray XE6
USA

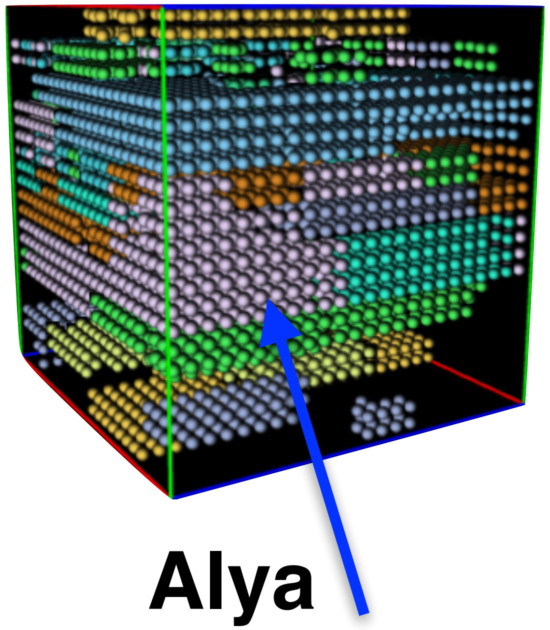


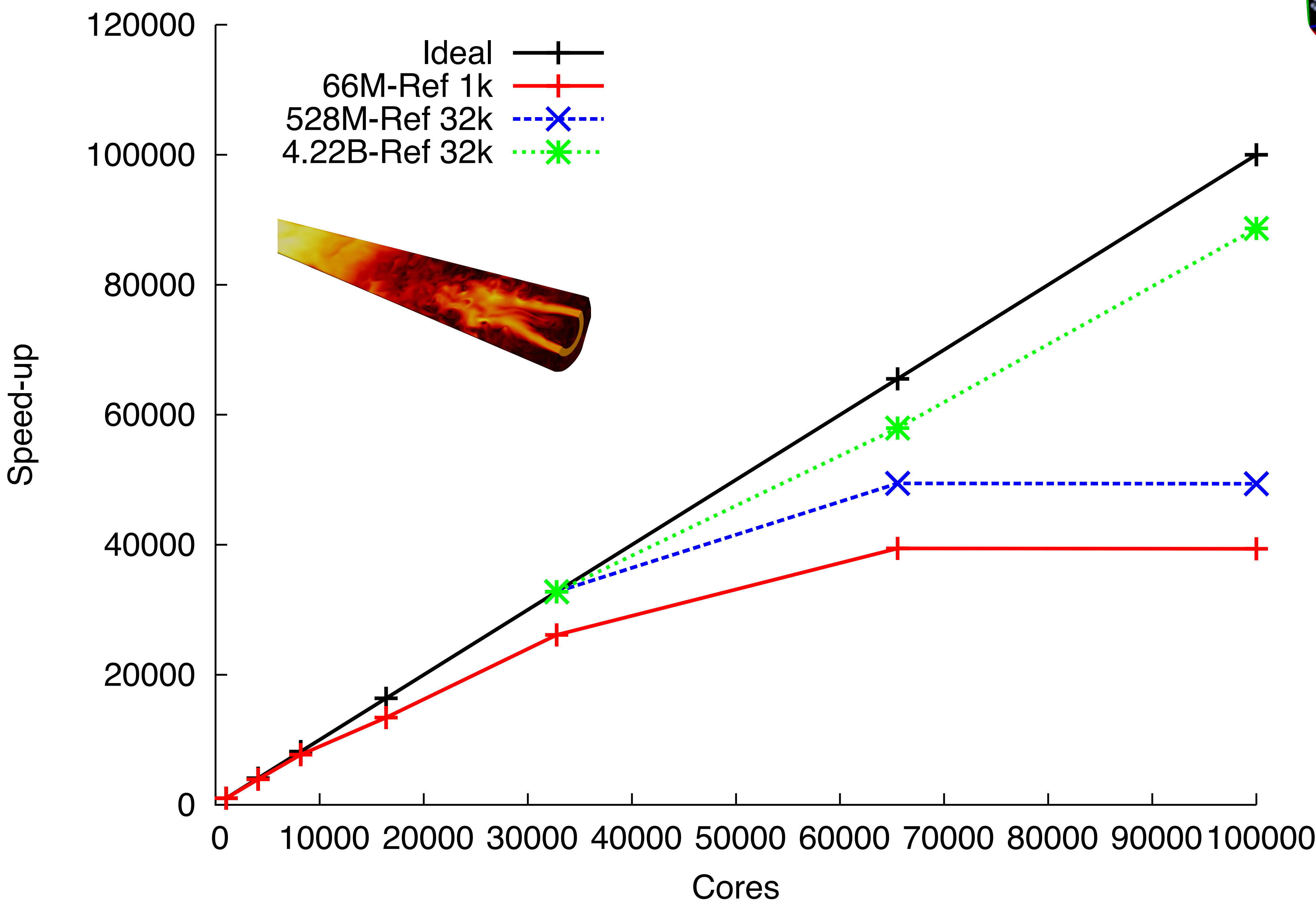






Parallel performance





Blue Waters

Vázquez et al. (2016)

Combustion systems

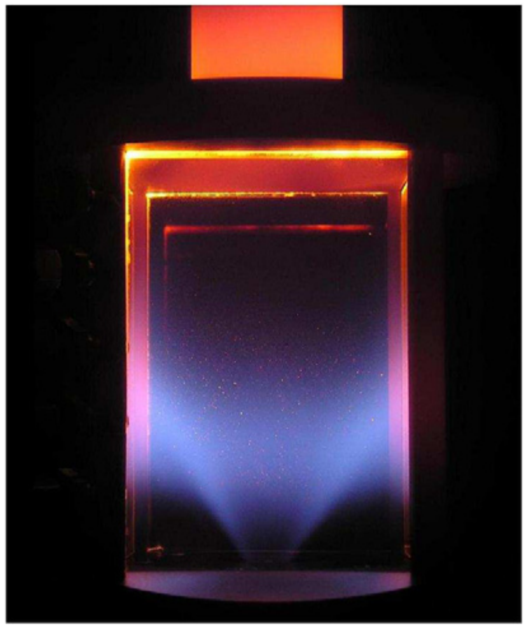
PREdiction and **C**ontrol of **C**ombustion **INSTA**bilities in Industrial Gas Turbines (**PRECCINSTA**)

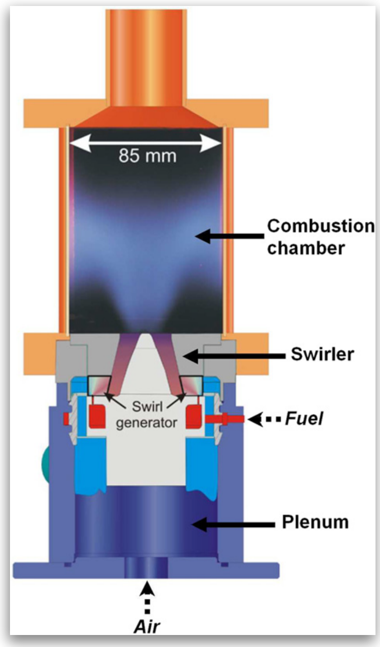
Collaboration with:

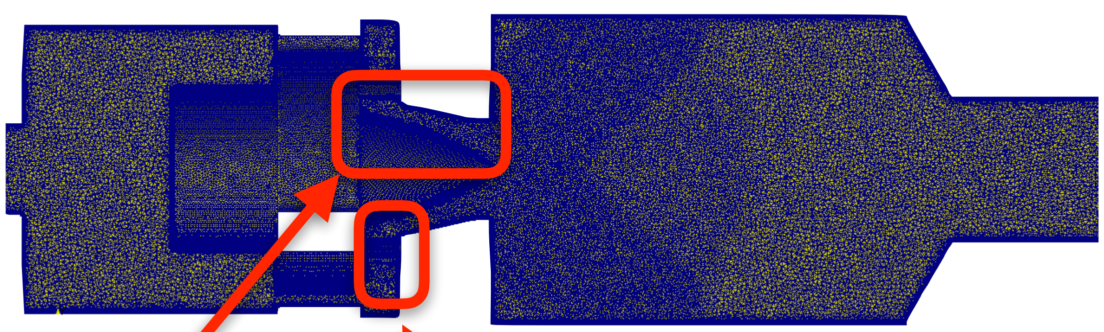
Simon Gövert and J.W.B. Kok, *Department of Thermal Engineering, University of Twente*
B. Cuenot and L.Y. Giquel, *Combustion Group, CERFACS*
W. Meier, *Institute of Combustion Technology, DLR German Aerospace Centre*

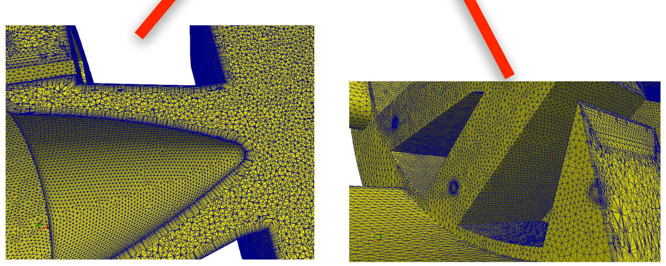
BSC CERFACS UNIVERSITY OF TWENTE.

