BPEA 2025: Use of Methanol as a Potential Alternative Fuel in a Power Generation Gas Turbine

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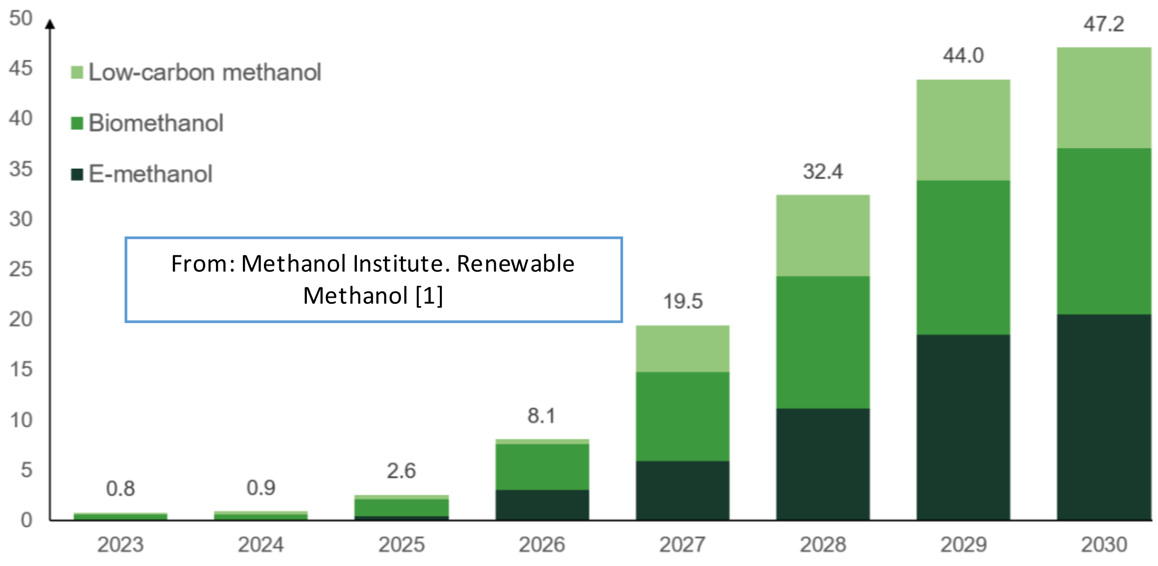
Introduction

Fuel Characteristics

- **Methanol** as a fuel compared to **methane** is characterized by:
  - **wider flammability limit**
  - **2.5 times lower LHV (Lower Heating Value)**

