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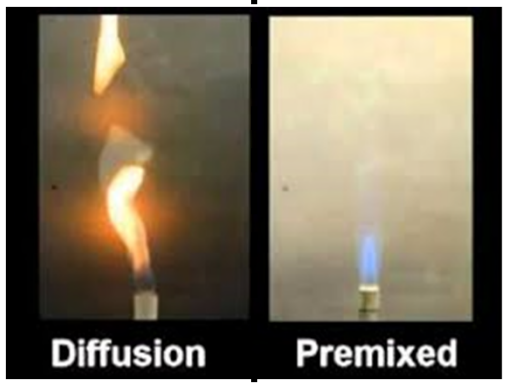
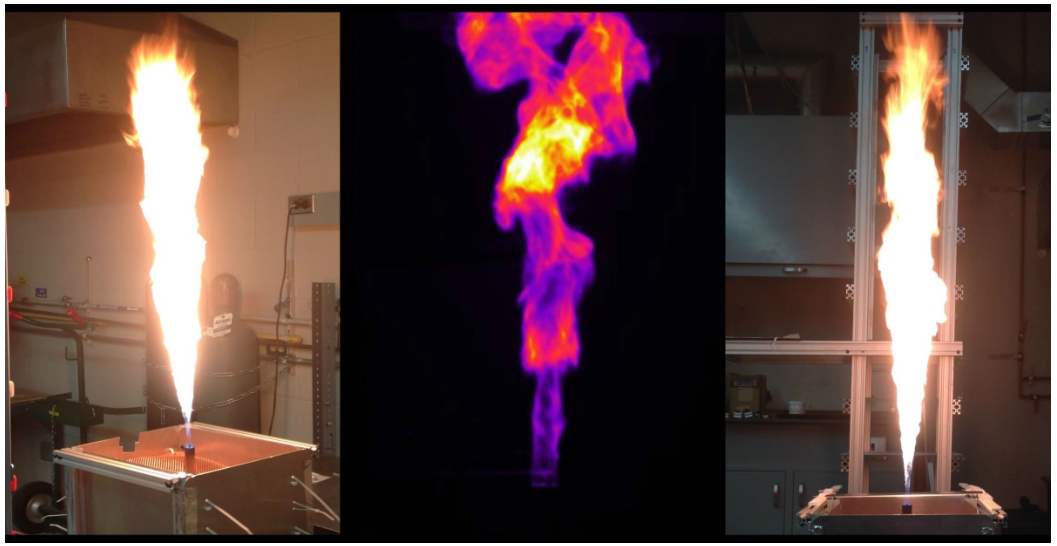
Pierre Q Gauthier PhD
Visiting Professor of Low Emissions Combustion Modelling

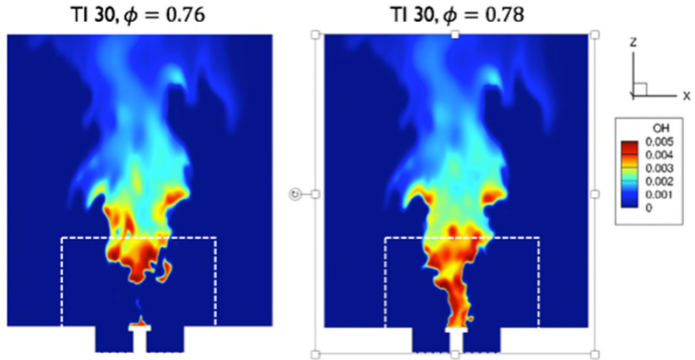
Low Emissions Design Concepts for Industrial Gas Turbines

Flame Types





Jet Flames



Sensitive!

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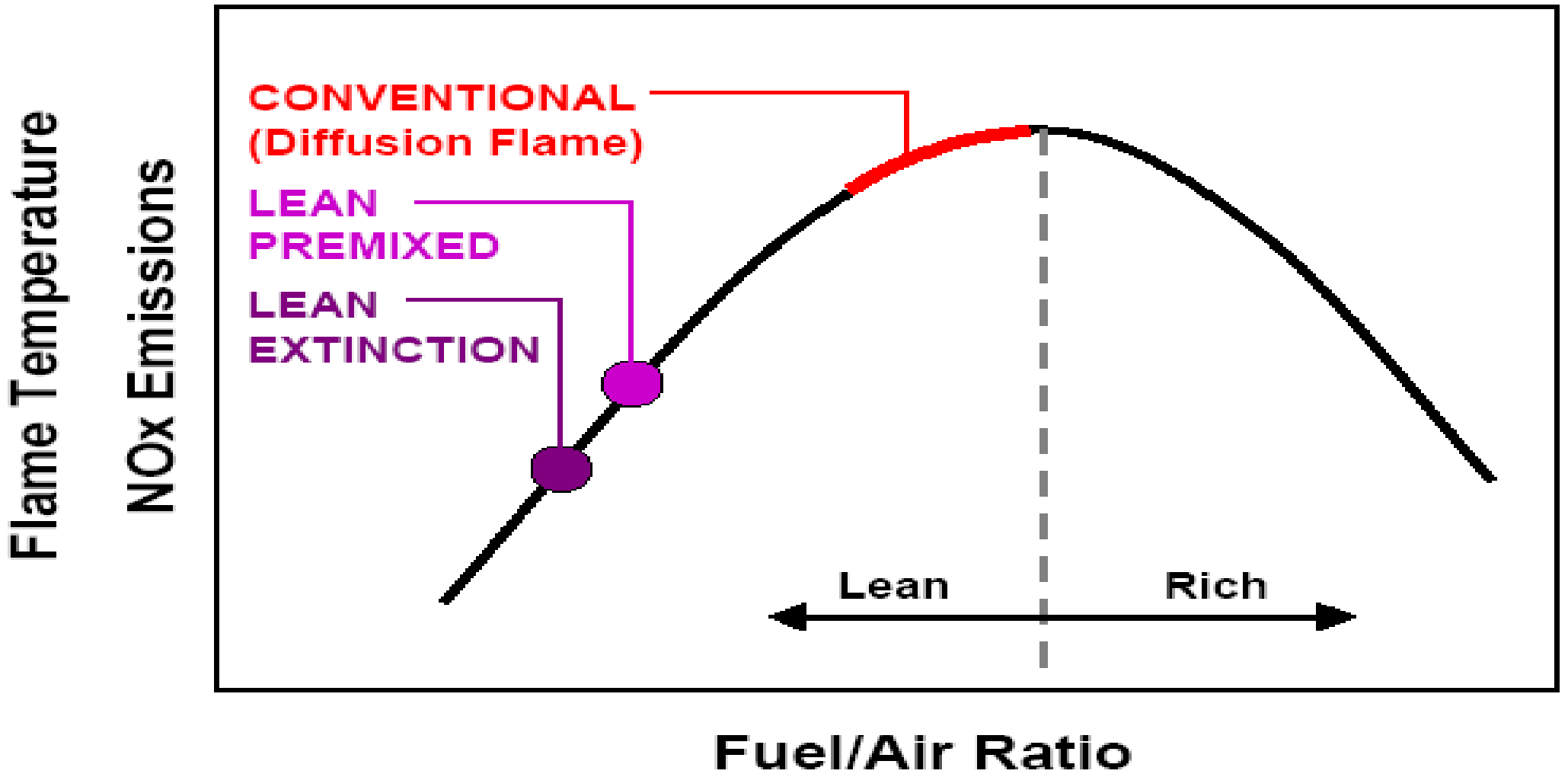
Effect of Stoichiometry on Flame Temperature and NOx Emissions



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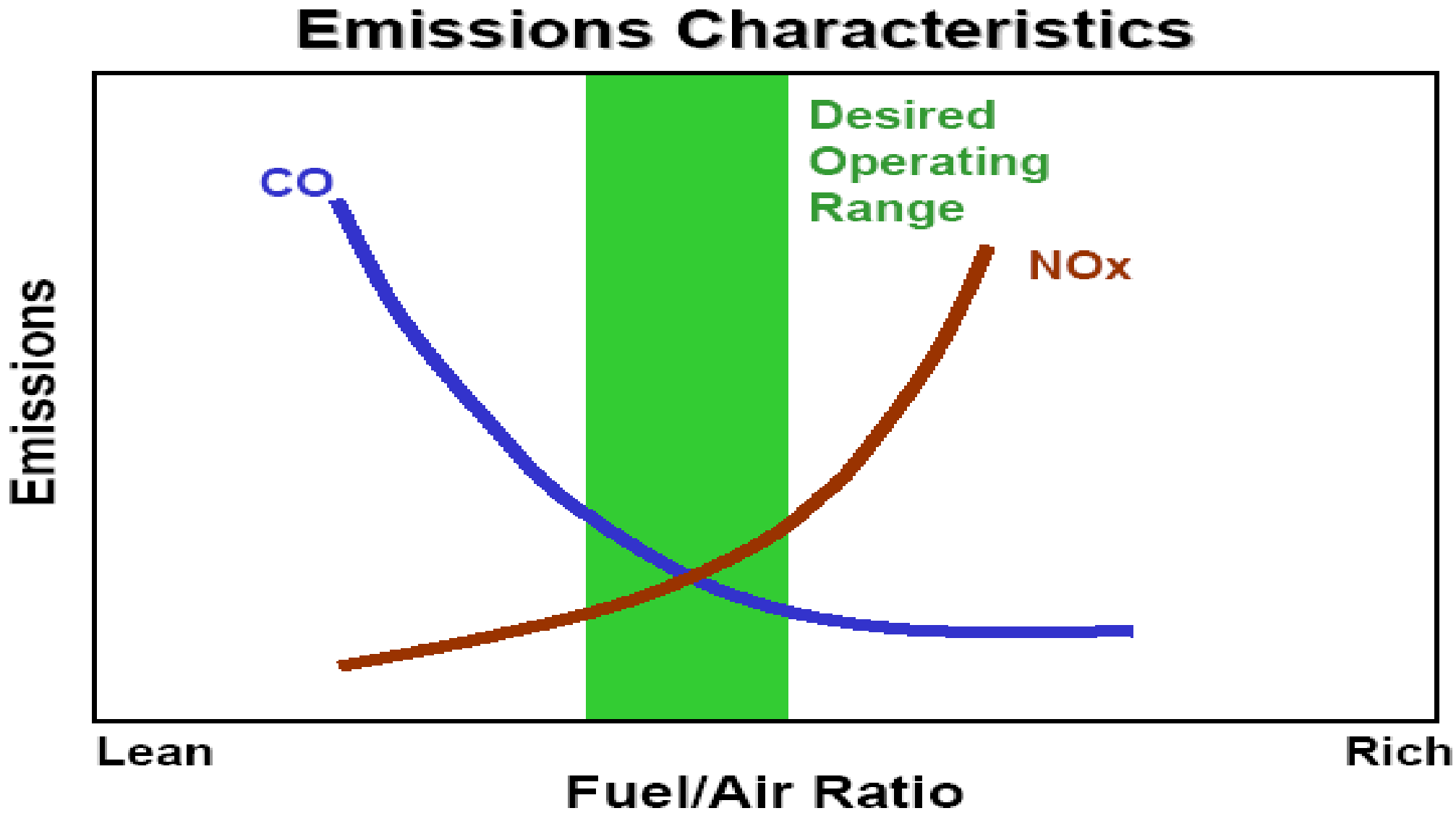
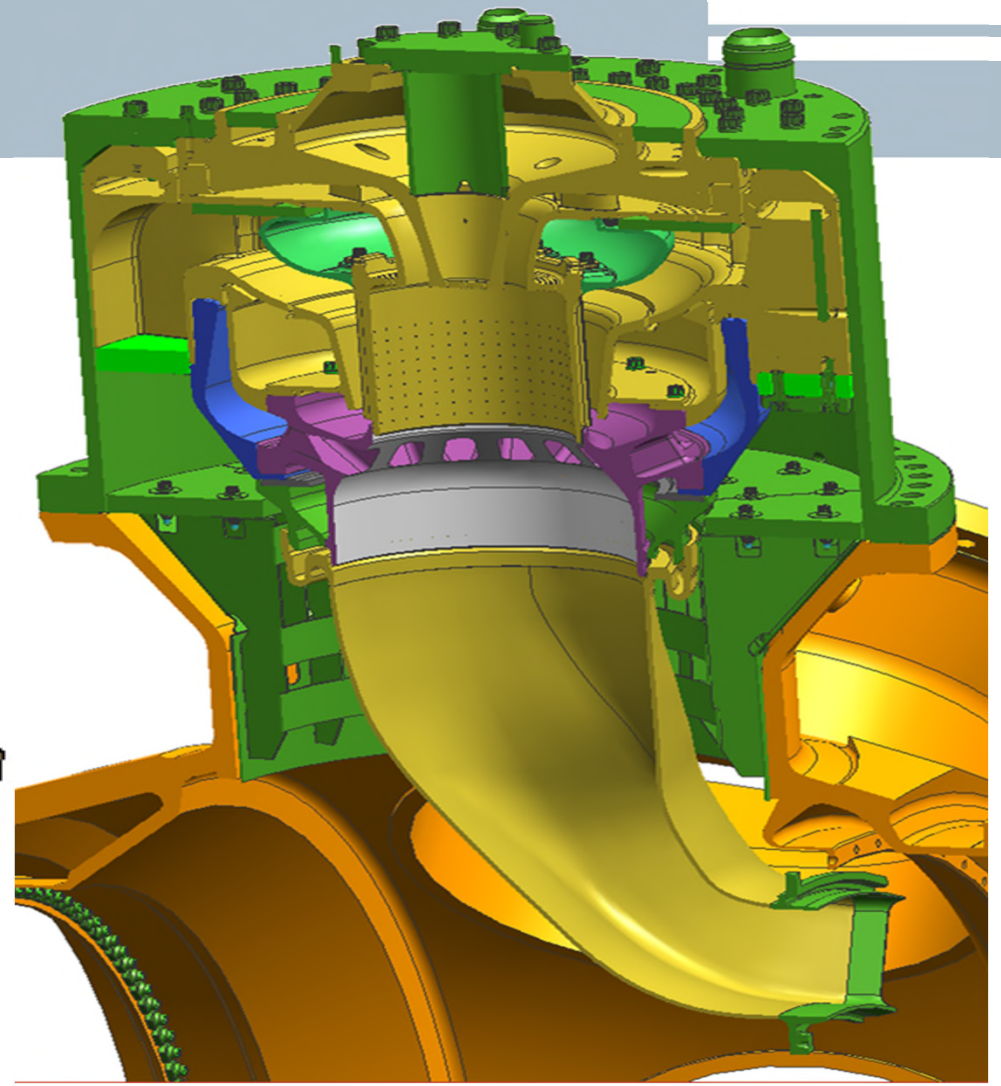
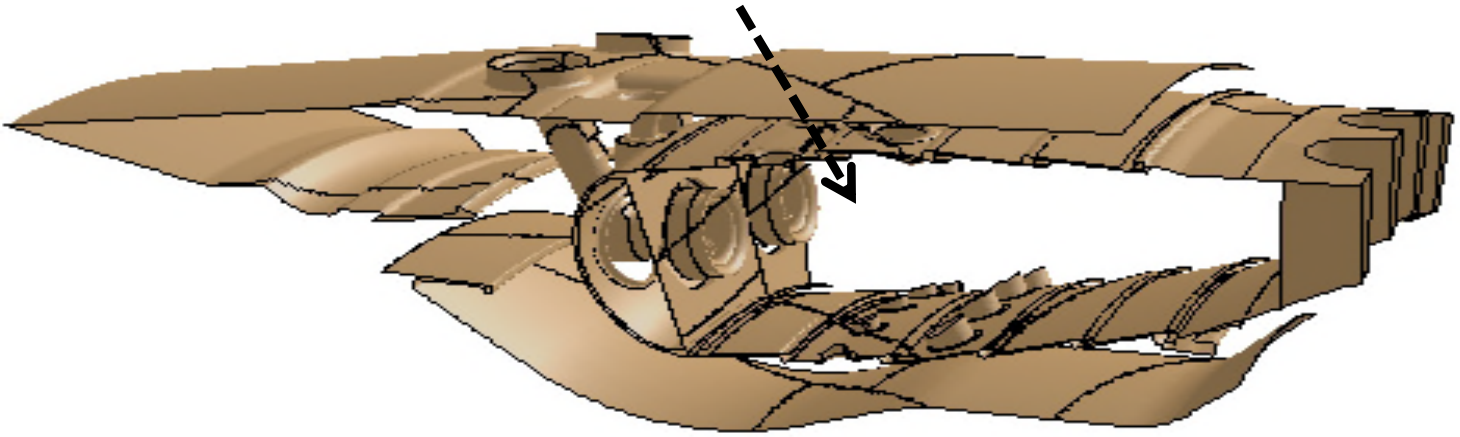

Emissions Characteristics
Desired
Operating
Range
CO
NOx
Emissions
Lean
Rich
Fuel/Air Ratio

Industrial Applications

Intricate ‘plumbing’ required to
Mix the fuel and the air before
entering the combustor