Experimental configuration

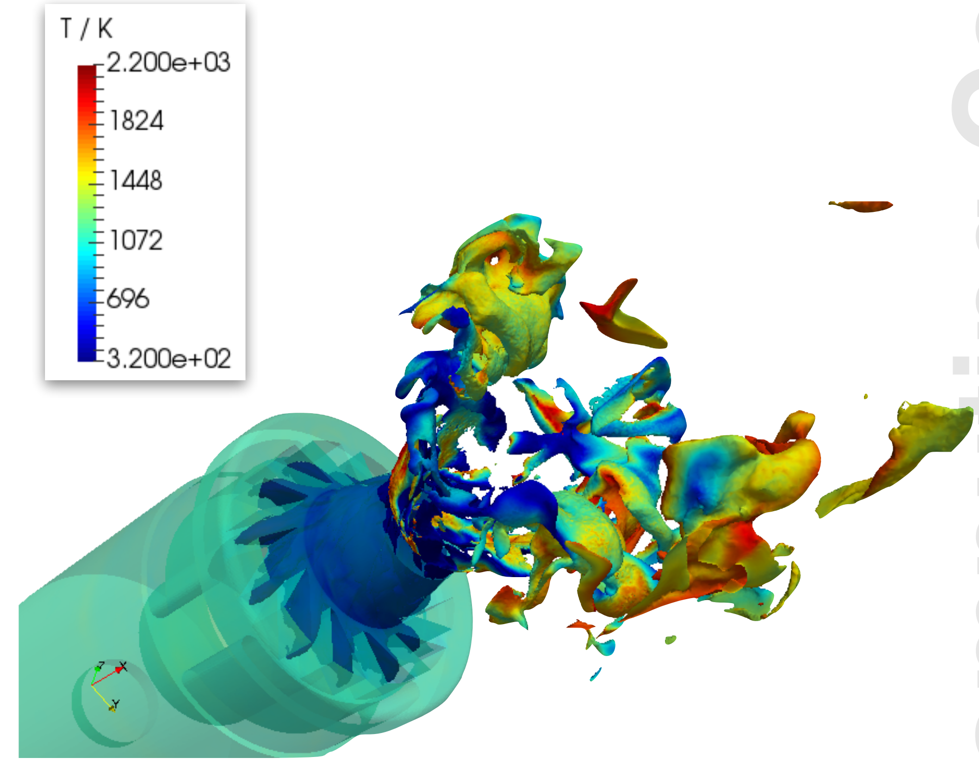




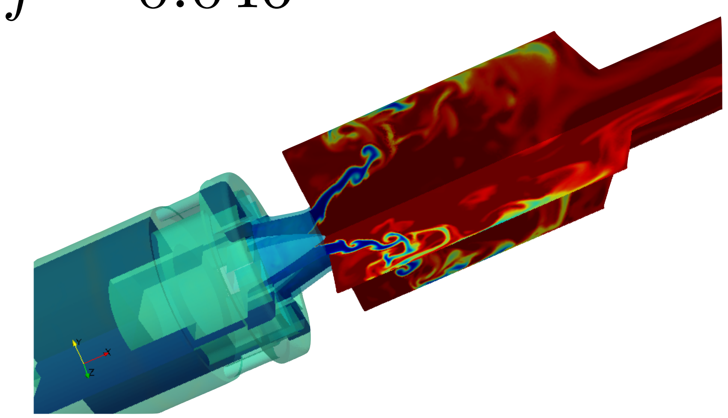


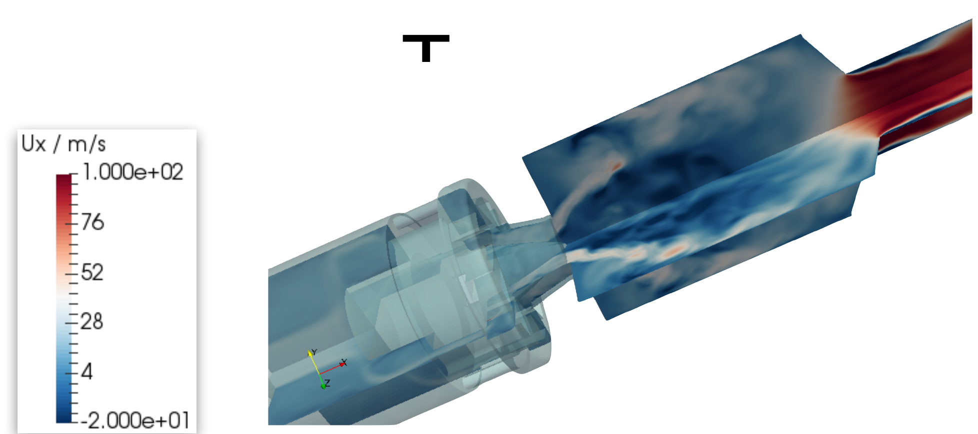


	No.
Mesh 1	8M
Mesh 2	14M
$\boxed{\text{Mesh 3}}$	$\boxed{\text{20M}}$