Analysed Power Station

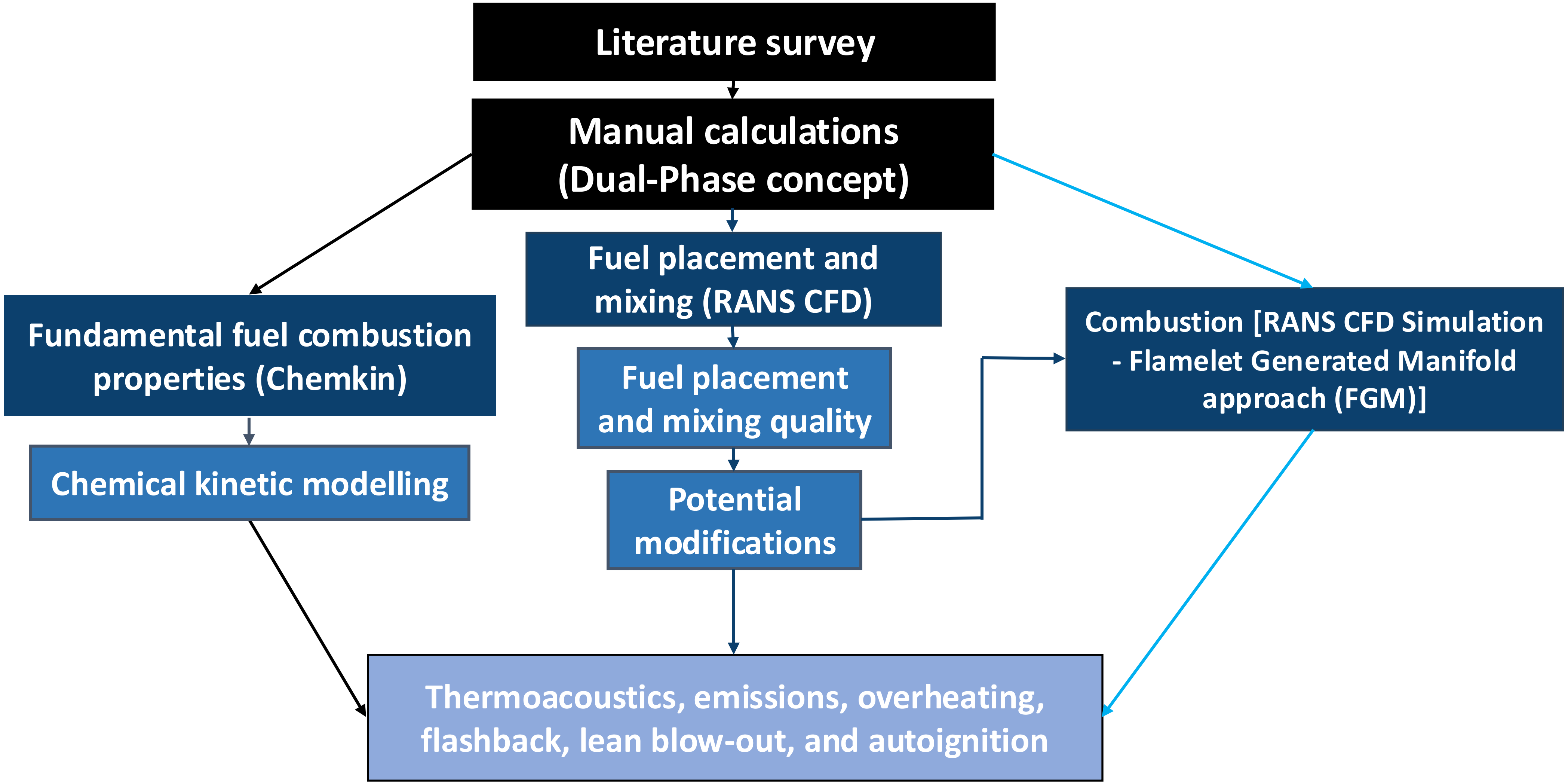
- **Killingholme Power Station :**
  - Equipped with four **Siemens STG5-2000E** gas turbines
  - Own by **Uniper,** operates on **capacity market** framework



Previous studies

- Previous tests comparing **liquid methanol** (diffusion-based) to **kerosene** showed up to **80% NOx reduction** (Clifford et al. [2]).