Fuel and Air meet for the first time
Inside the combustor



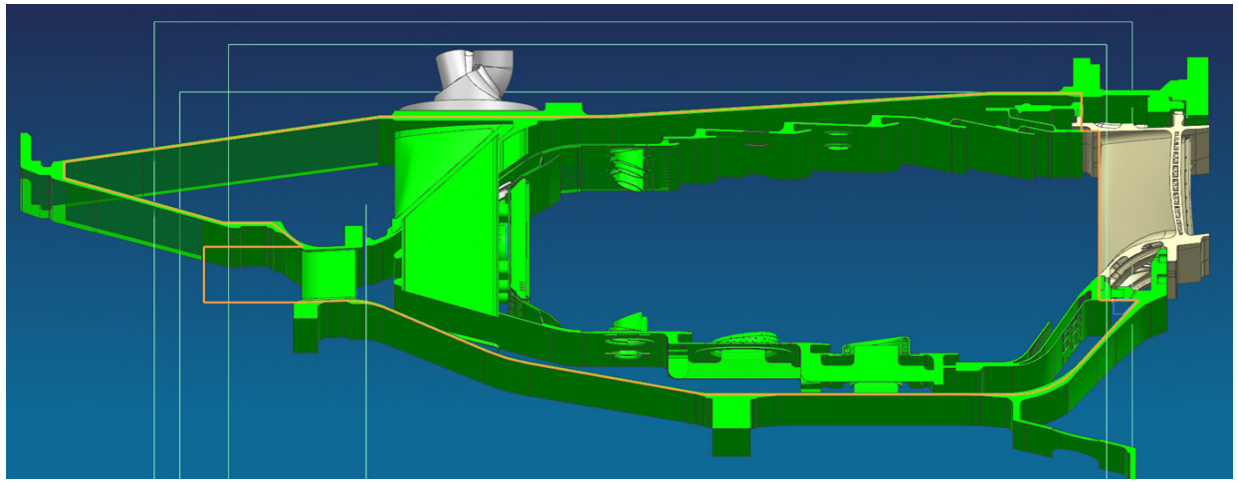
Typical Aero Combustion System

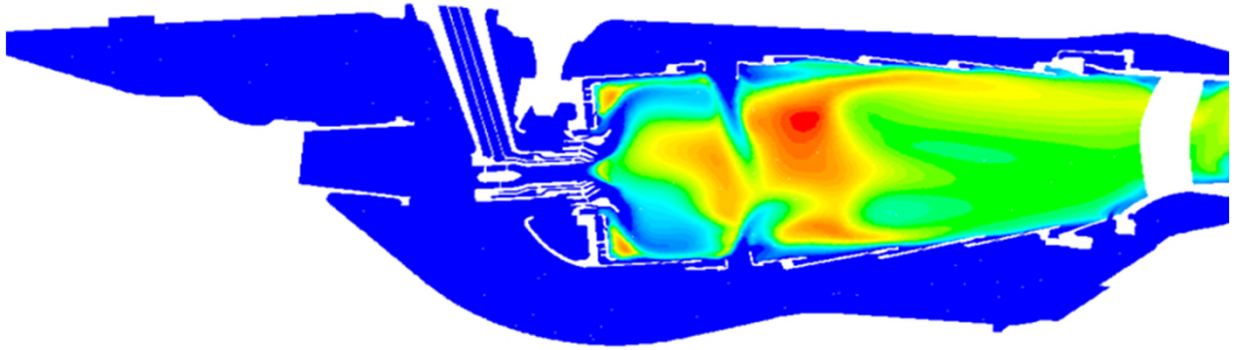
Diffusion Flames

Industrial Combustion System

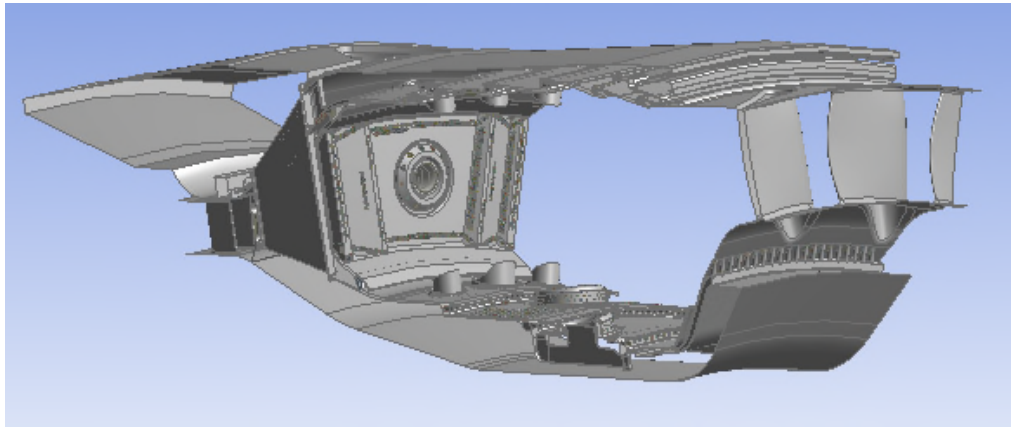
Premixed Flames

CFD Models: Full Combustor Simulations (Diffusion Flames)

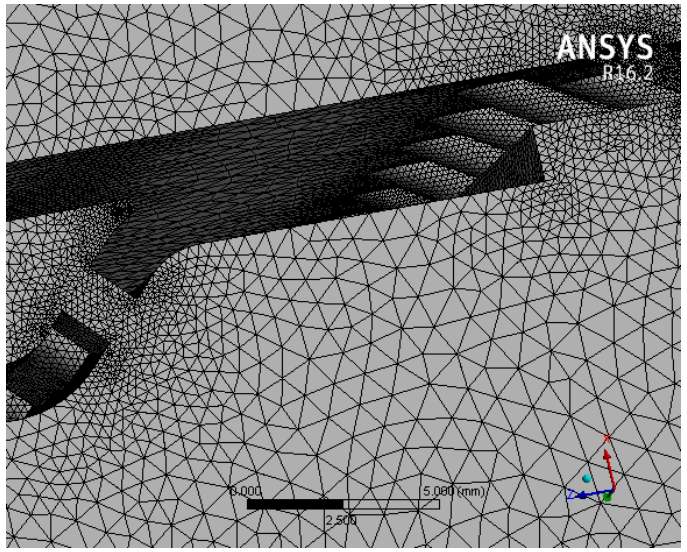




High fidelity CFD Model of a Typical Annular Combustion System

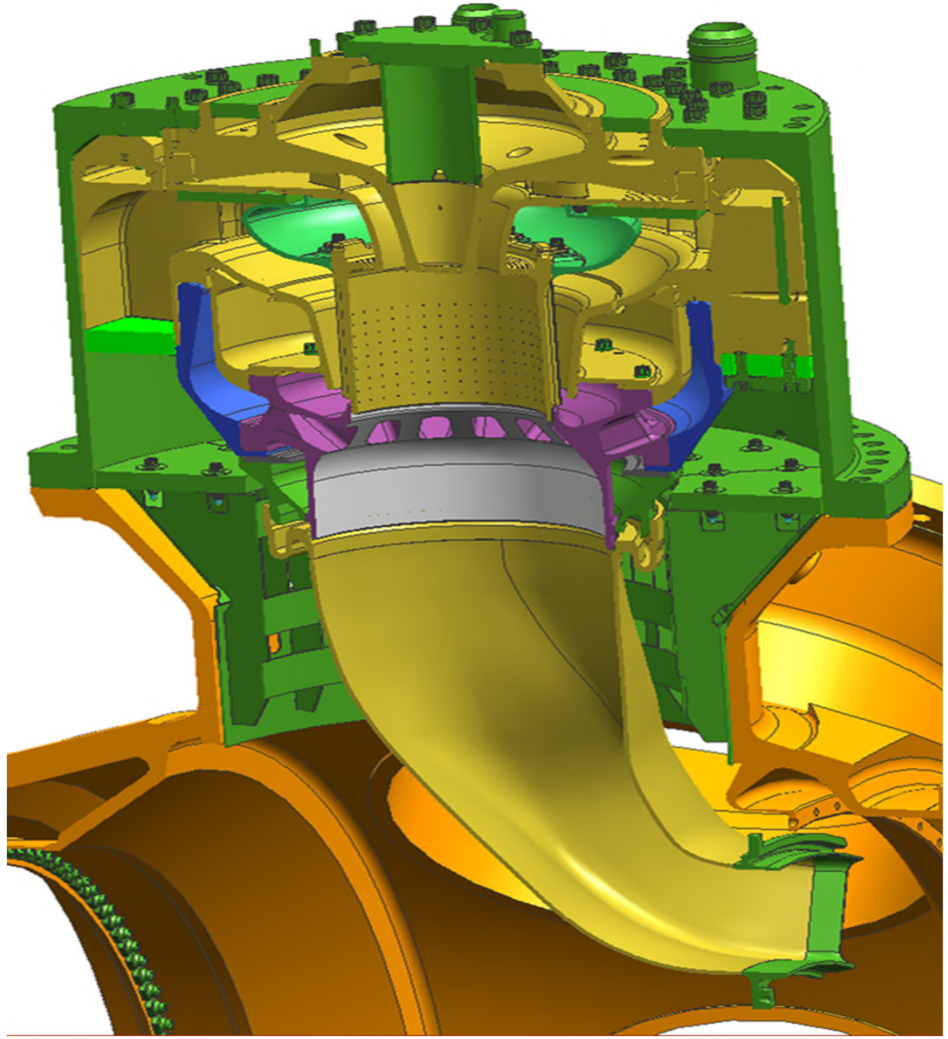


Injector details, Liner cooling details, Exit Guide Vanes…

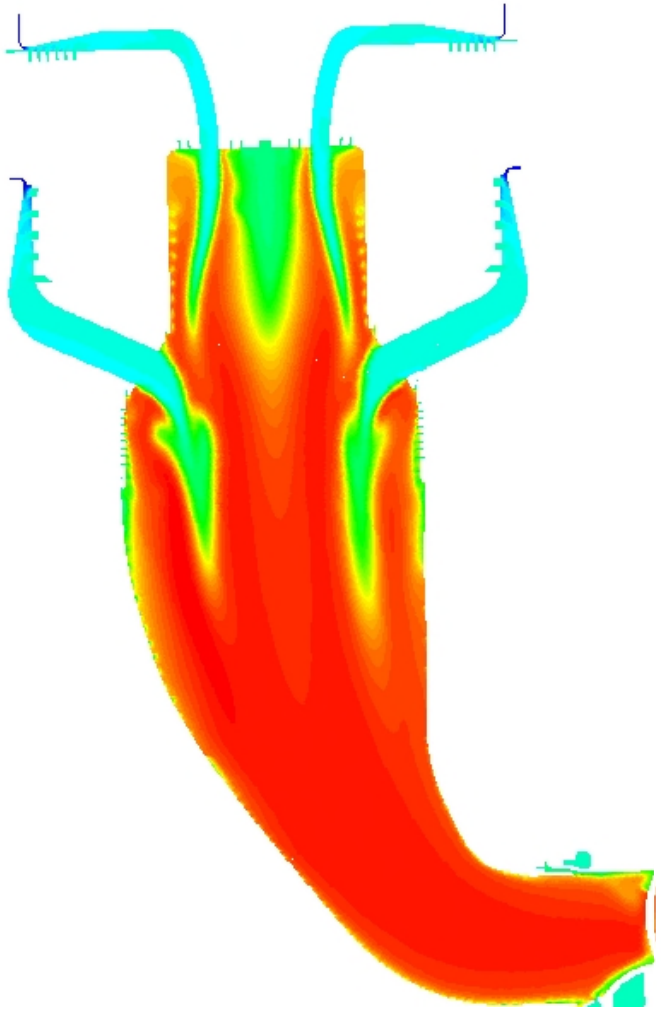


Millions of cells CFD Models

CFD Models: Full Combustor Simulations (Premixed Flames)



SGT-A65



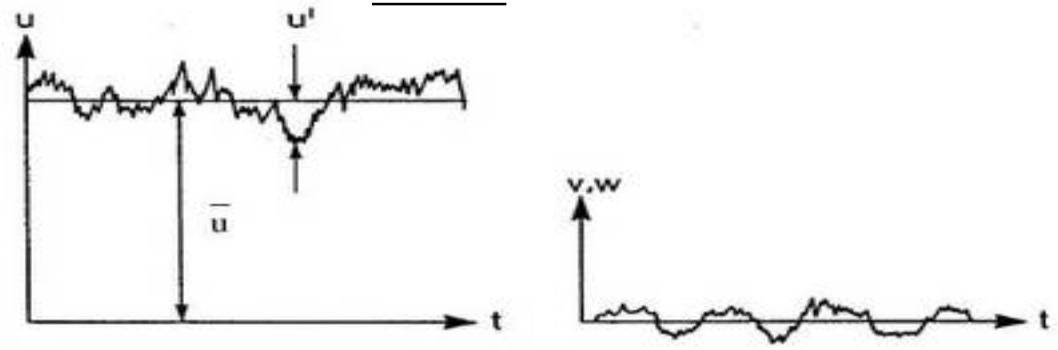
RANS

LES

Turbulence

"Big whirls have little whirls, That feed on their velocity;
And little whirls have lesser whirls, And so on to viscosity."
Lewis Fry Richardson

RANS



$$u = \bar{u} + u', \quad v = \bar{v} + v', \quad w = \bar{w} + w', \quad p = \bar{p} + p'$$

$$\rho \frac{D\bar{u}_i}{Dt} = F_i - \frac{\partial \bar{p}}{\partial x_i} + \mu \Delta \bar{u}_i - \rho \underbrace{\left(\frac{\partial \overline{u_i' u_j'}}{\partial x_j} \right)}_{\text{Reynolds-stress}}$$

$$\tau_{ij} = \mu \frac{\partial u_i}{\partial x_j} - \rho \overline{u_i' u_j'} = \mu \frac{\partial u_i}{\partial x_j} + \rho \left(\nu_T \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} k \delta_{ij} \right)$$

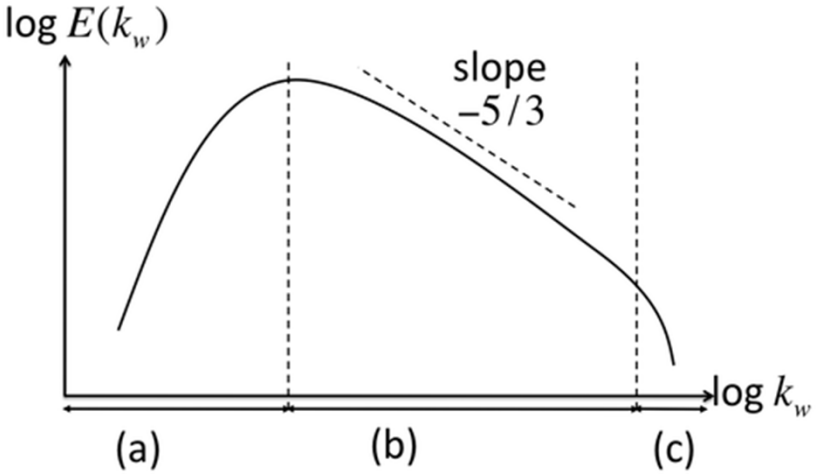
$$\nu_t = \left| \frac{\partial u}{\partial y} \right| l_m^2 \longrightarrow \mu_t = \rho C_\mu \frac{k^2}{\epsilon} \longrightarrow \mu_t = \frac{\rho a_1 k}{\max(a_1 \omega, \Omega F_2)}$$

Mixing Length **k-ε models** **k-ω models**

LES

$$\overline{\phi(\boldsymbol{x}, t)} = \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \phi(\boldsymbol{r}, t') G(\boldsymbol{x} - \boldsymbol{r}, t - t') dt' d\boldsymbol{r},$$

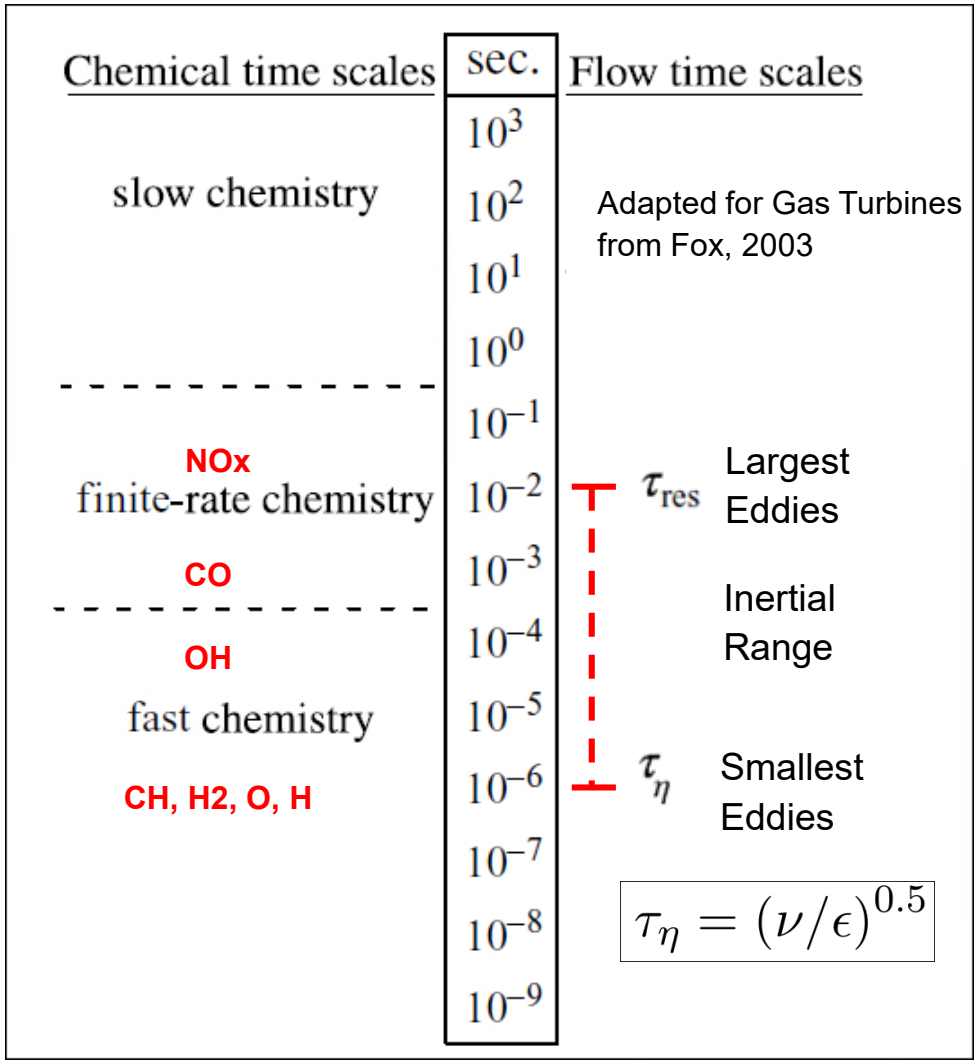
G(**x**) or G(**k**) are Filtering Functions