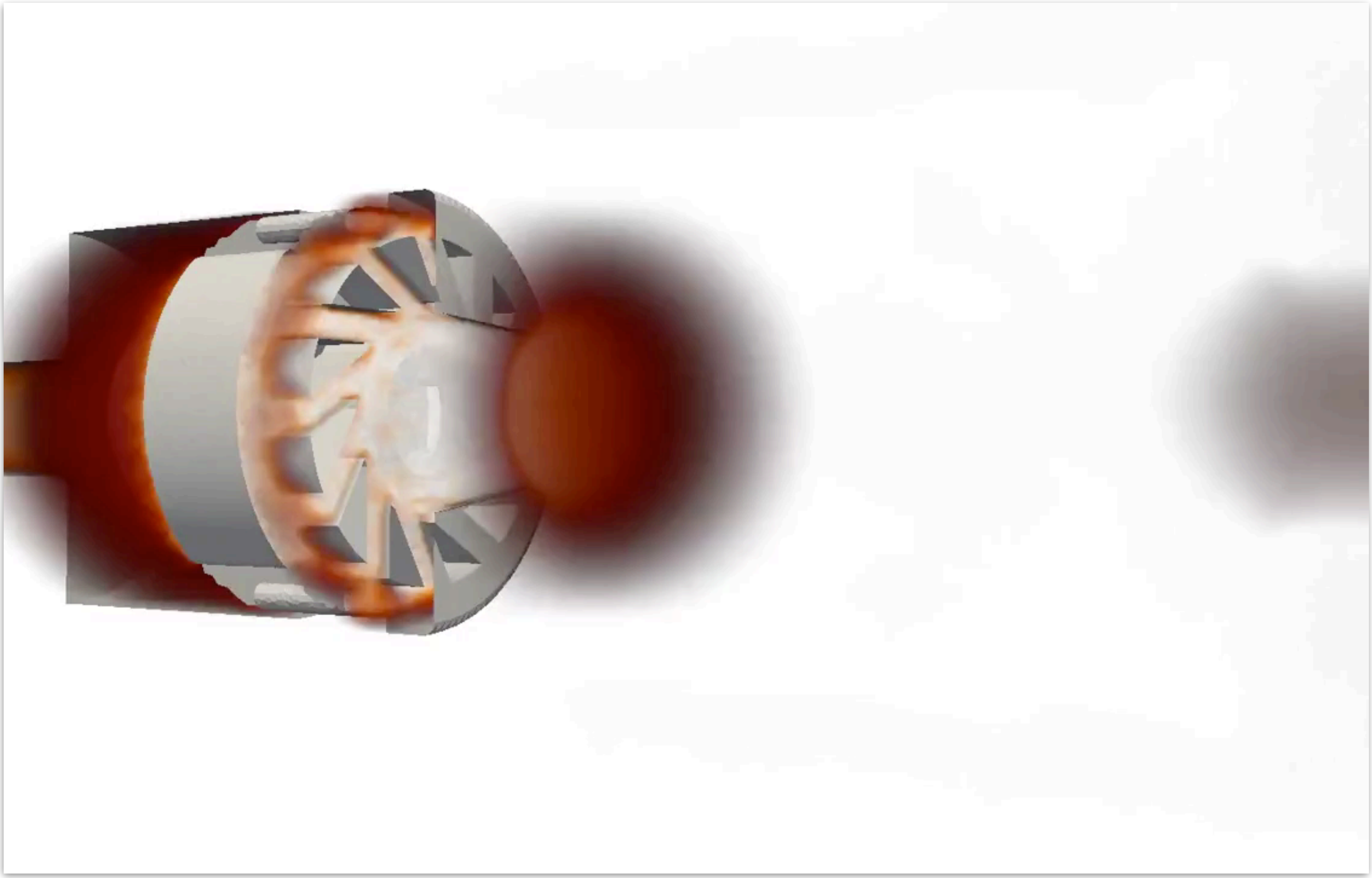


$$f = 0.046$$

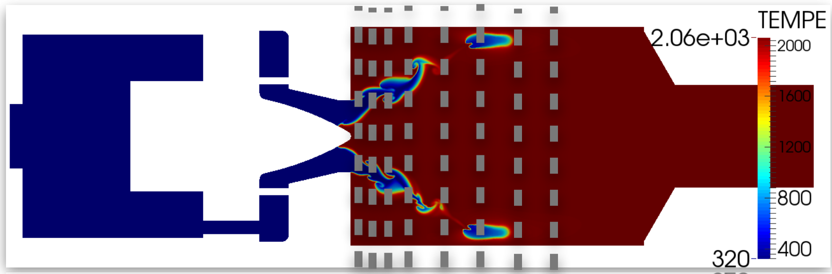


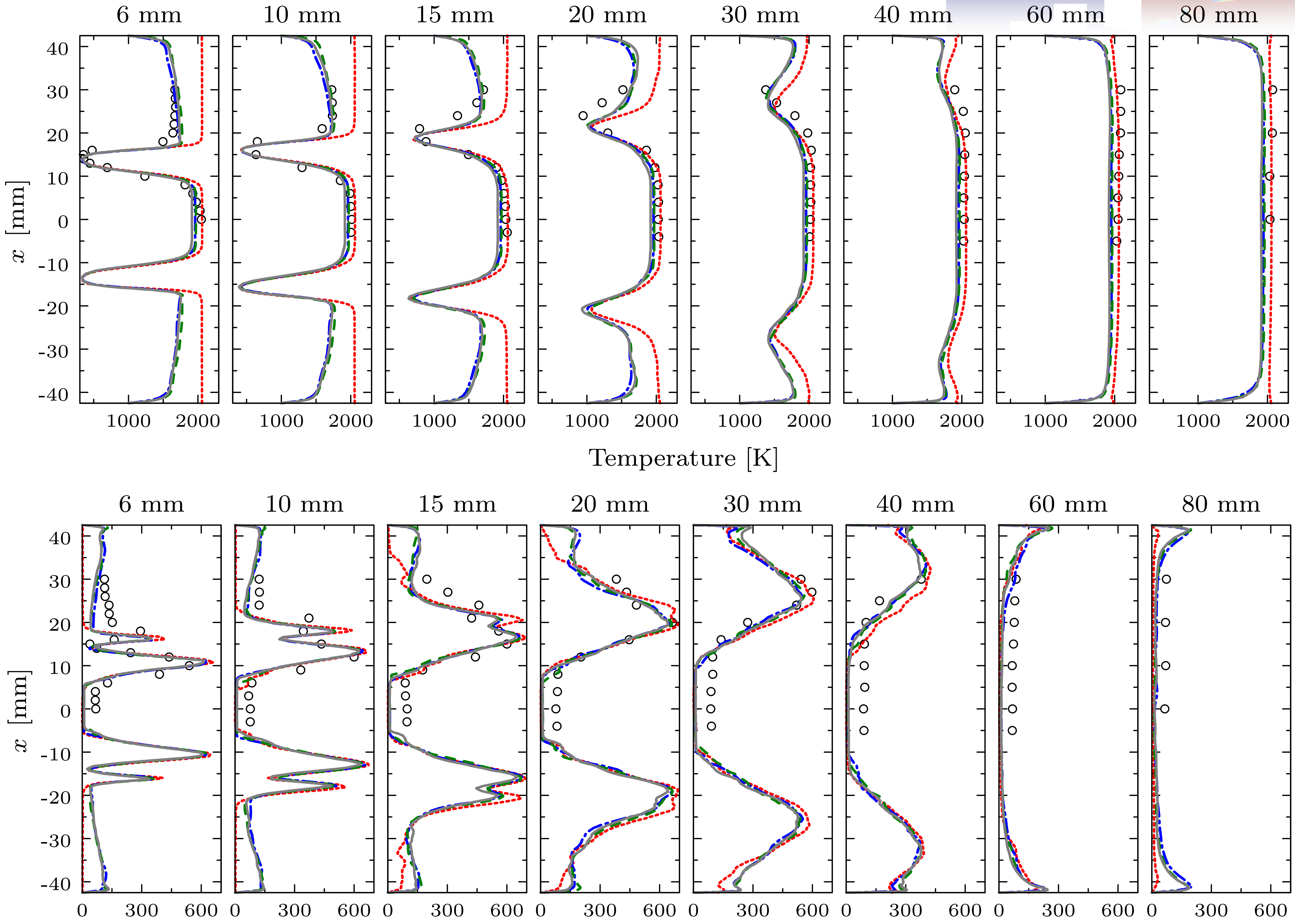


PRECCINSTA

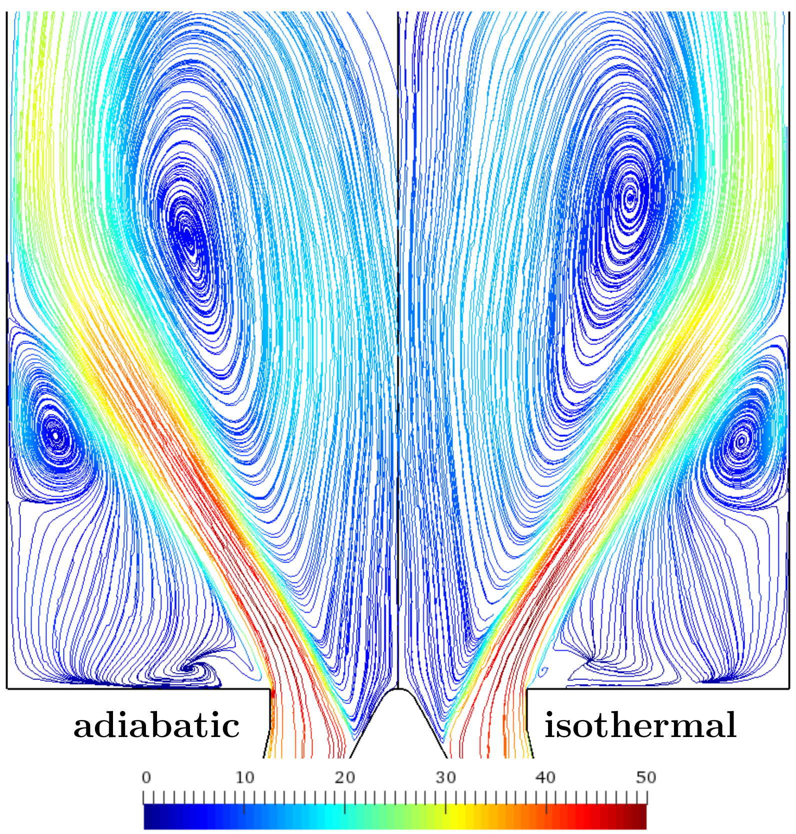


Validation LES (mean temperature)