Methodology



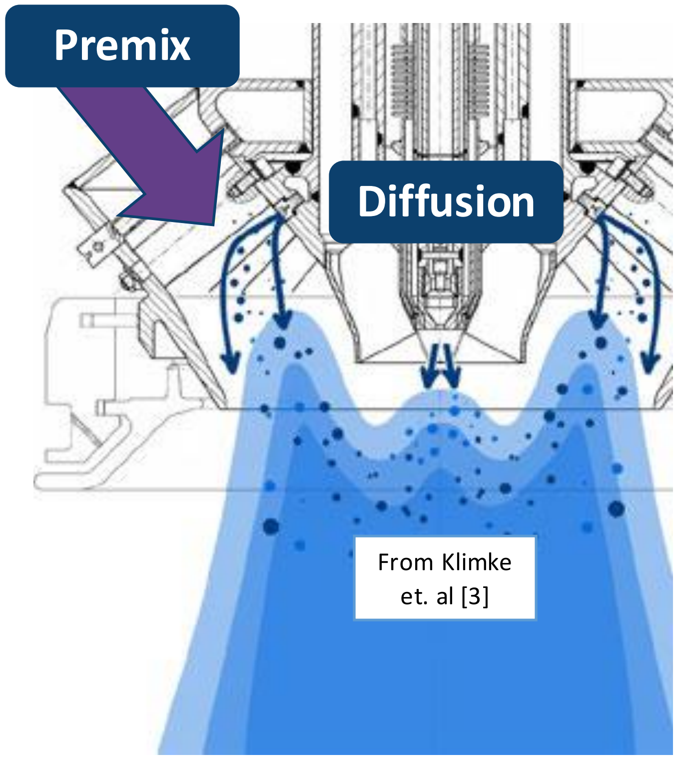
Dual-Phase Concept

Hybrid Burner in SGT5-2000E:

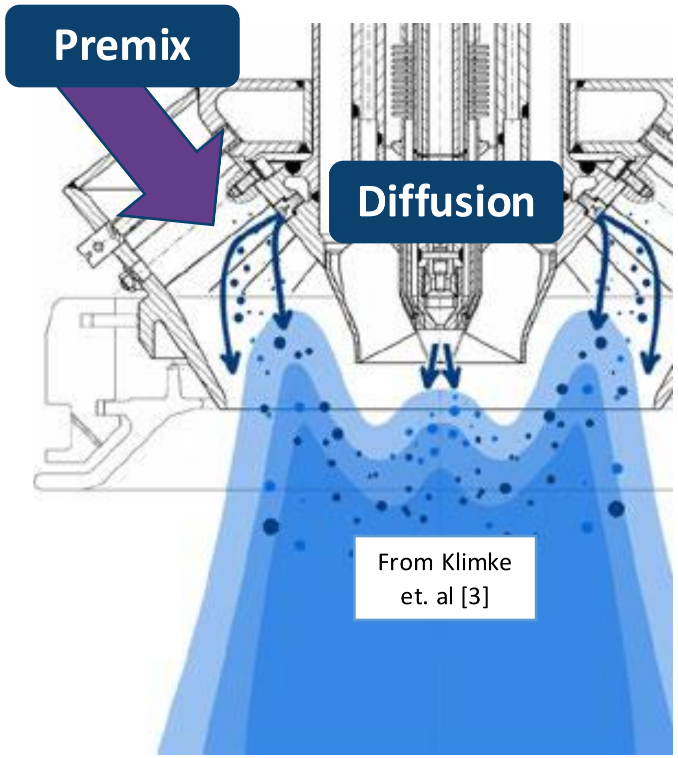
- Can operate on both **liquid and gaseous fuel**
- Operations on **methanol** will require **increase in injection nozzles**

Use of liquid methanol (based on correlations from [4]):

- **Methanol vs Diesel:**
  - **Methanol** shows **a 2.14× higher transfer number (indicating faster evaporation)**
  - **Methanol** firing required **a 1.5× larger nozzle** to match **standard pressure loss,** yet still produced a **2.62× smaller Sauter Mean Diameter (SMD)**