Eddies in turbulent flows contain Energy resulting in a level of turbulent mixing and shear forces.
Kolmogorov's Energy cascade Theory: Energy is passed from eddies with larger wave numbers, to eddies with smaller wave numbers.
(1941 paper 'The local Structure of Turbulence at High Reynolds Number', in which he sites T. Von Karman and G.I. Taylor)

Sub-Grid Scale Turbulence Models are still required

Scales…scales and more scales

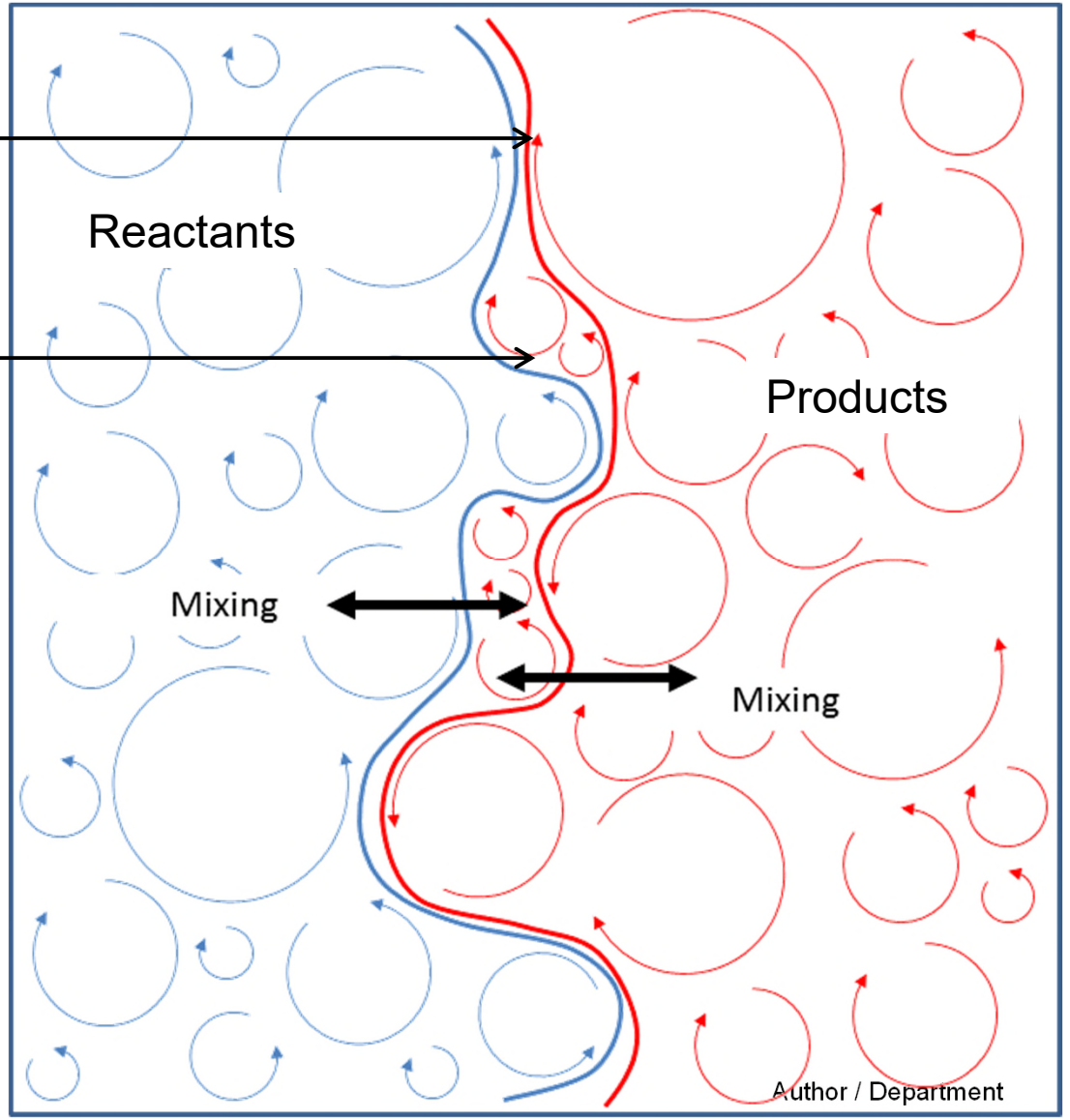


Adapted for Gas Turbines from Fox, 2003

Flamelet behavior

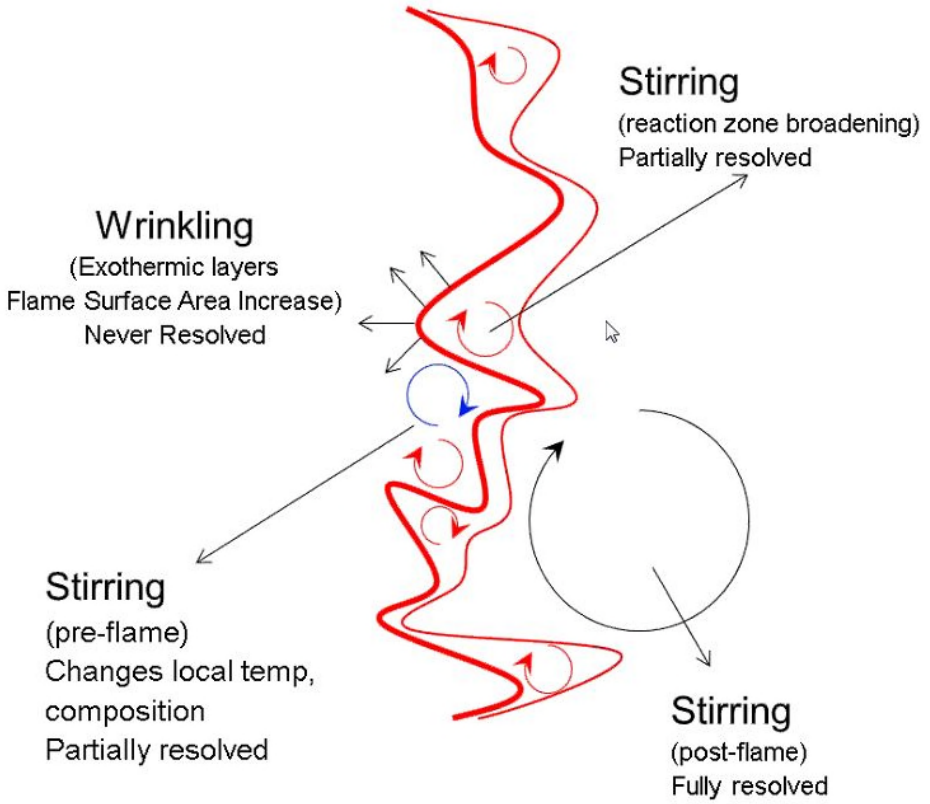
Non-flamelet behavior

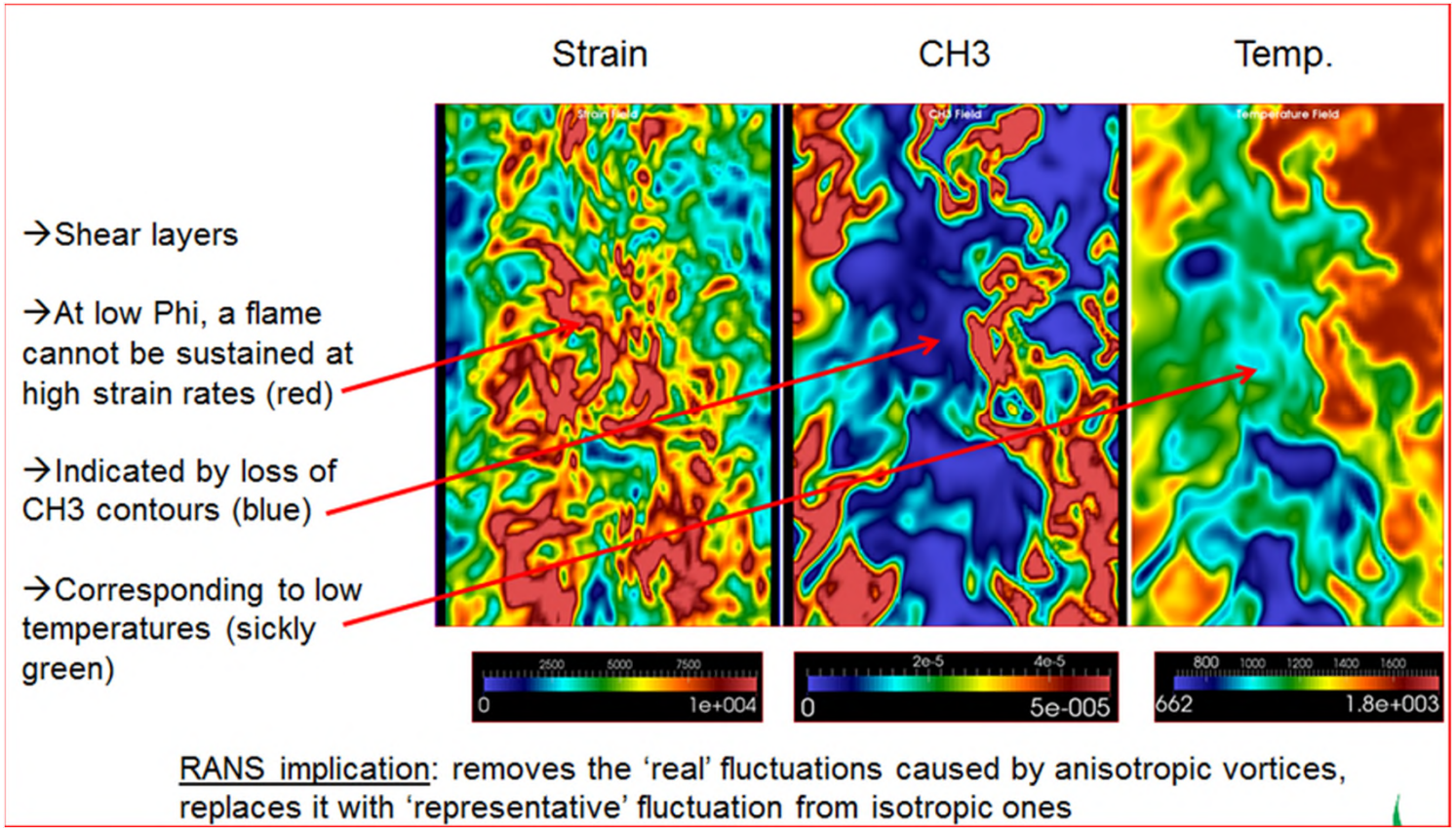
Species <u>will</u> interact with turbulence



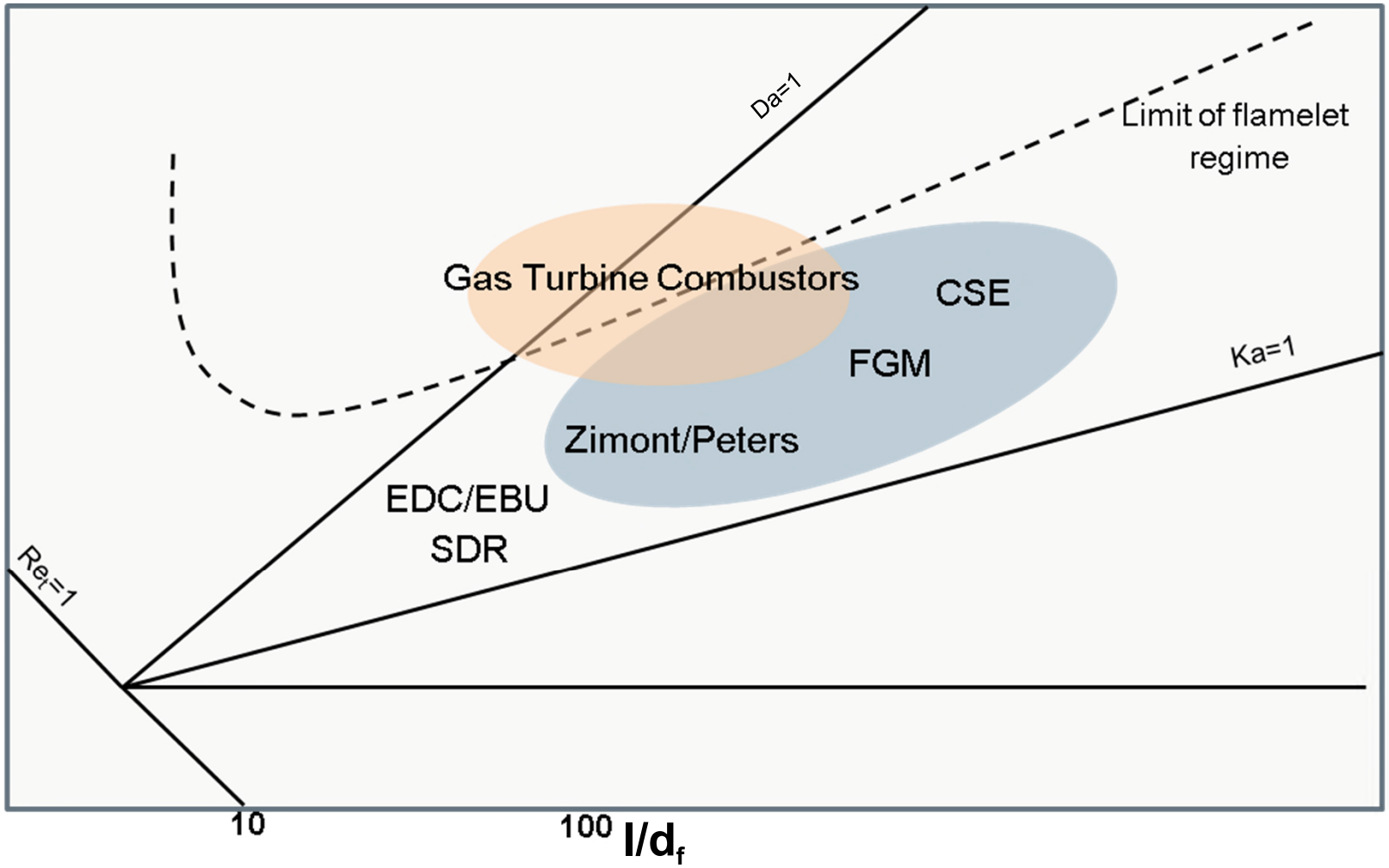
Fuel Type will essentially modify the overlap of chemical and turbulent time-scales.

Flame Physics





Flame Regimes: Borghi Diagrams



U'
Turbulence Velocity Scale

S_L
Laminar Flame Speed Scale

l
Intergral Length Scale

d_f
Flame Length Scale

Karlovitz Number

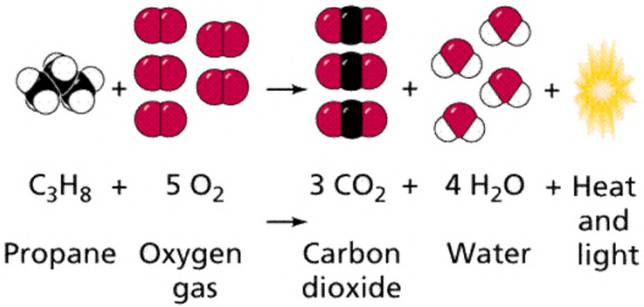
$Ka = \tau_c / \tau_\nu$

Damkohler Number

$Da = \tau_T / \tau_c$

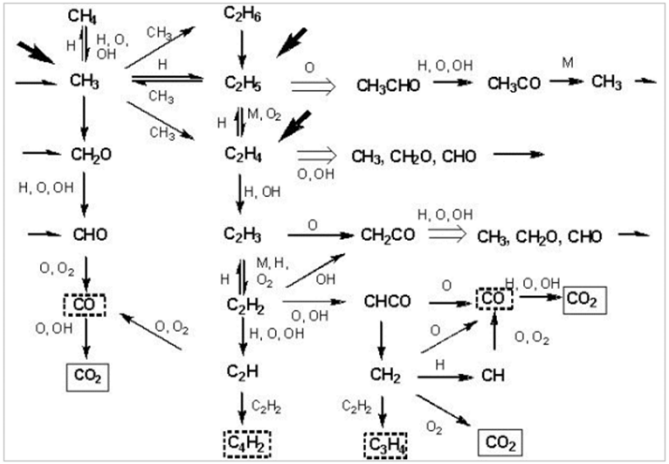
Chemistry (Mechanisms)

Global Reactions → One or more 'reactions' tuned to reproduce Thermo-Chemical effects



(FUEL + Oxidizer → Products)