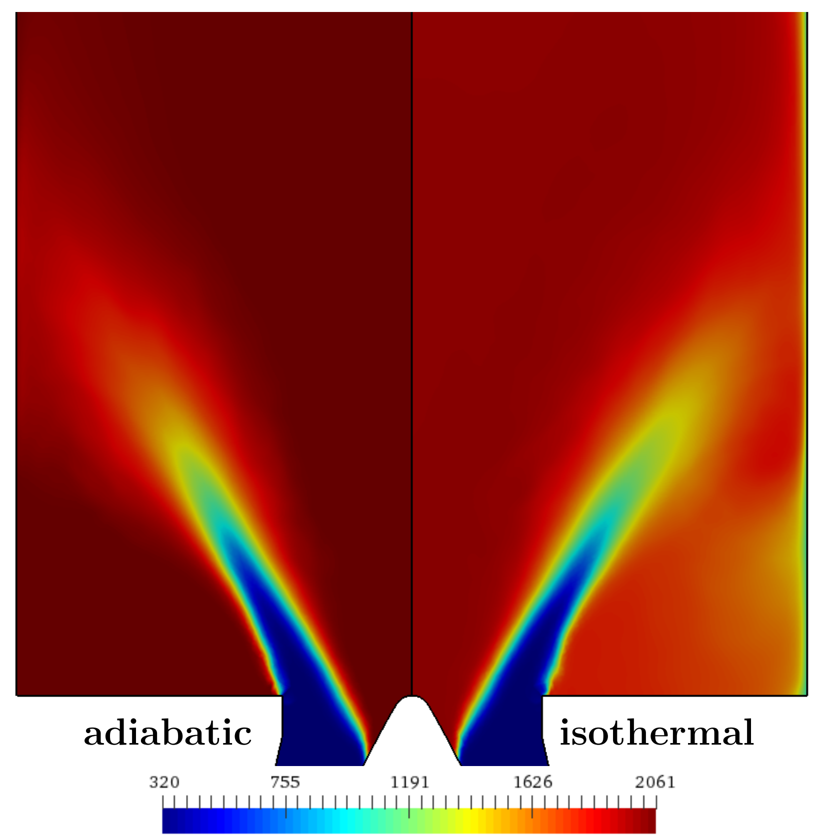




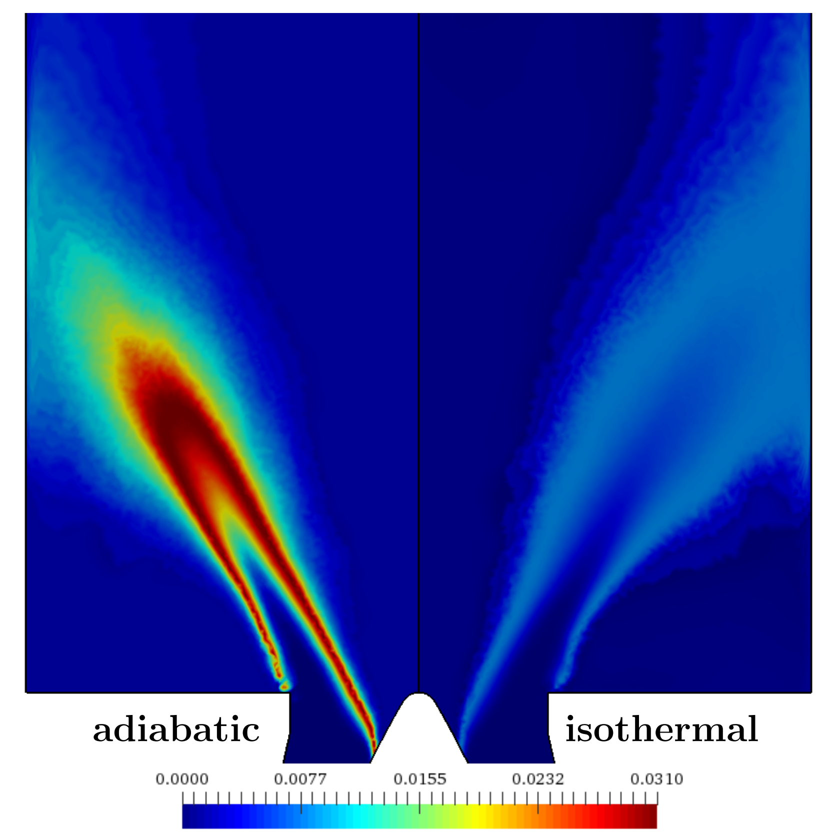
Effects of heat losses



Velocity



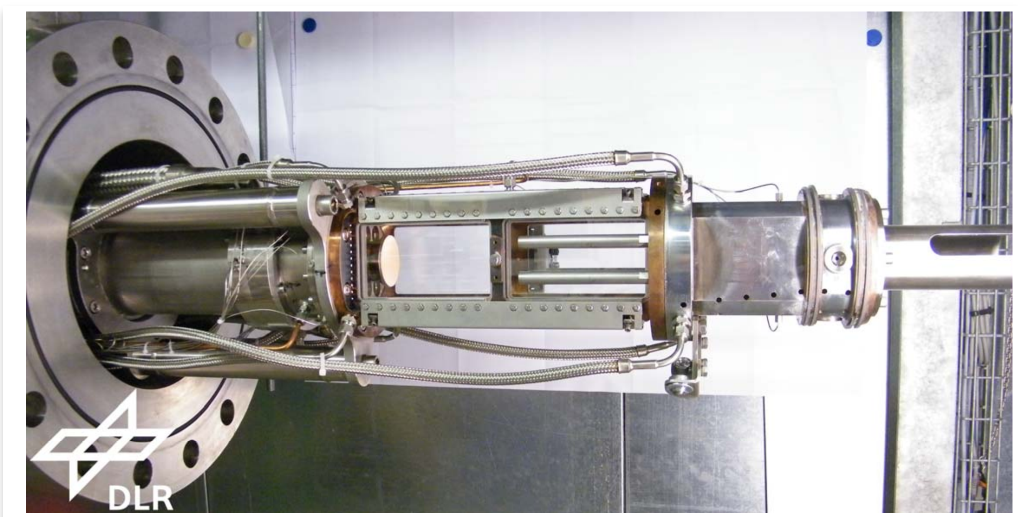
Temperature

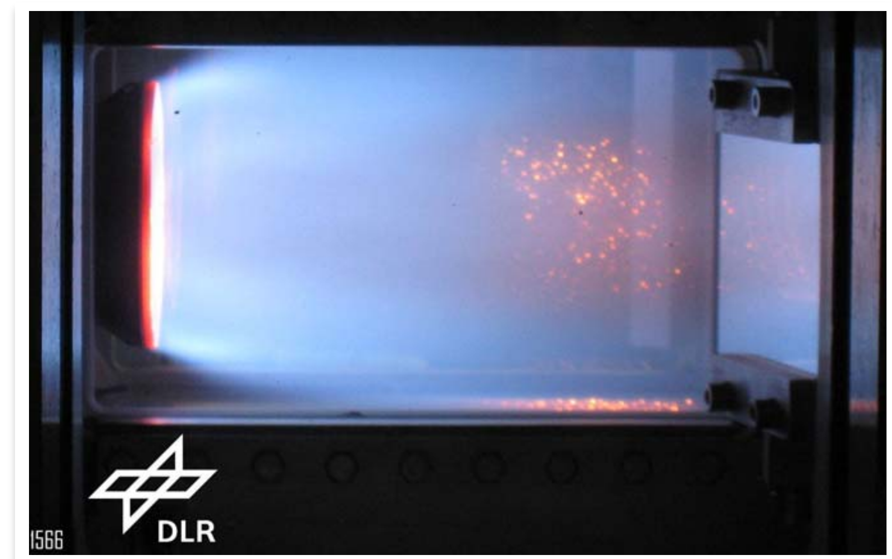


CO mass

Combustion systems

Scaled combustor **SGT5800H** - SIEMENS





Collaboration with:
Enric Illana and Lukasz Panek, *Siemens AG, Energy Sector*
Simon Gövert and J.W.B. Kok, *Department of Thermal Engineering, University of Twente*