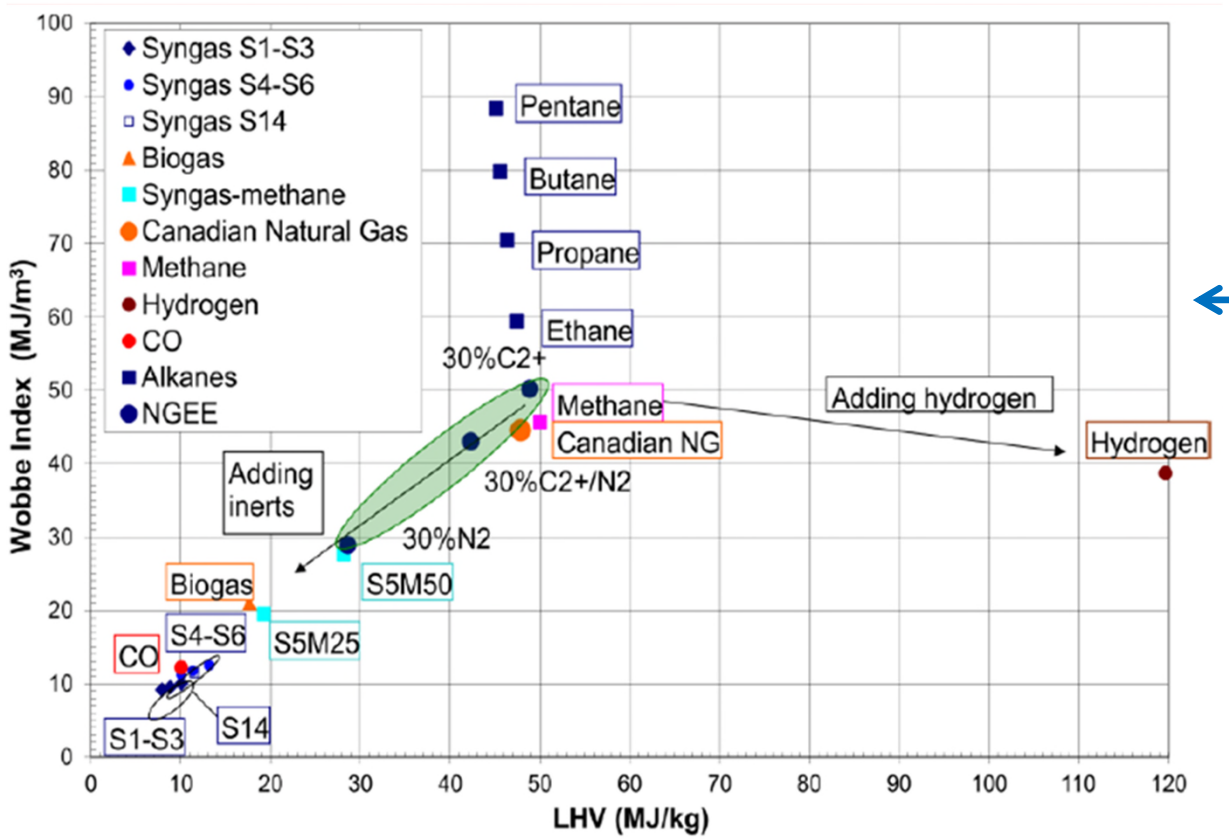
Detailed Chemistry → Chain-Initiating, Chain-Carrying, Chain-Branching...Chain-Terminating



Reduced Chemistry → Keep Important Pathways...even add a little NOx!

(R_1)	$H_2 \leftrightarrow 2H$
(R_2)	$H_2 + O_2 \leftrightarrow 2OH$
(R_3)	$2H_2 + O_2 \leftrightarrow 2H_2O$
(R_4)	$2CO + O_2 \leftrightarrow 2CO_2$
(R_5)	$2CH_4 + O_2 \leftrightarrow 2CO + 4H_2$
(R_6)	$2CH_4 \leftrightarrow 2CH_3 + H_2$
(R_7)	$2CH_4 + 3O_2 \leftrightarrow C_2H_2 + 6OH$
(R_8)	$2HCN + O_2 \leftrightarrow 2CO + H_2 + N_2$
(R_9)	$O_2 + N_2 \leftrightarrow 2NO$
(R_{10})	$O_2 + 2N_2 \leftrightarrow 2N_2O$

Chemistry (fuels)

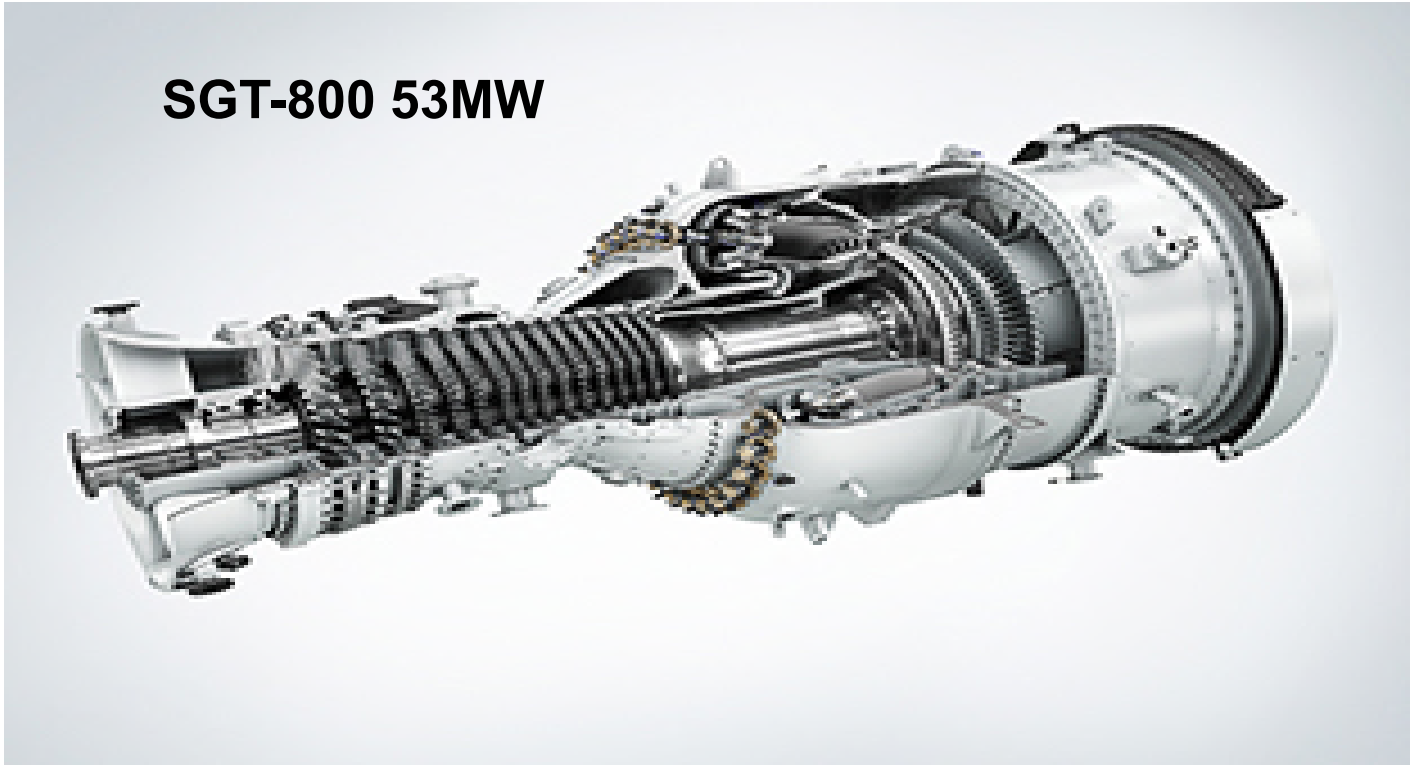


Combustion Turbine Fuels

- Conventional Fuels
  - Natural Gas
  - Liquid Fuel Oil
- Nonconventional Fuels
  - Crude Oil
  - Refinery Gas
  - Propane
- Synthetic Fuels
  - Chemical Process
  - Physical Process

Examples

- Introduction
- Combustion test rig
- Computational models
- Computational results
- Summary



Introduction: SGT-800 3rd generation DLE burner
Swirl stabilized main flame with 12 pilot flames

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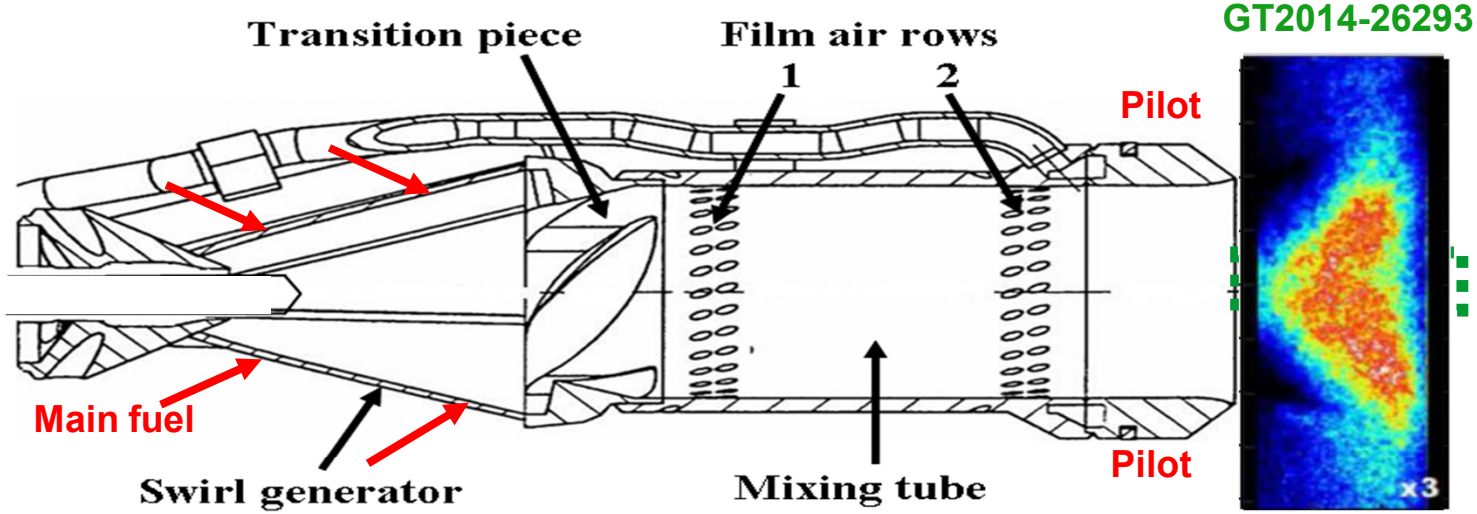
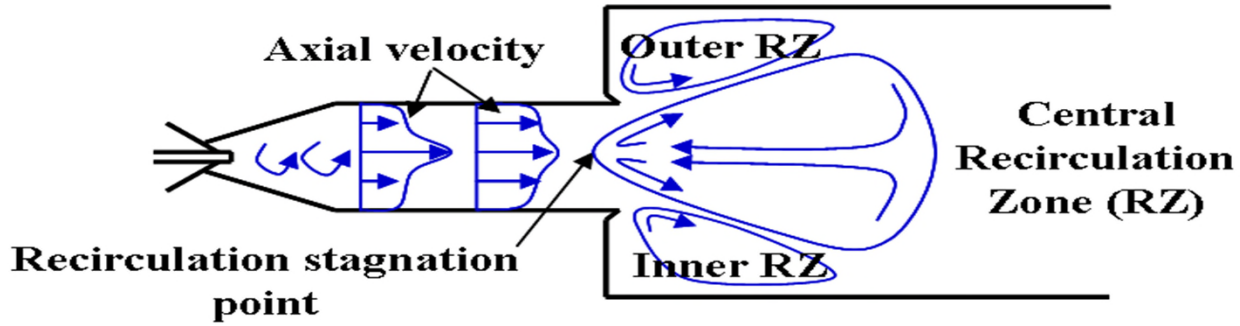
SGT-800 DLE burner

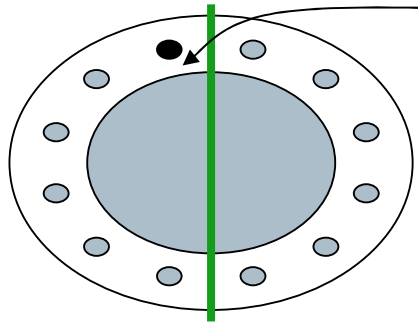


Laser sheet
OH PLIF
GT2014-26293

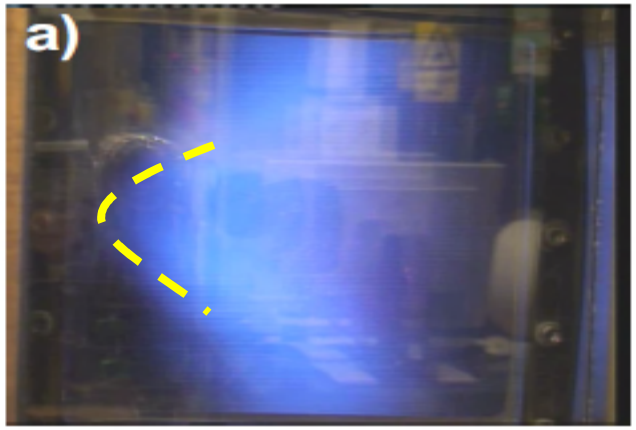
PDF of OH gradient



Burner front view & pilot nozzles



Atm. rig measurements
Low PFR, natural gas

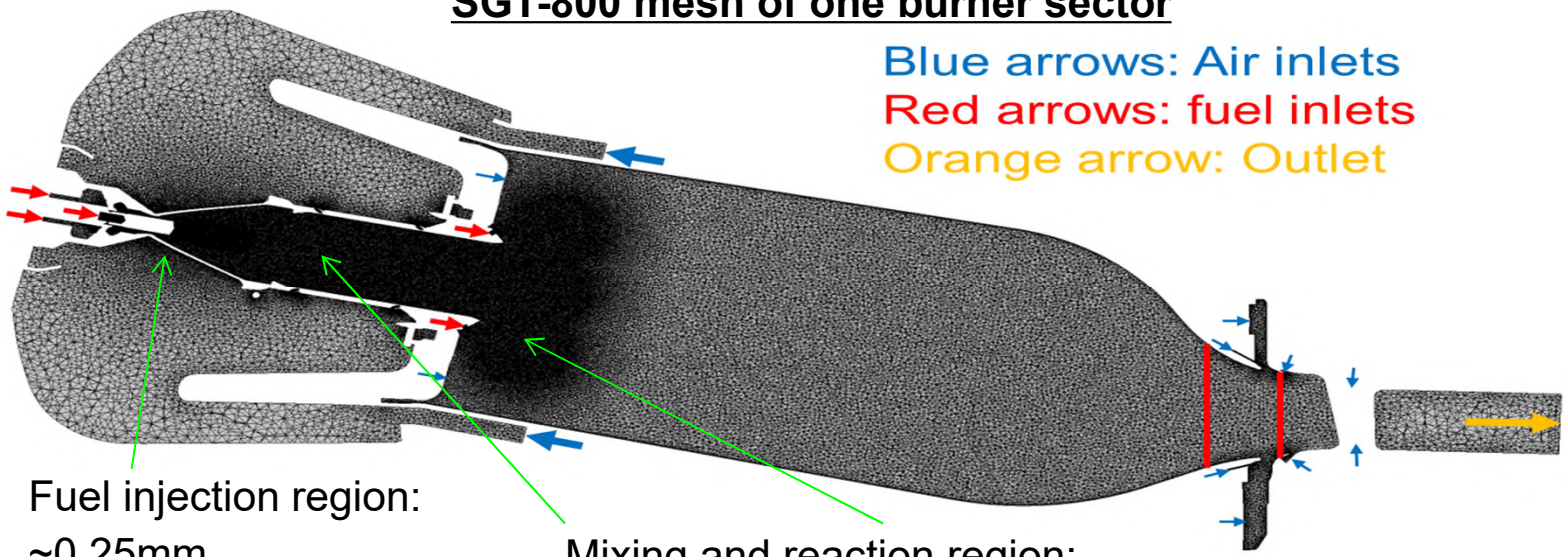


Numerical method:
Turbulence & combustion models, mesh and BC

Advantages of SAS compared to LES:
- Automatic wall boundary treatment
- May use larger time steps since LES requires CFL≤1 in whole domain while SAS may use CFL>1 if RANS like behavior is acceptable in high CFL regions

- **Turbulence models**
  - Steady RANS k-ω SST
  - Scale Adaptive Sim. k-ω SST
- **Combustion models**
  - Flamelet based models: Lindstedt & Vaos Fractal & Zimont Burning Velocity model
  - Eddy Dissipation Model – Finite Rate Chemistry (see GT2016-57423 and GT2016-45853)
- **Mesh**
  - 42M tetrahedron cells
  - 0.6M prisms at liner walls
  - Previous mesh evaluation:
    - GT2013-95478
    - GT2015-44040
- **Solver: Ansys CFX16.0**
- **Boundary conditions**
  - From 50.5MW engine test

SGT-800 mesh of one burner sector



Computational results (EDM-FRC M4_HP):
Velocity and temperature

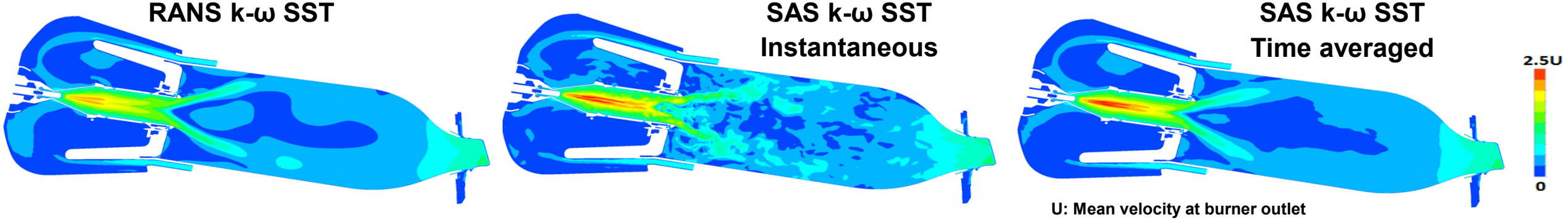
- Velocity field similar between RANS k-ω SST and time averaged SAS-SST
- Temperature gradient in flame region is much higher for k-ω SST than for time averaged SAS-SST

Velocity magnitude

RANS k-ω SST

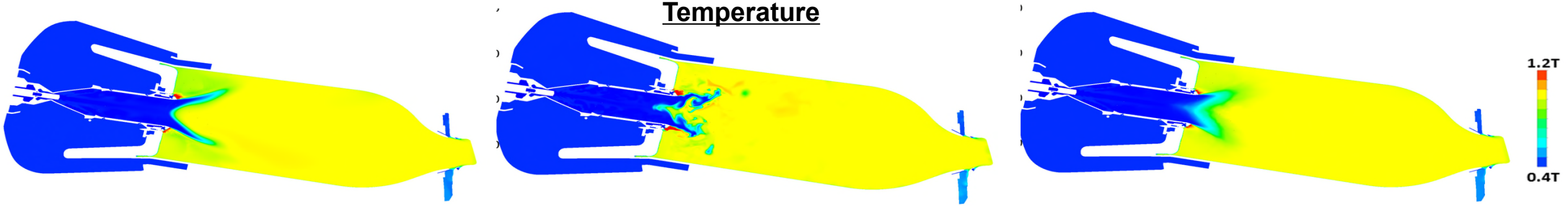
SAS k-ω SST Instantaneous

SAS k-ω SST Time averaged



U: Mean velocity at burner outlet

Temperature



T: Mean temperature at combustor outlet

Computational results (EDM-FRC M4_HP):
Turbulent kinetic energy and eddy frequency field

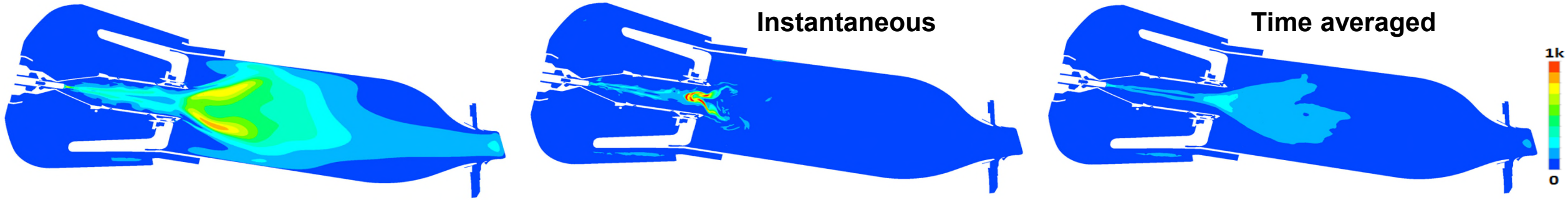
- Time averaged kinetic energy for SAS-SST is much lower than for k-ω SST while the time averaged eddy frequency is higher

Turbulent kinetic energy

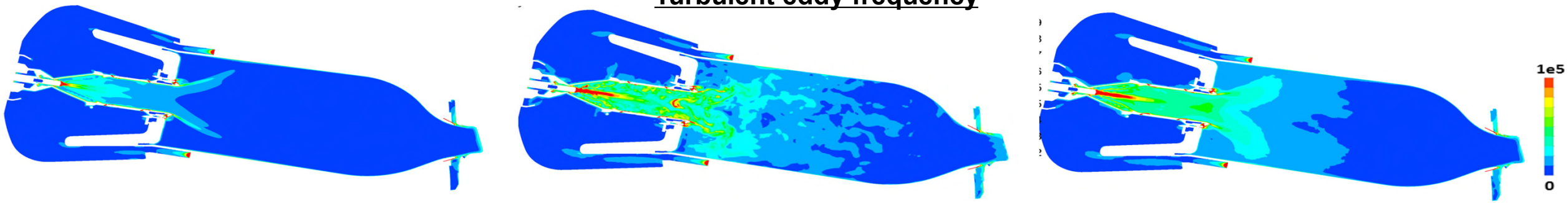
RANS k-ω SST

SAS k-ω SST Instantaneous

SAS k-ω SST Time averaged



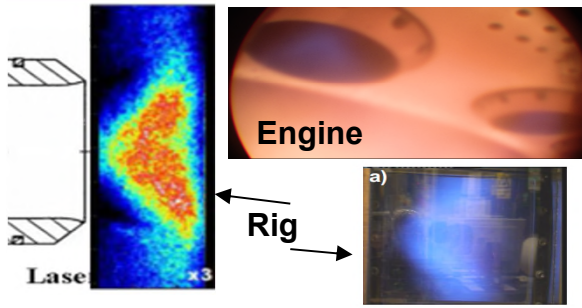
Turbulent eddy frequency



Computational results (EDM-FRC M4_HP):
CO2, CO and progress variable fields

Difference 1 & 20 bar in rig, see GT2016-57423

- Qualitatively flame position agrees with measurement data
- Time averaged SAS-SST predicts smoother gradients than k-ω SST → in better agreement with OH gradient PDF field



CO2

RANS k-ω SST

SAS-SST

2C

0

CO

RANS k-ω SST

SAS-SST

0.02

0

Progress variable

RANS k-ω SST

SAS-SST

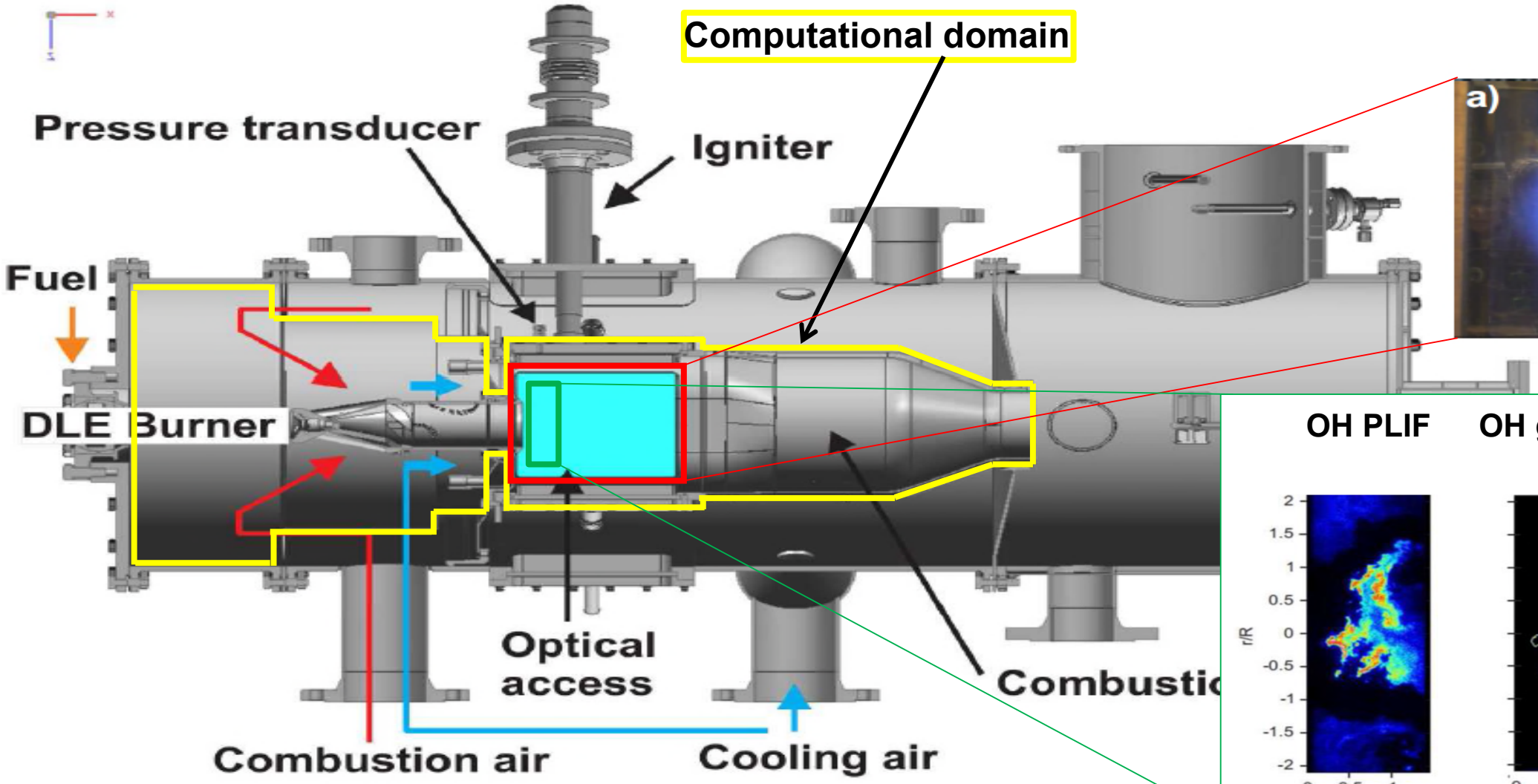
1

0

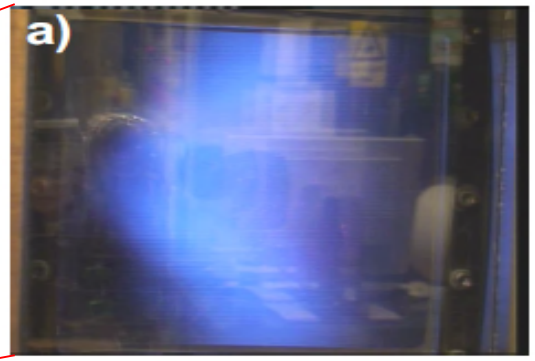
C: Averaged concentration at combustor outlet

PV is based on fuel mass fraction relative to its value in both reactants and products

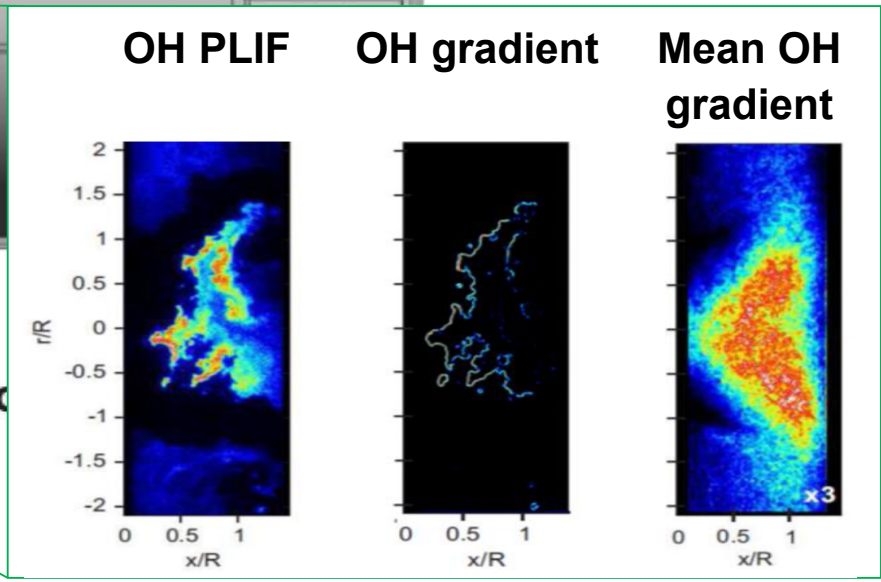
SGT-800 burner in an atmospheric combustion rig



Natural gas
Low pilot

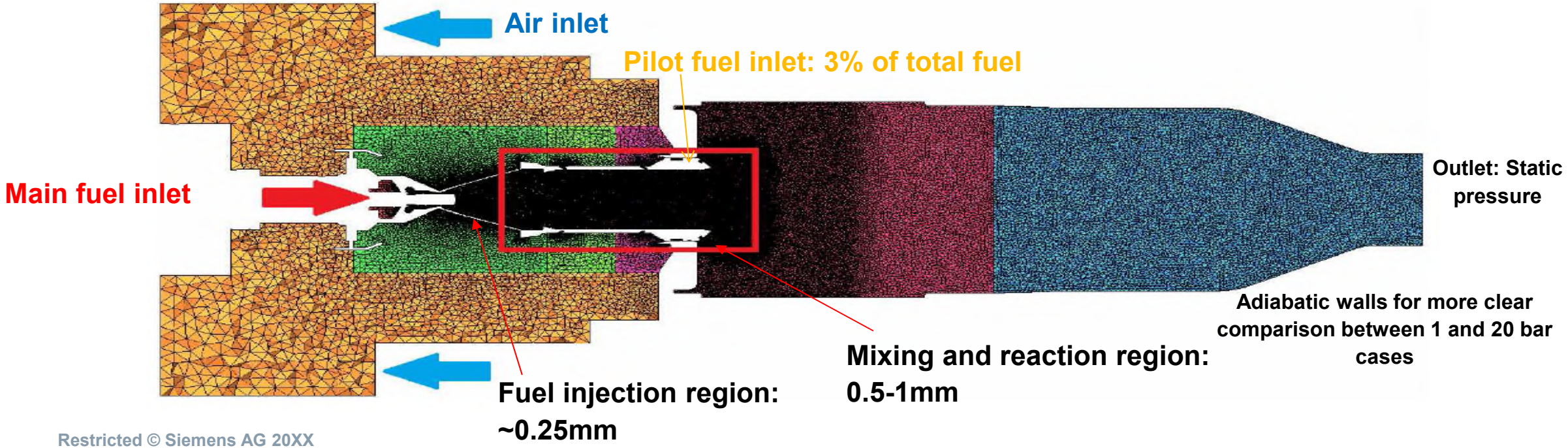


GT2014-26293



CFD modeling
Geometry, meshing and boundary conditions

- Software: ICEMCFD ~32M tetra cells
  - Same mesh as GT2015-44040 where grid study performed
    - Same boundary conditions for atmospheric case
    - For 20 bar case, mass flows scaled (same U_{out} & T_{out})



Chemical kinetic modeling
Reduced schemes

- Detailed reaction mechanisms for common fuels are huge
  - Contain hundreds of species and thousands of reactions
  - Need to simplify this for practical use in CFD
    - Global reaction mechanisms
- Reduced schemes can predict reasonably well
  - Laminar flame speed, adiabatic flame T & ignition delay
  - Wide range of operating conditions
- Global mechanisms consist of a small number of reactions, each controlled by A_i, B_i, E_{ai} and $\mu_{j,i}$ according to Arrhenius rate expression:

$$\dot{\omega}_i = A_i \prod_{j \in \mathcal{A}} \left(\frac{\rho Y_j}{W_j} \right)^{\mu_{j,i}} T^{B_i} \exp\left(-E_{a_i}/(RT)\right)$$

A_i: pre-exponential factor
B_i: Temperature exponent
E_{ai}: Activation energy
$\mu_{j,i}$: Reaction orders

- Optimization has been used to obtain these parameters.

Chemical kinetic modeling
M4_20bar scheme

	Reaction	A	E_a [cal/mole]	β
1	$CH_4 + 0.5O_2 \rightarrow CO + 2H_2$	0.98e12	36500	0.8
2	$H_2 + 0.5O_2 \leftrightarrow H_2O$	2.076e17	40000	-1.48
3	$CO + 0.5O_2 \leftrightarrow CO_2$	1.633e13	35500	-0.4
4	$CO + H_2O \leftrightarrow CO_2 + H_2$	1.985e13	32857	0.4

M4_20bar is based on M4_1bar (see GT2013-95454)

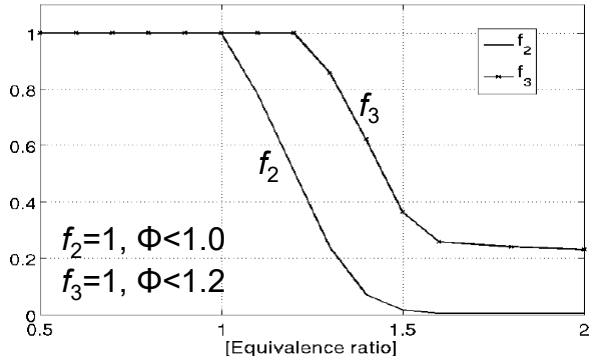
It was sufficient to optimize the pre-exponential factors A to take into account for the pressure effect

$$RR_1 = A_1 T^{\beta_1} e^{\frac{-E_{a1}}{RT}} [CH_4]^{0.7} [O_2]^{0.97}$$

$$RR_2 = A_2 T^{\beta_2} f_2(\Phi) e^{\frac{-E_{a2}}{RT}} [H_2]^{0.55} [O_2]^{1.01}$$