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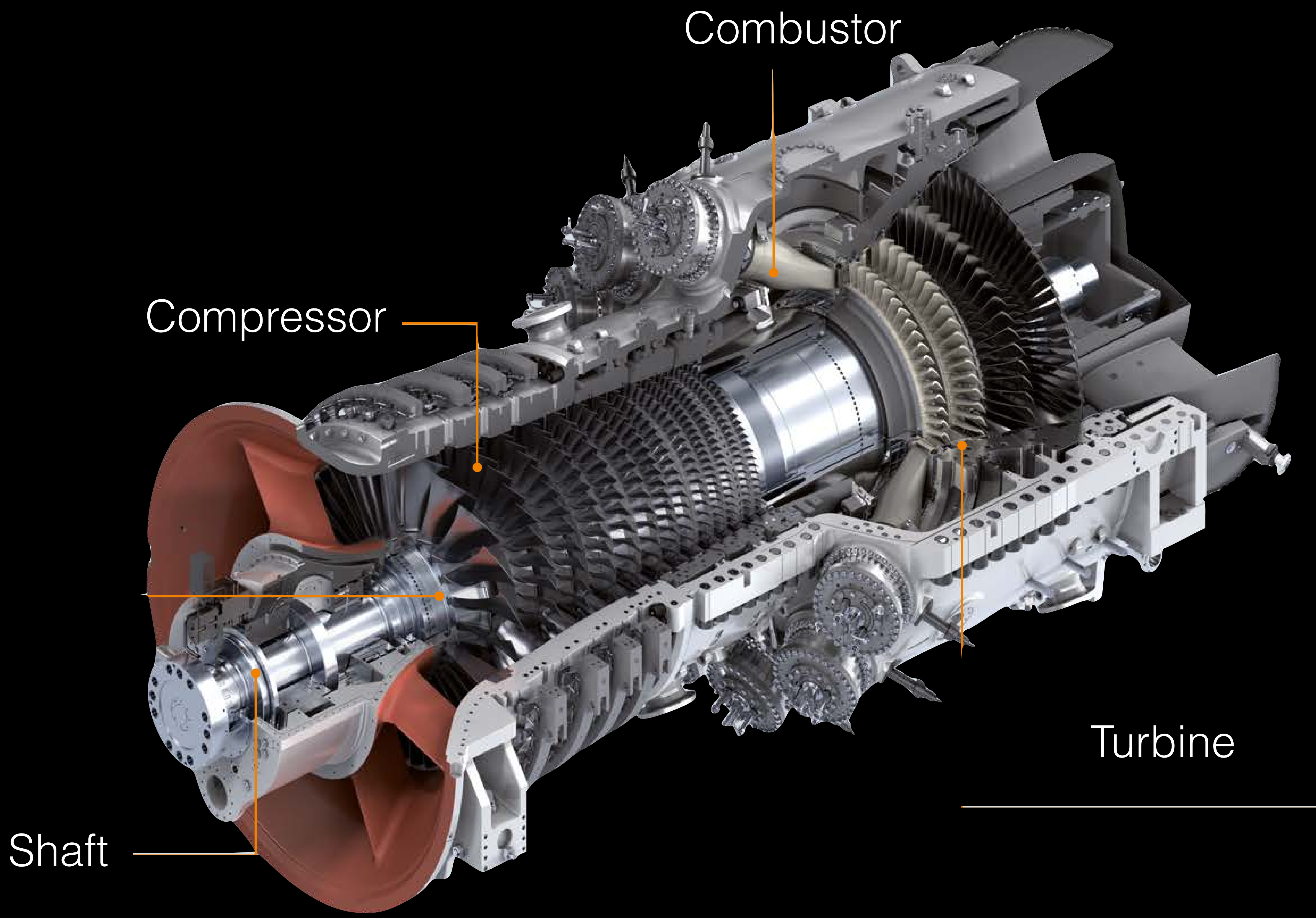
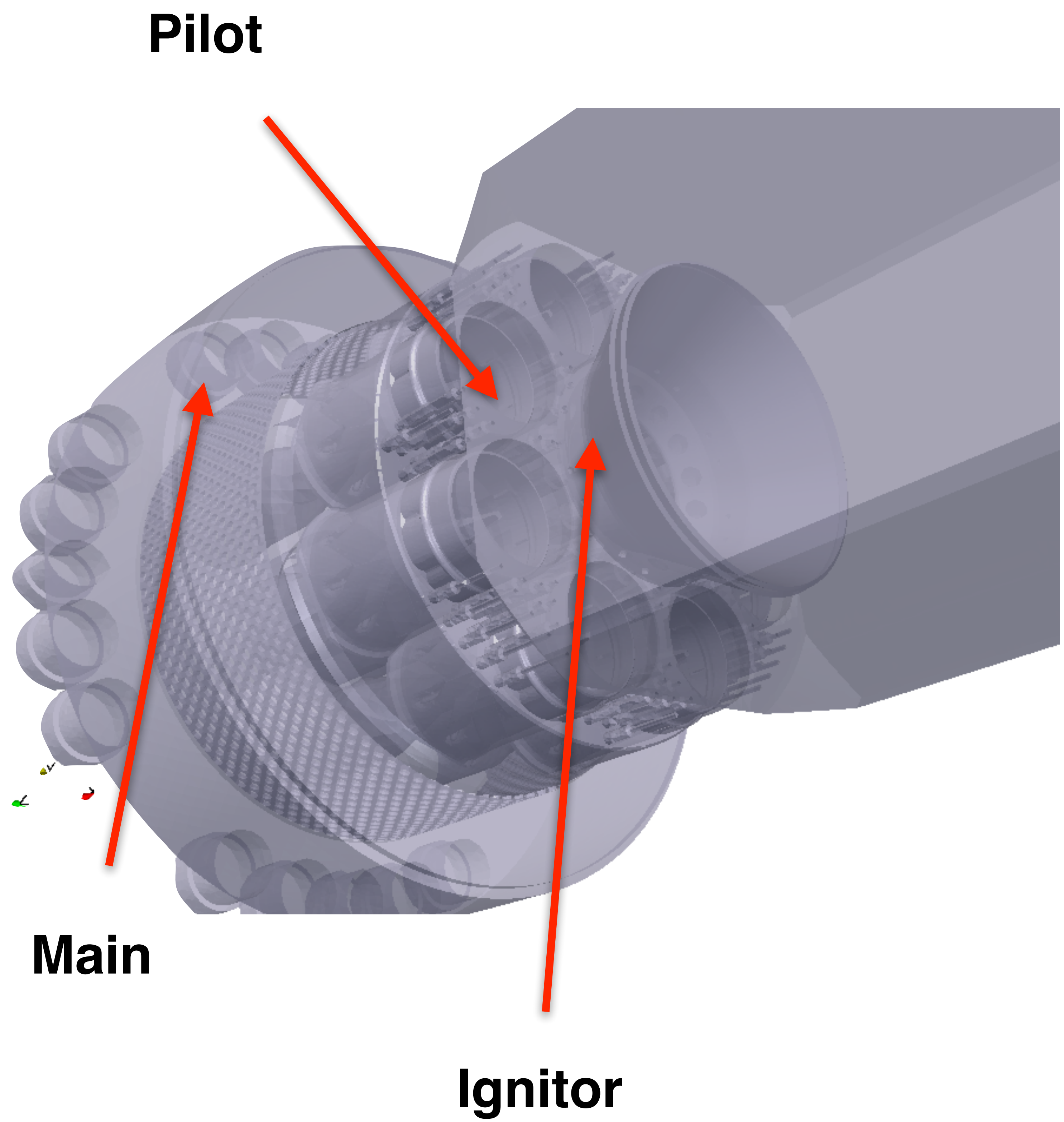
Siemens SGT-8000H series