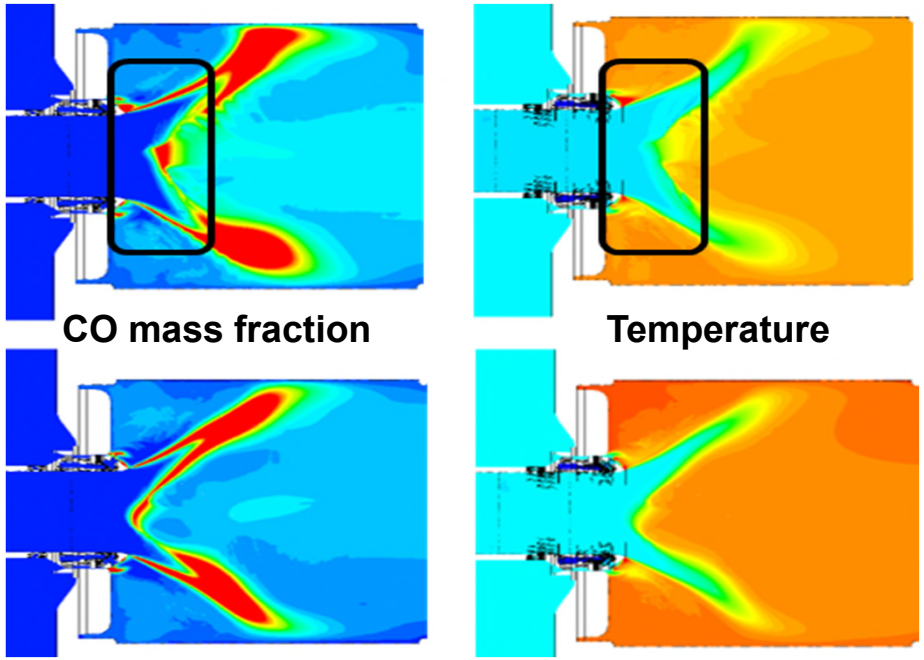
$$RR_3 = A_3 T^{\beta_3} f_3(\Phi) e^{\frac{-E_{a3}}{RT}} [CO]^1 [O_2]^{0.5}$$

$$RR_4 = A_4 T^{\beta_4} e^{\frac{-E_{a4}}{RT}} [CO]^1 [H_2O]^1$$



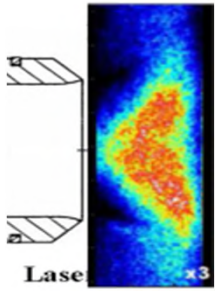
Results and discussion
CO and Temperature

k-ω SST turbulence model



CO mass fraction | Temperature

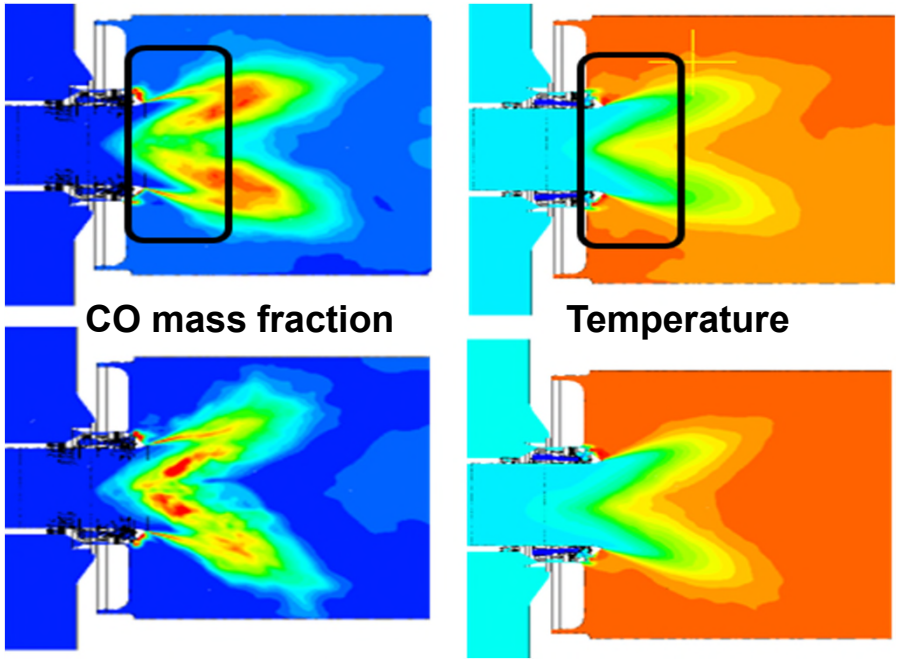
PDF OH gradient



1 bar

20 bar

SAS-SST turbulence model

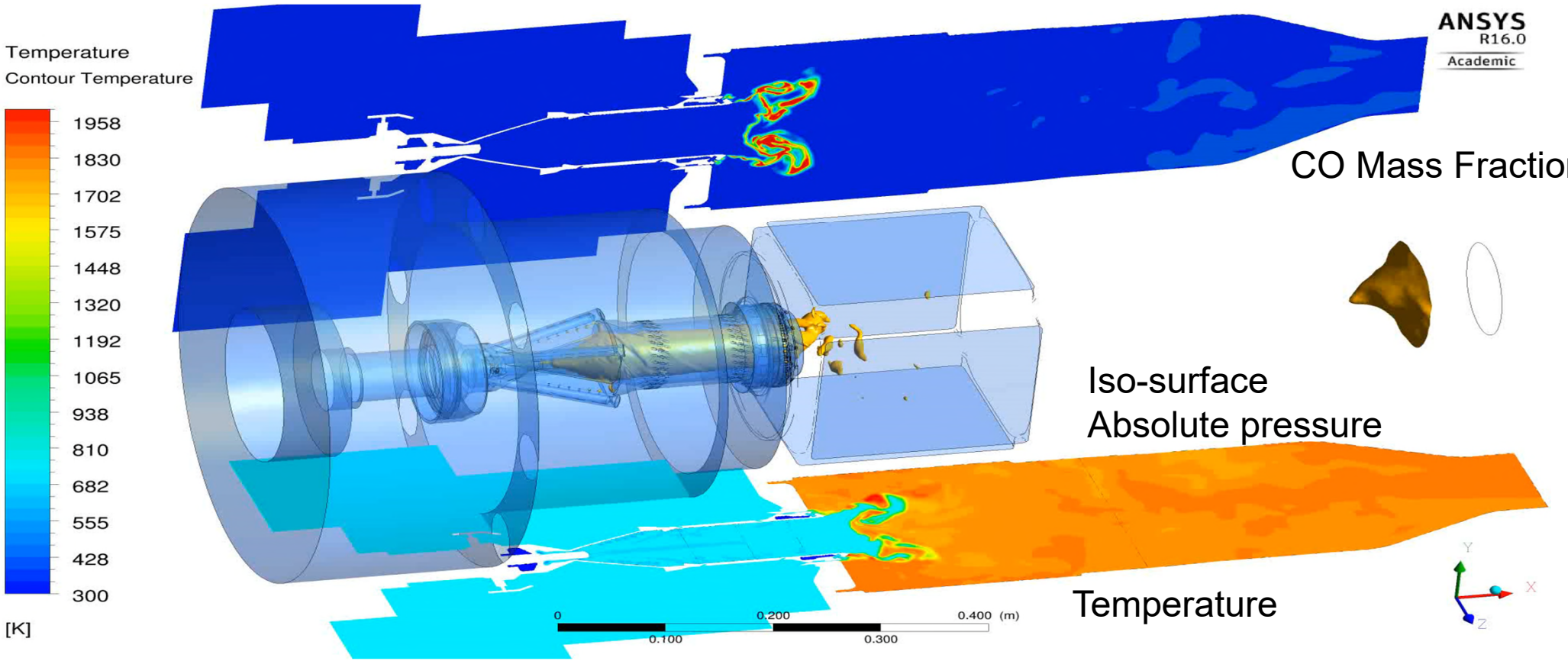


CO mass fraction | Temperature

- A fairly steady flame without any wrinkling.
- Highest CO outside the experimental window and close to the burner walls.
- Atm flame front location: x/R ≈ 0.5±0.15
  - Location in agreement with OH gradient density but gradients too high
- HP flame similar

- Atm flame front location: x/R ≈ 0.8±0.9
  - In agreement with the OH gradient density.
- HP flame in similar location but narrower
  - In agreement with visual location in rig and engine.
- Adiabatic walls in CFD may explain stronger external RZ

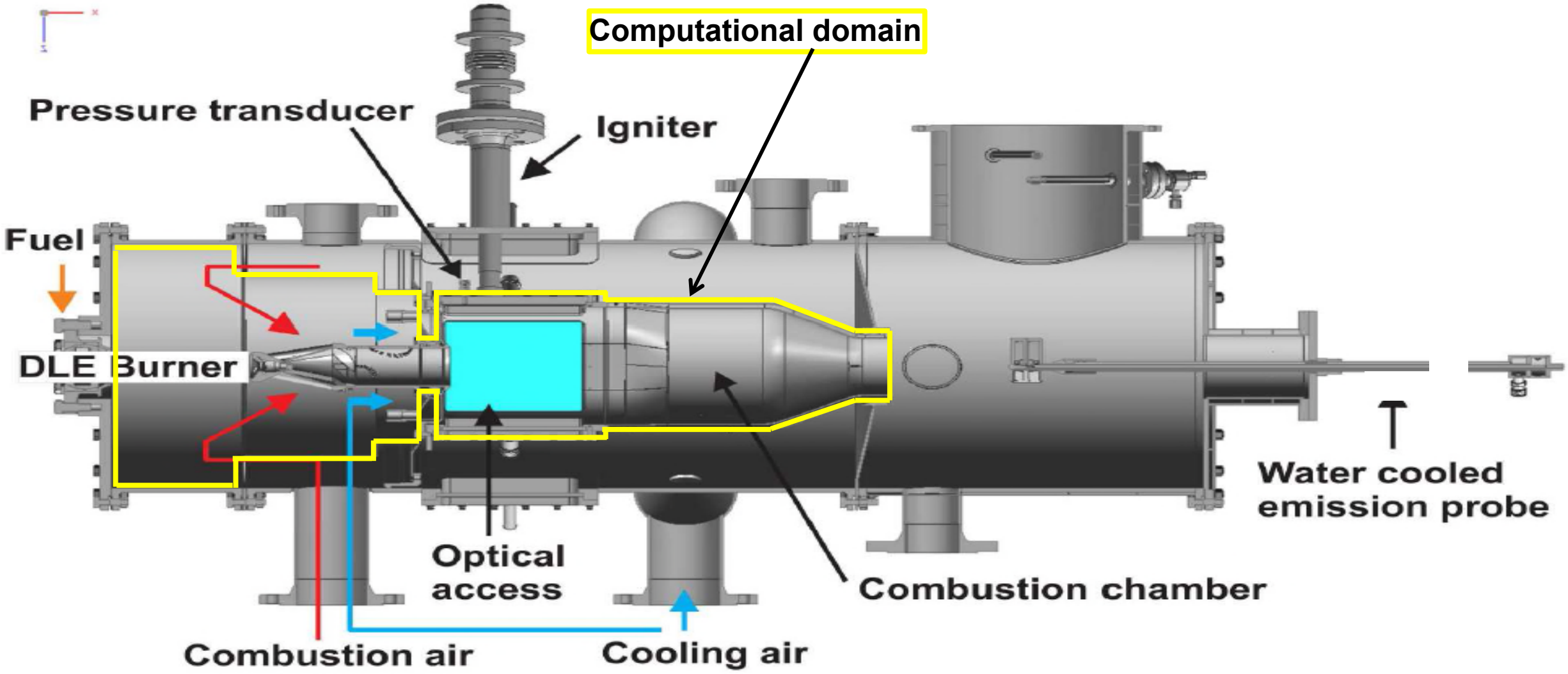
Results and discussion
20bar, SAS-SST model



- Complex flow field structure, presence of a rotating PVC and a CRZ, extending up to approximately one burner exit diameter downstream.
- The central flame root location is determined by the location where the flow starts to break down into smaller flow structures in the burner. This breakdown results in an axial movement of the location where the flame is anchored.

NUMERICAL INVESTIGATION OF HYDROGEN ENRICHED NATURAL GAS IN THE SGT-800 BURNER *(GT2015-44040)*

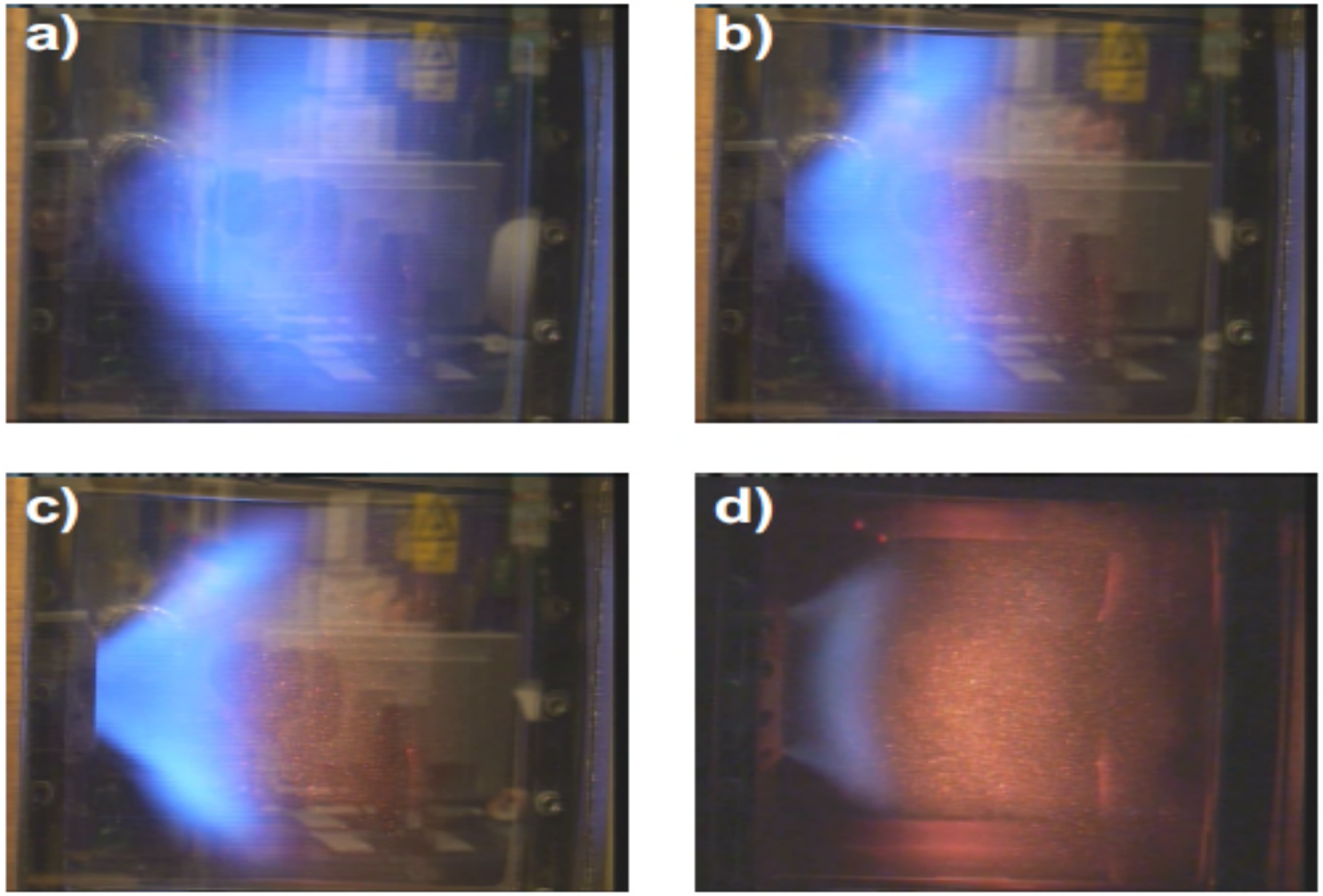
SIEMENS



Combustion test rig: Results
Visual flame behavior

- Flame shape and position with different amount of hydrogen addition, volume percent:
  a) 100% CH4
  b) 70% CH4 + 30% H2
  c) 40% CH4 + 60% H2
  d) 100% H2

- With increased amount of hydrogen
  - Flame position is moving upstream
  - Flame appears more compact



From GT2014-26293

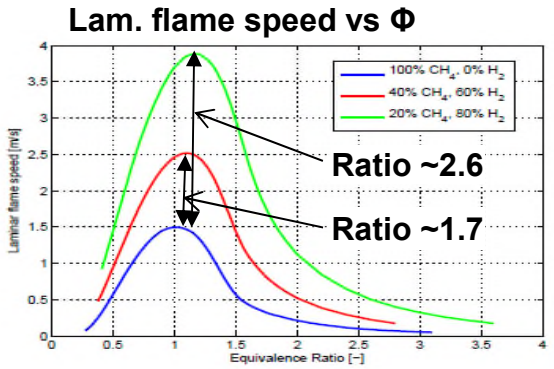
Computational model
Description

- Flow solver Ansys CFX v14.5

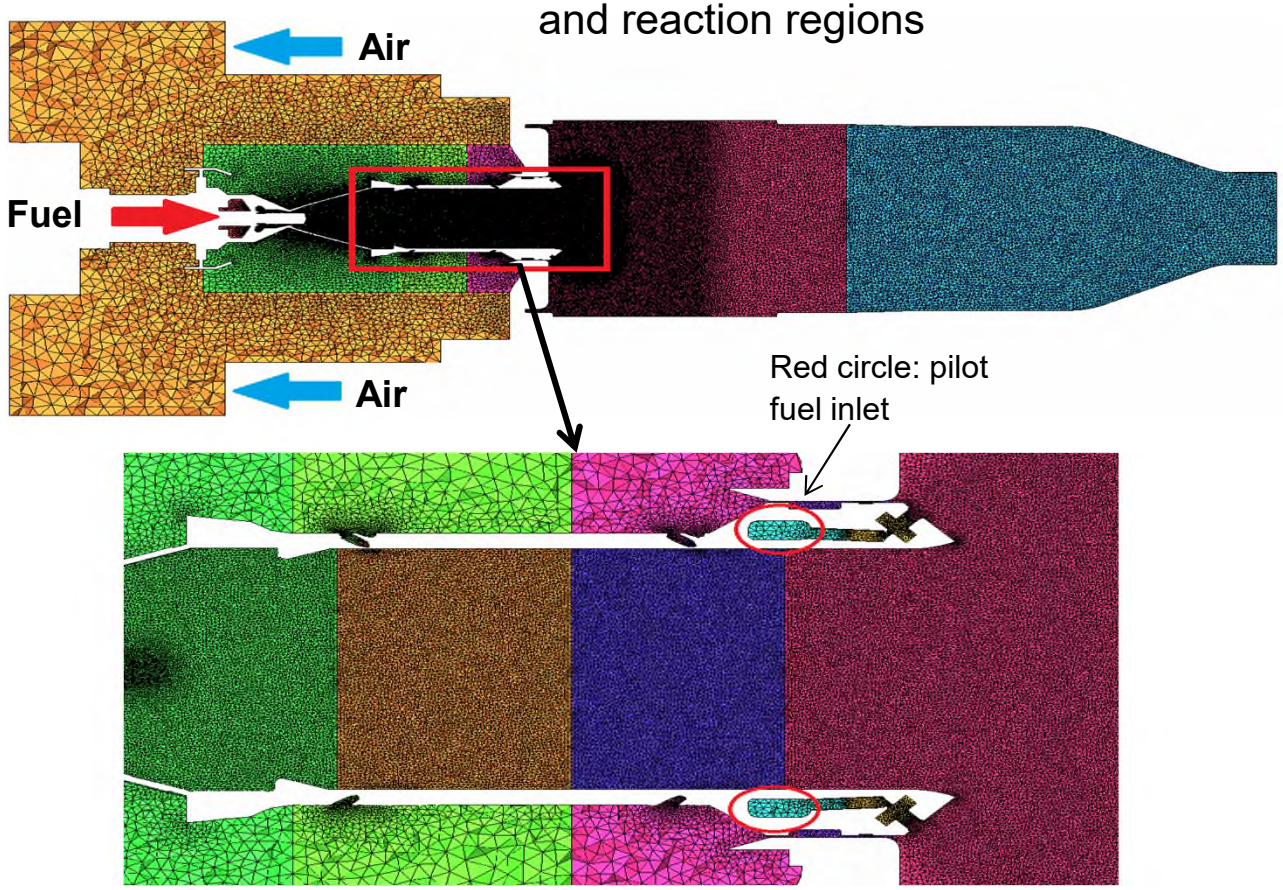
- Three different fuel compositions
  - CH4: 100%
  - H2/CH4: 60/40%
  - H2/CH4: 80/20%

- Turbulence model
  - k – ω SST
  - SST-SAS

- Combustion model
  - Flamelet along with Fractal mean reaction rate model. Two different reaction rate constants, CR:
    - CR = 2.6 (Only 100% CH4)
    - CR = 1.0



Total mesh size of 32M cells with maximum cell size of 1mm in mixing and reaction regions



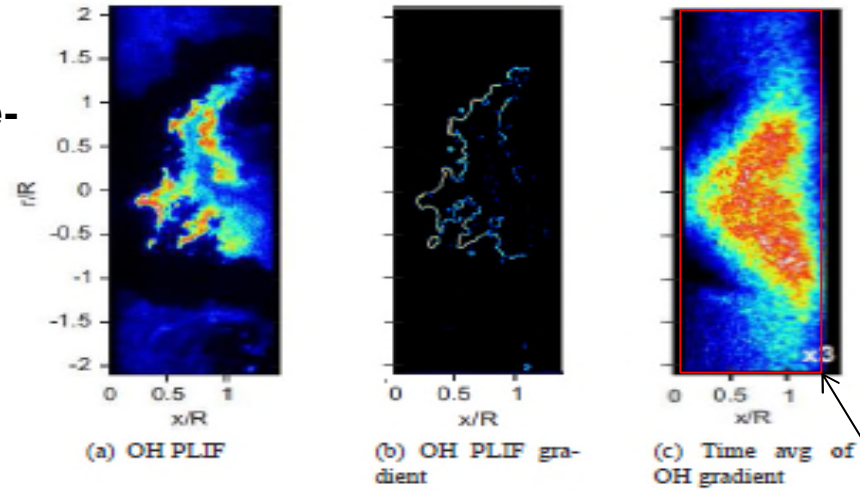
CFD results: (Methane/air combustion)
Different turbulence models and mean reaction rates

- k - ω SST
  - No change in centerline flame position with different CR reaction rate constants
- SST-SAS CR = 2.6
  - Time averaged flame position too far upstream
- SST-SAS CR = 1.0
  - Better agreement with experimental data

$$\overline{S_c} = C_R \rho_u \frac{u_L^0}{V_K} \frac{\tilde{\varepsilon}}{\tilde{k}} \tilde{c}\,(1-\tilde{c})$$

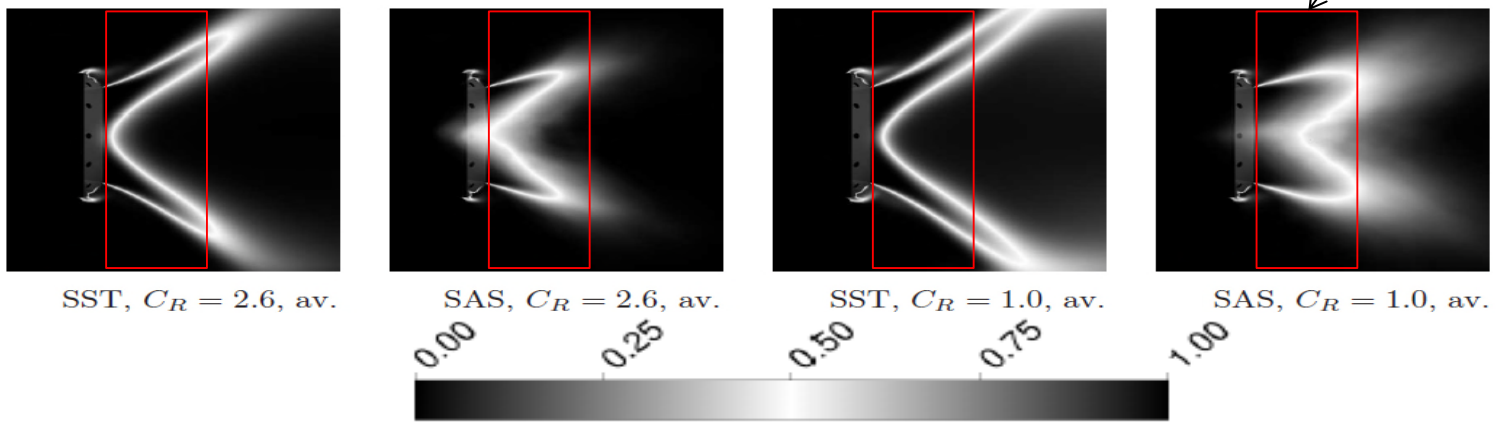
Note: CR and laminar flame speed affect CFD solution similarly. Influence of CR gives indication of influence of fuel flexibility effects.

OH PLIF of methane-air flame
(GT2014-26293)



Close agreement

Time averaged Reaction progress

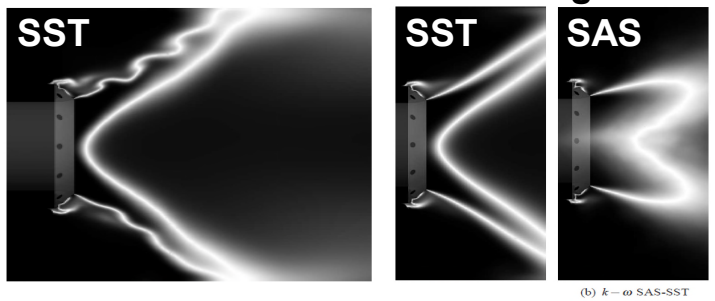


CFD results: (Methane/air combustion)
Dynamic behavior of flame using SST-SAS, Cr = 1.0

SIEMENS

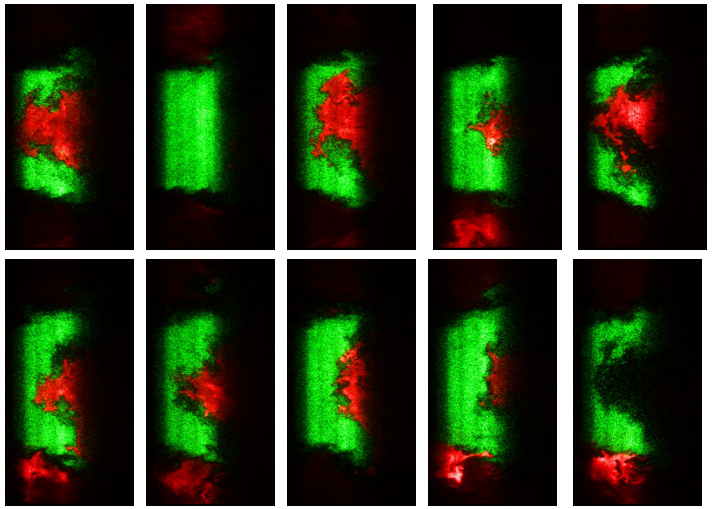
Reaction Progress

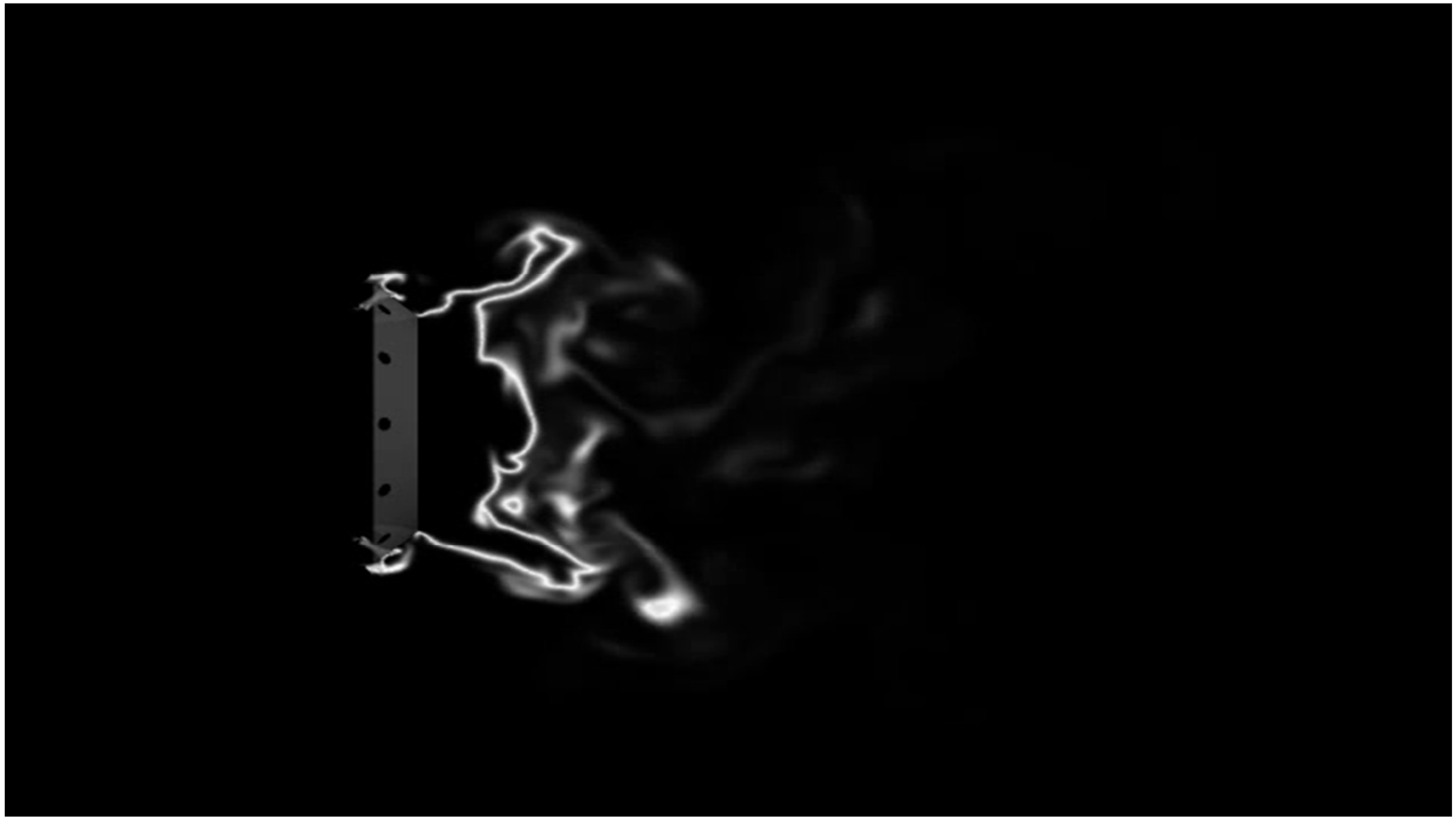
Instantaneous **Time averaged**



(b) $k-\omega$ SAS-SST

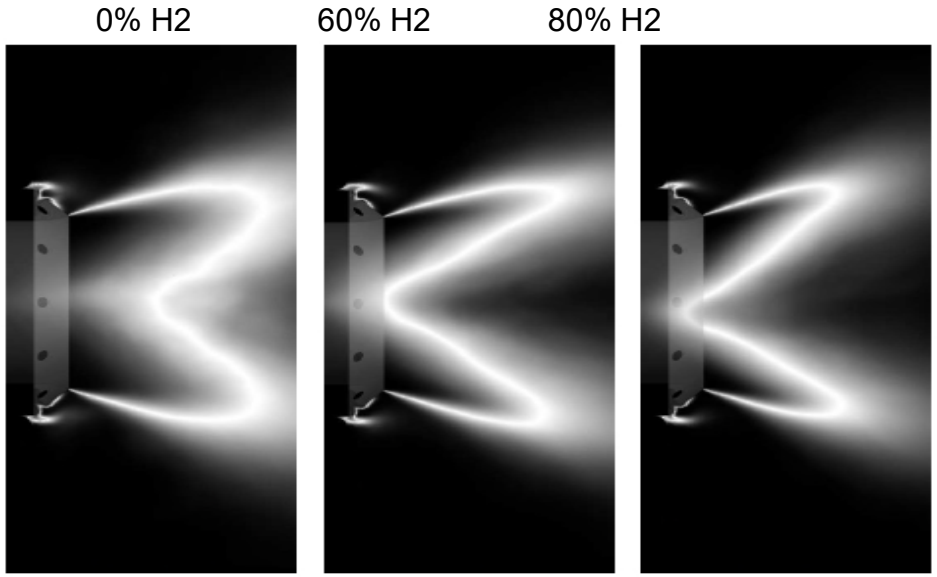
Instant. Acetone / OH PLIF
GT2012-69936



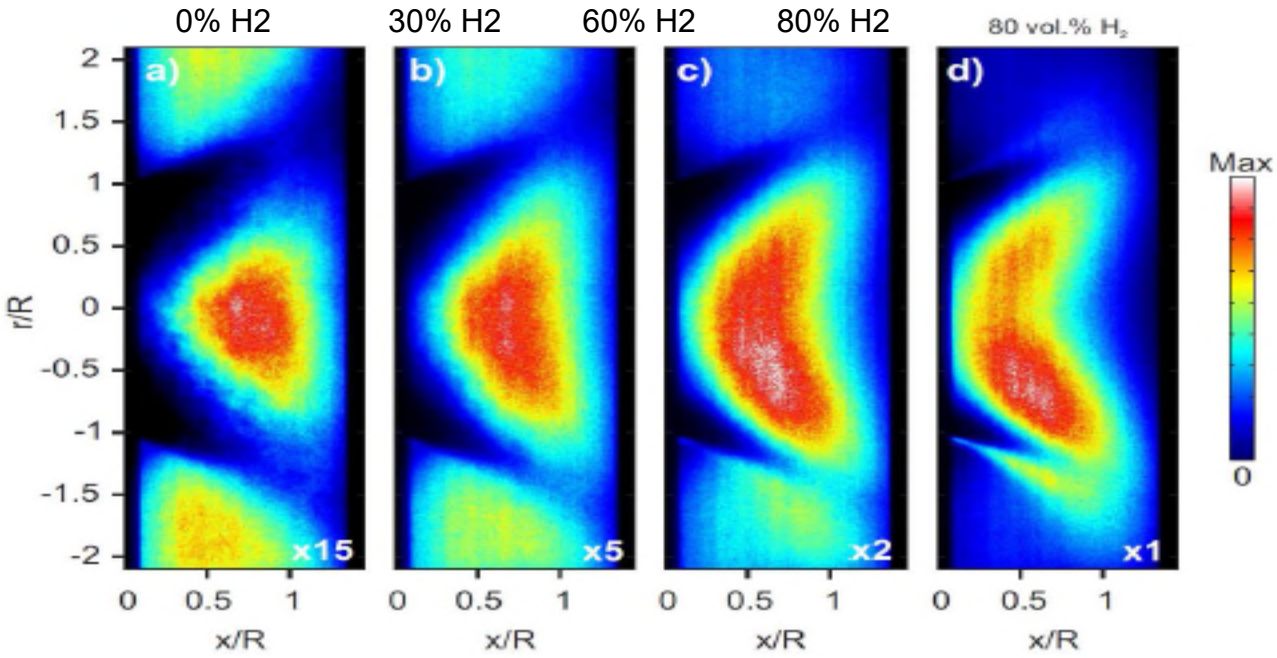


CFD results: (Hydrogen enriched combustion):
Predicted flame location compared to measurements

- Only SST-SAS with reaction rate CR=1.0 used for studying hydrogen addition.
- The flame stabilization point is moving upstream with hydrogen content
  - Qualitatively same trend in CFD and OH PLIF measurements
  - Flame center position moves upstream with hydrogen content
  - Flame gets shorter with hydrogen content