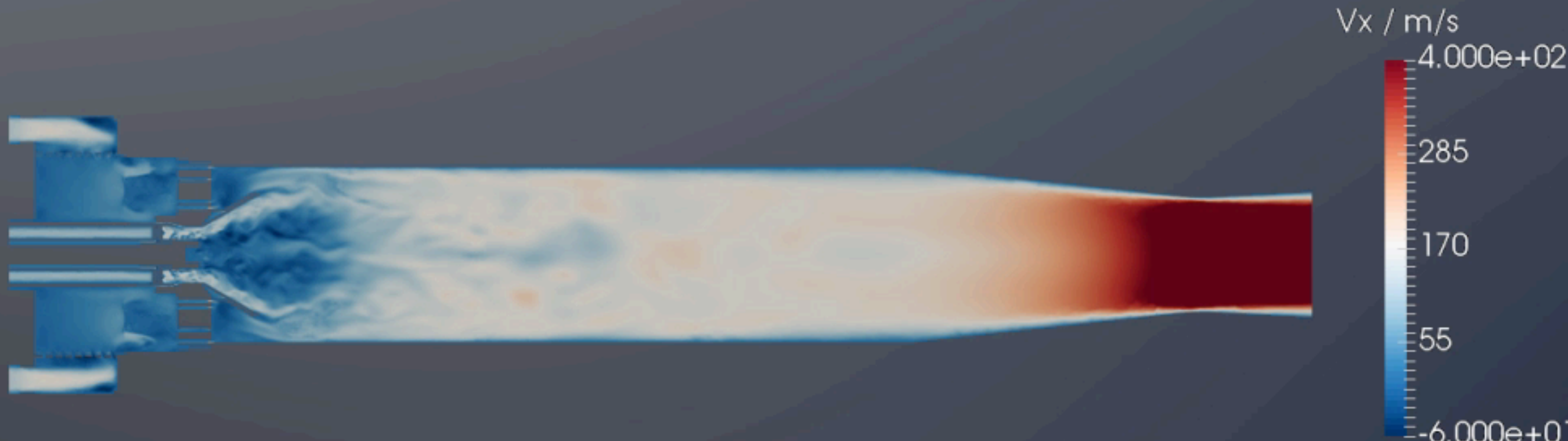


SGT5800H Siemens

Flow description

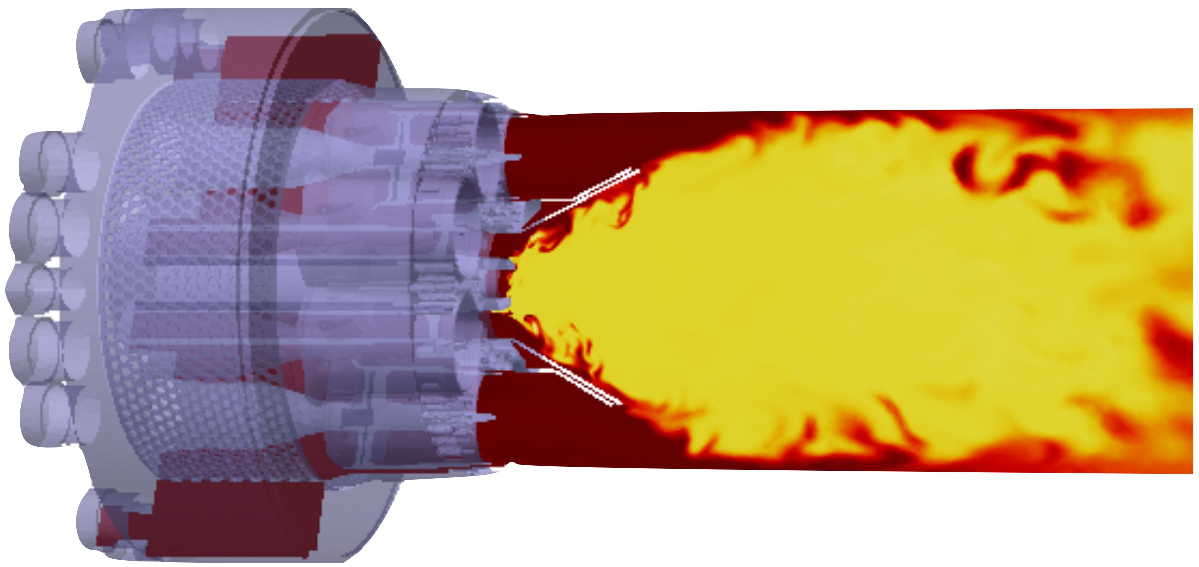


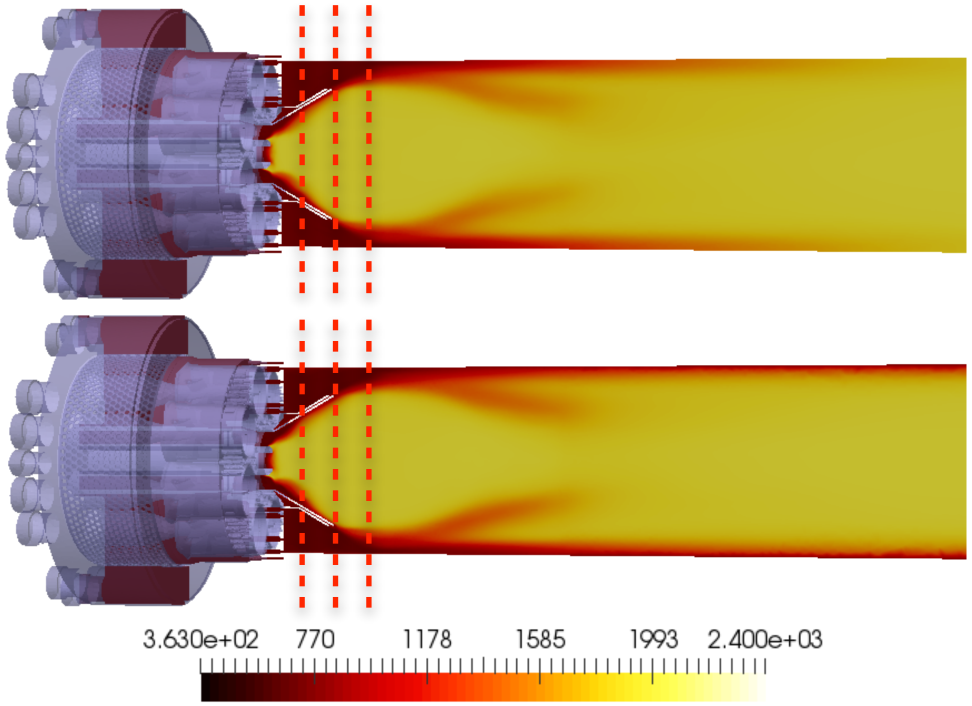
SGT5-8000H Downscaled can combustor

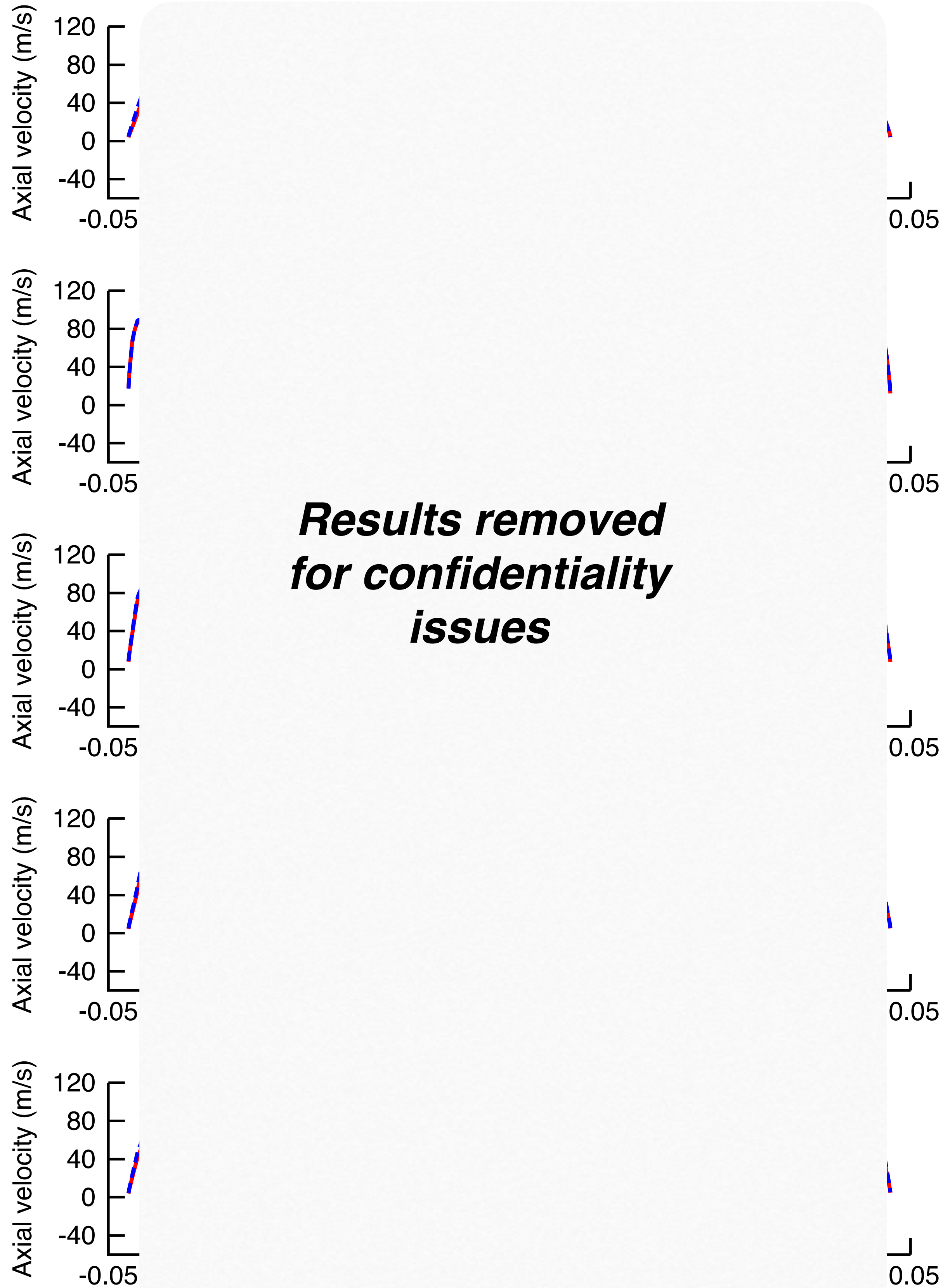


SGT5800H Siemens

Validation

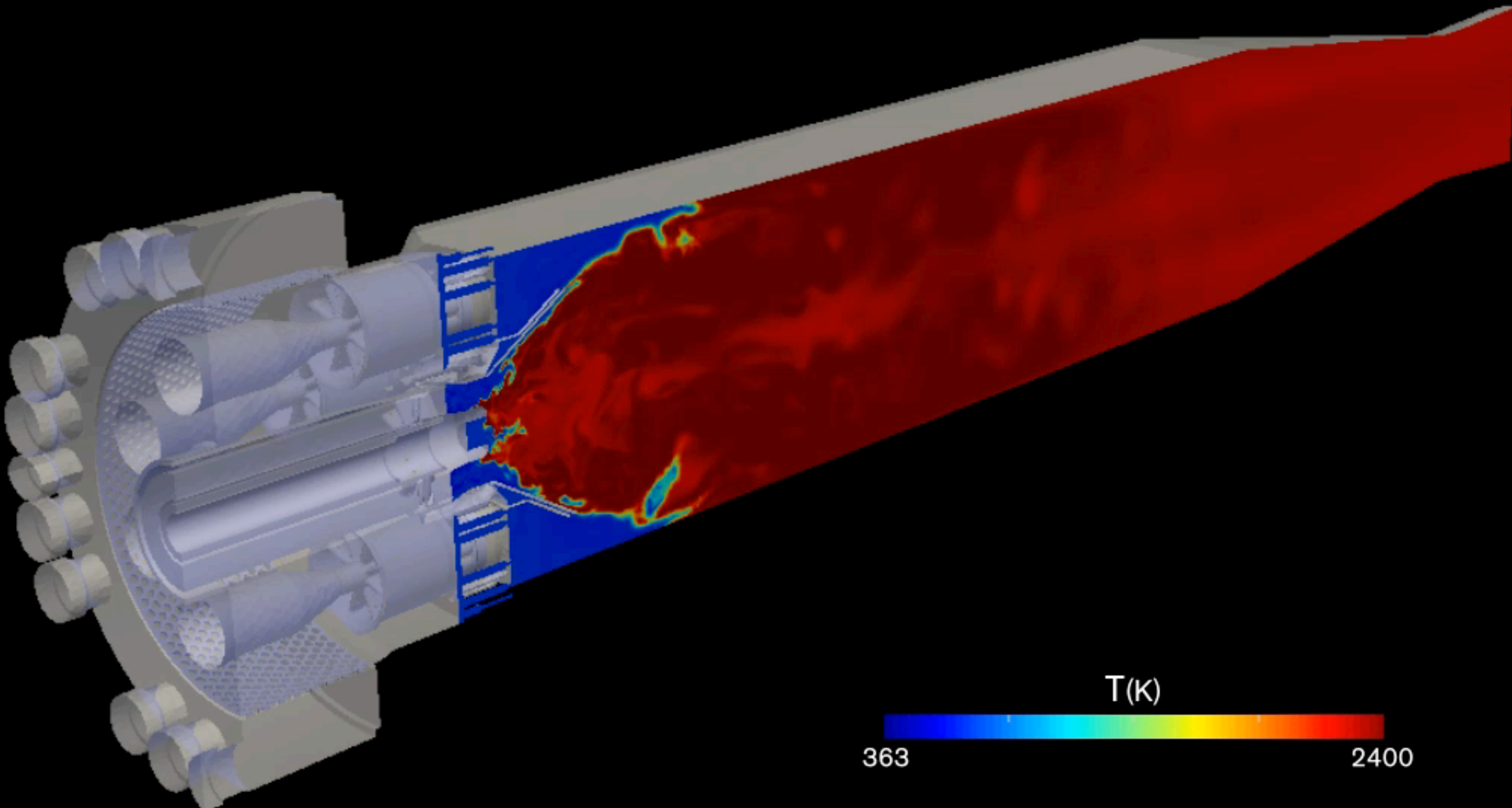






SGT5-8000H

Siemens Combustor



Conclusions

- Combustion is one of the main responsible of the climate change for its use in propulsion and power.
- It requires not only correct description of fluid mechanics, but also chemistry.
- It adds the complexity of large chemical kinetics to the problem of turbulent flows: ***turbulent combustion modelling***.
- Turbulent combustion modelling is based in chemistry reduction and turbulent/flame interactions.
- Combustion demands high computing power, in particular, turbulent combustion can only be targeted using HPC.

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- **HPC4E Project, grant agreement No. 689772 (H2020)**

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