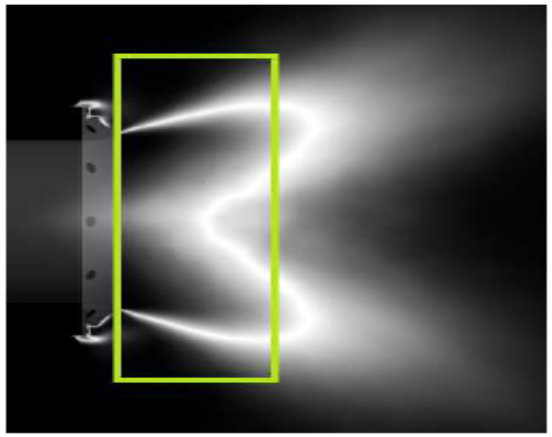


Averaged OH PLIF of methane-hydrogen-air flames
(GT2014-26293)

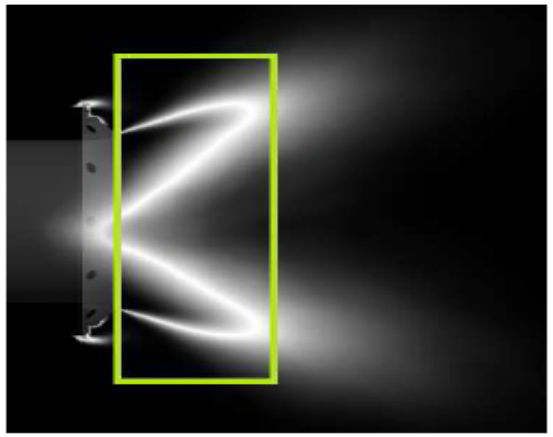


CFD results: (Hydrogen enriched combustion):
Predicted flame location compared to measurements

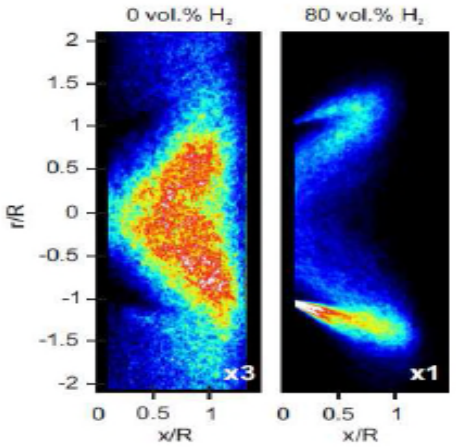
- Averaged OH gradient may be a better indicator of flame position
  - Qualitative comparison to reaction progress
- The flame stabilization point is moving upstream with hydrogen content
  - Qualitatively same trend in CFD and OH PLIF measurements



0% H2



80% H2

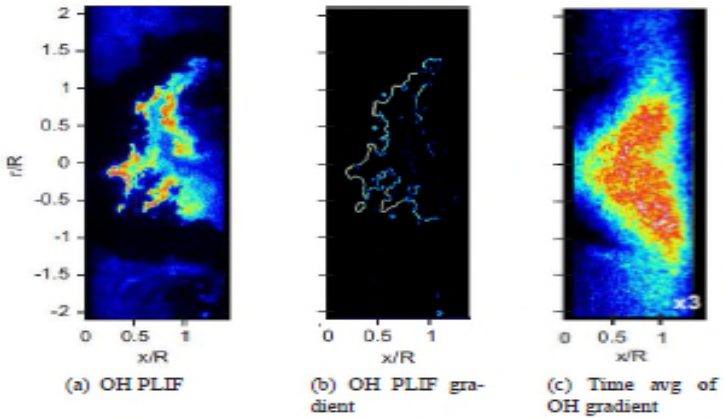


PDF of OH PLIF Gradient

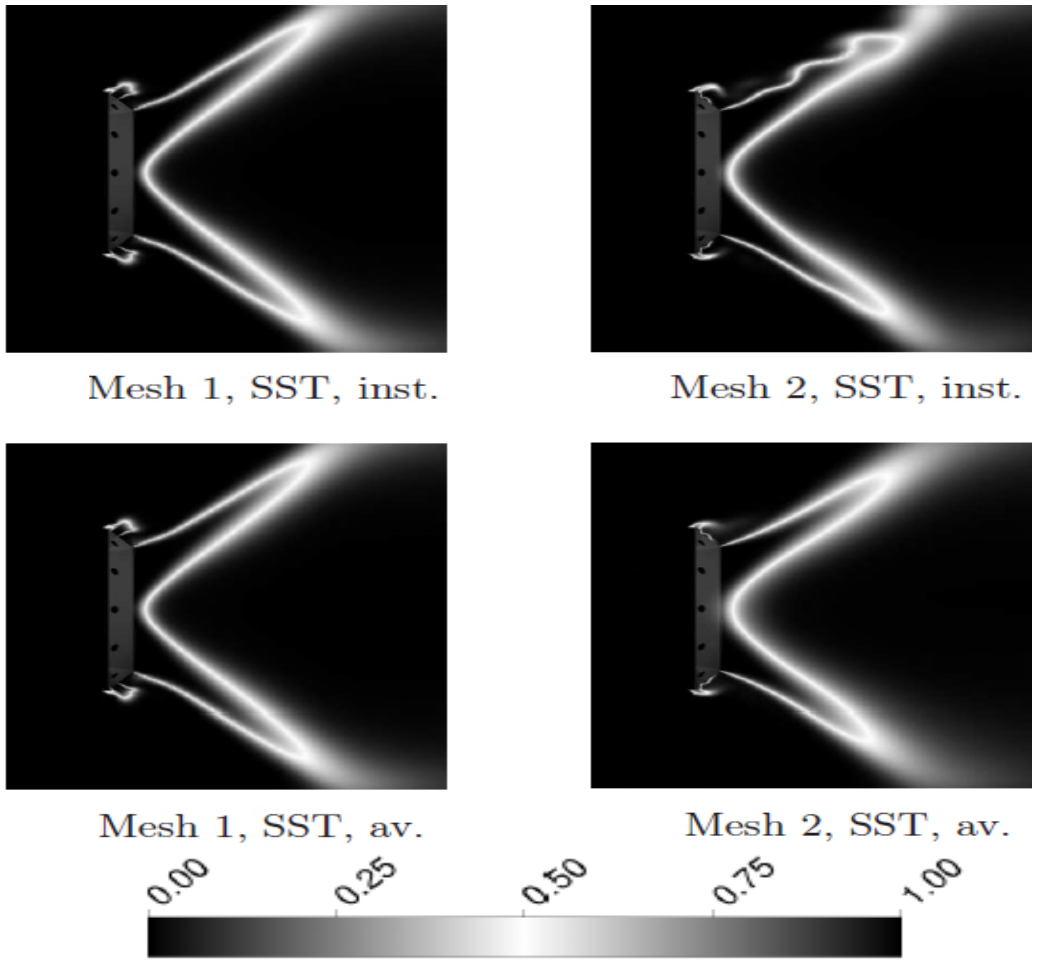
OH PLIF of methane-hydrogen-air flames
(GT2014-26293)

CFD Results: (Grid Study – k-ω SST)
Reaction progress

- k-ω SST time averages very similar with both grids
- No dynamic behavior close to central stagnation point using any grid

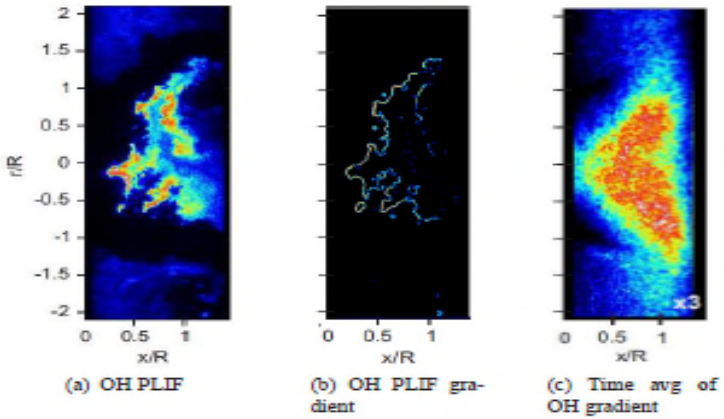


OH PLIF of methane/air flame
[Lantz et. al ASME Turbo Expo 2014]

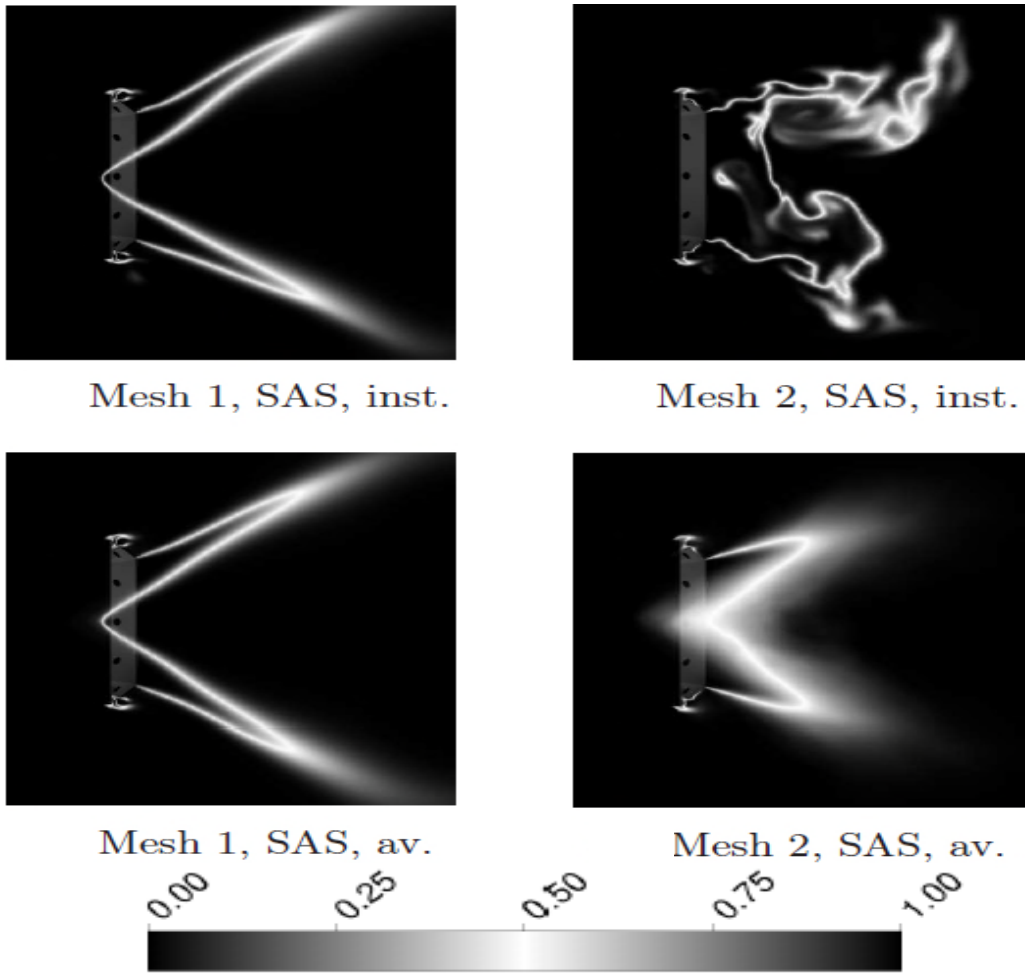


CFD Results: (Grid Study- SST-SAS)
Reaction progress

- SAS SST time averages differs, finer grid resolution gives a much more compact flame
- Increased dynamic levels using a finer grid

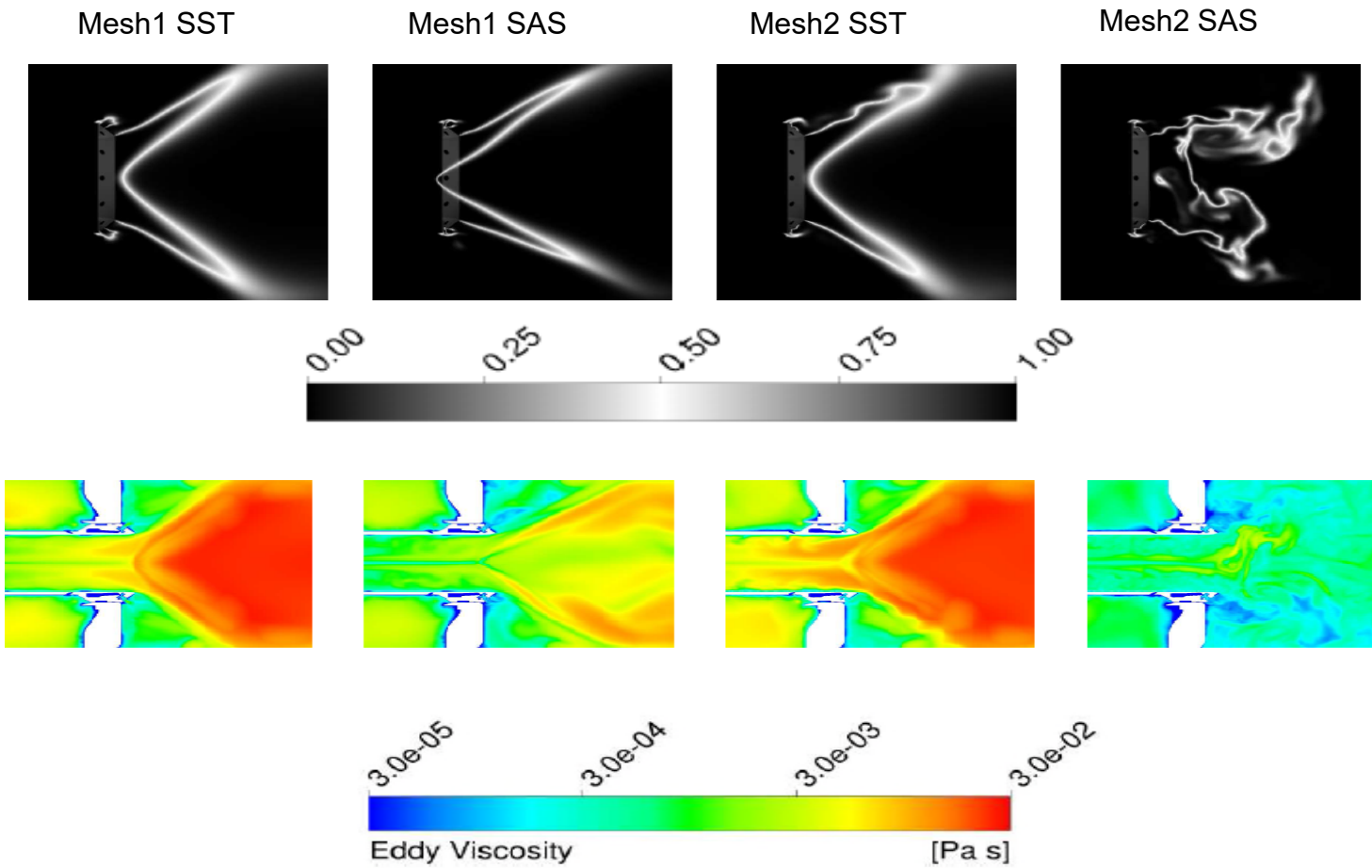


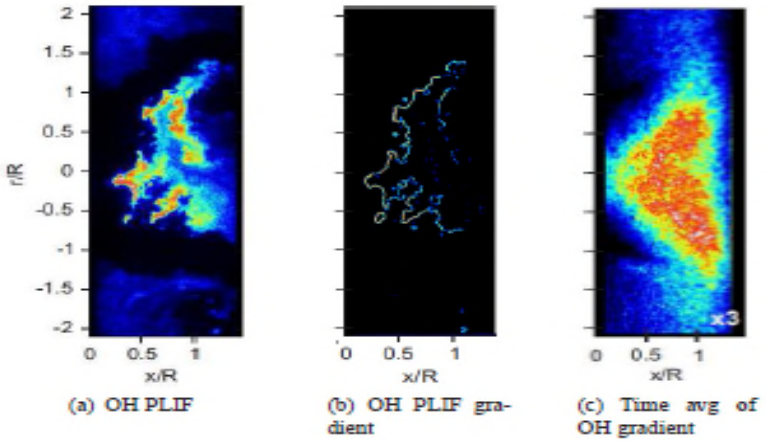
OH PLIF of methane/air flame
[Lantz et. al ASME Turbo Expo 2014]



CFD Results: (Grid Study)
Reaction progress and Eddy viscosity

- Using SAS with the finer grid decreases the eddy viscosity and thereby increases the dynamic motions of the flame front





OH PLIF of methane/air flame

[Lantz et. al ASME Turbo Expo 2014]

Summary and conclusions

- The SGT-800 combustor has been evaluated using different models:
  - Turbulence: RANS k-ω SST & SAS-SST
  - Combustion: EDM-FRC M4_HP, Fractal-Lindstedt & Vaos and BVM-Zimont
- k-ω SST: Shows reasonable results but flame region gradients seems over predicted
- SAS-SST using EDM-FRC and using calibrated constants also Fractal and BVM
  - Close agreement to available exp. data for flame position and shape
  - BVM question marks: insufficient burn out and spurious PV~1 in fuel system
  - Both Fractal & BVM using larger constants causes the flame too far upstream
- All results using the flamelet based models causes question marks about the mixing of cooling air entering already reacted gases
  - Affects the predicted turbine inlet temperature
- **SAS-SST with EDM-FRC M4_HP: Excellent results without need of calibration and without question marks concerning cooling air entering the reacted gases**
  - Computational cost ~40-50% higher than SAS-SST with Fractal or BVM

Summary and conclusions

Comparison between k-ω SST and SST-SAS turbulence models

- k-ω SST turbulence model unable to predict:
  - Dynamic behavior of the flame
  - Change in flame position due to changes in the mean reaction rate

- SST-SAS captures large scale dynamics
  - Similar level as compared to measurement data

Effects of hydrogen enrichment

- SST-SAS in combination with a fractal mean reaction rate closure:
  - Change in flame position due to hydrogen enrichment
    - Good qualitative agreement with measurements

Questions?