Dual-Phase Concept



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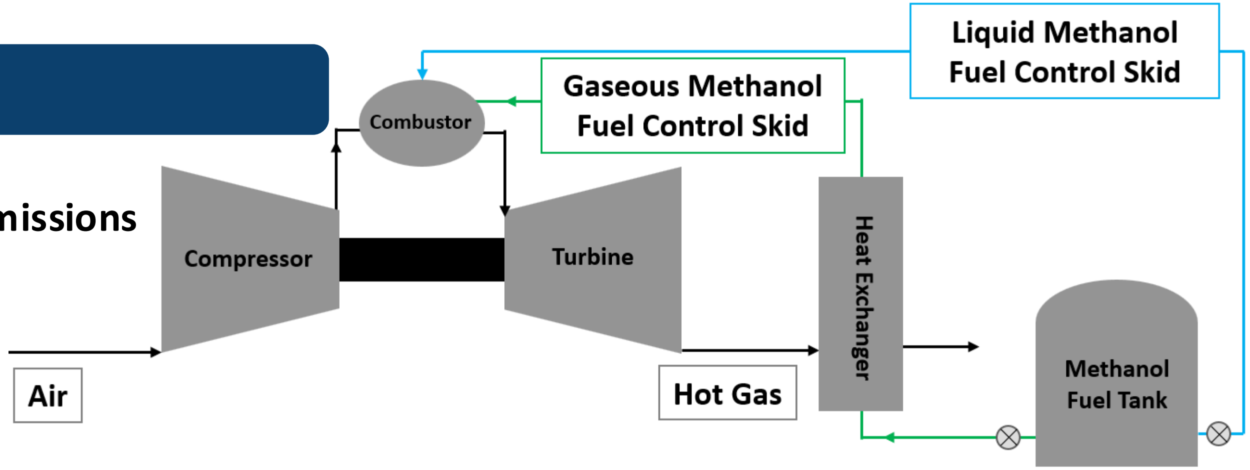
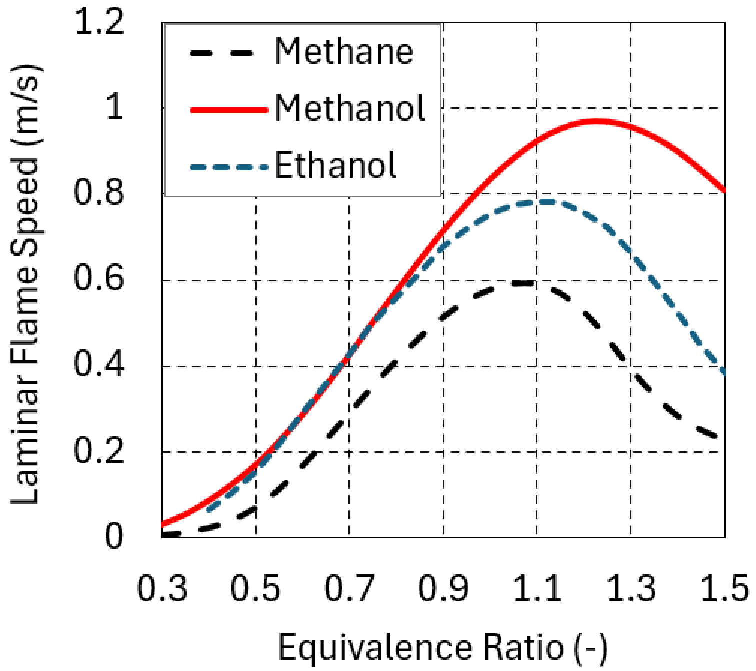
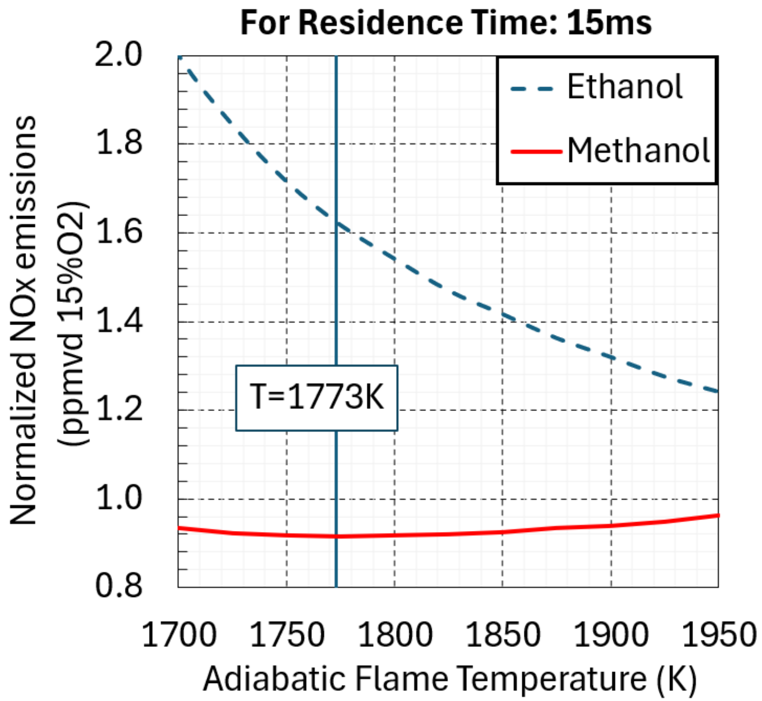
Use of evaporated methanol:

- Reduce **fuel consumption by 5-6%**
- Improve mixing and further **reduction in NOx emissions**



Chemical Kinetics

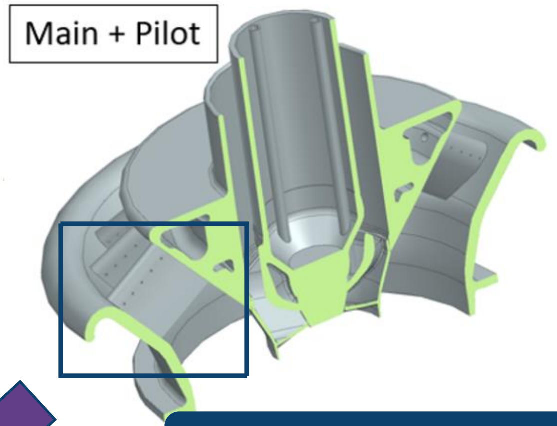




Based on results obtained in Chemical Kinetics study:

- Utilized mechanism **CRECK_2003_C1-C3_HT_NOX** [5]
- **Ethanol data** taken from **Caputo** [6]
- **Mean flame temperature 1773K** based on **Prade et al.** [7]

Potential Modifications for CFD Simulation



Burner Cross Section

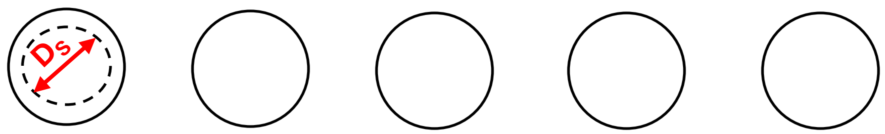
Modifications - Main Information:

- Potential modifications in fuel injection vane can include:

Uniform

D/D_S 1.44

Nozzle 1	Nozzle 2	Nozzle 3	Nozzle 4	Nozzle 5
D/D_S=1.44	D/D_S=1.44	D/D_S=1.44	D/D_S=1.44	D/D_S=1.44

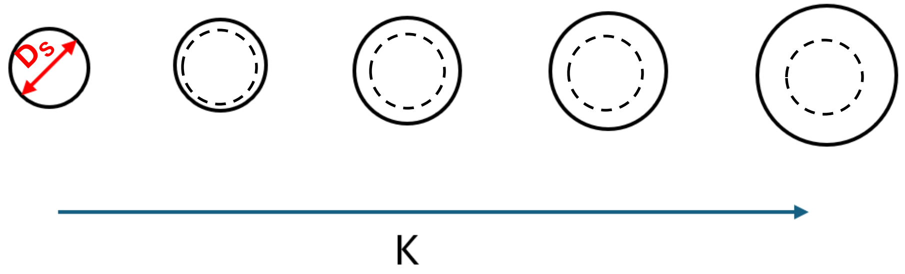


Outer annulus — Inner annulus

Non-uniform

K 1.17

Nozzle 1	Nozzle 2	Nozzle 3	Nozzle 4	Nozzle 5
D/D_S=1	D/D_S=1.17	D/D_S=1.37	D/D_S=1.60	D/D_S=1.87



Outer annulus — Inner annulus

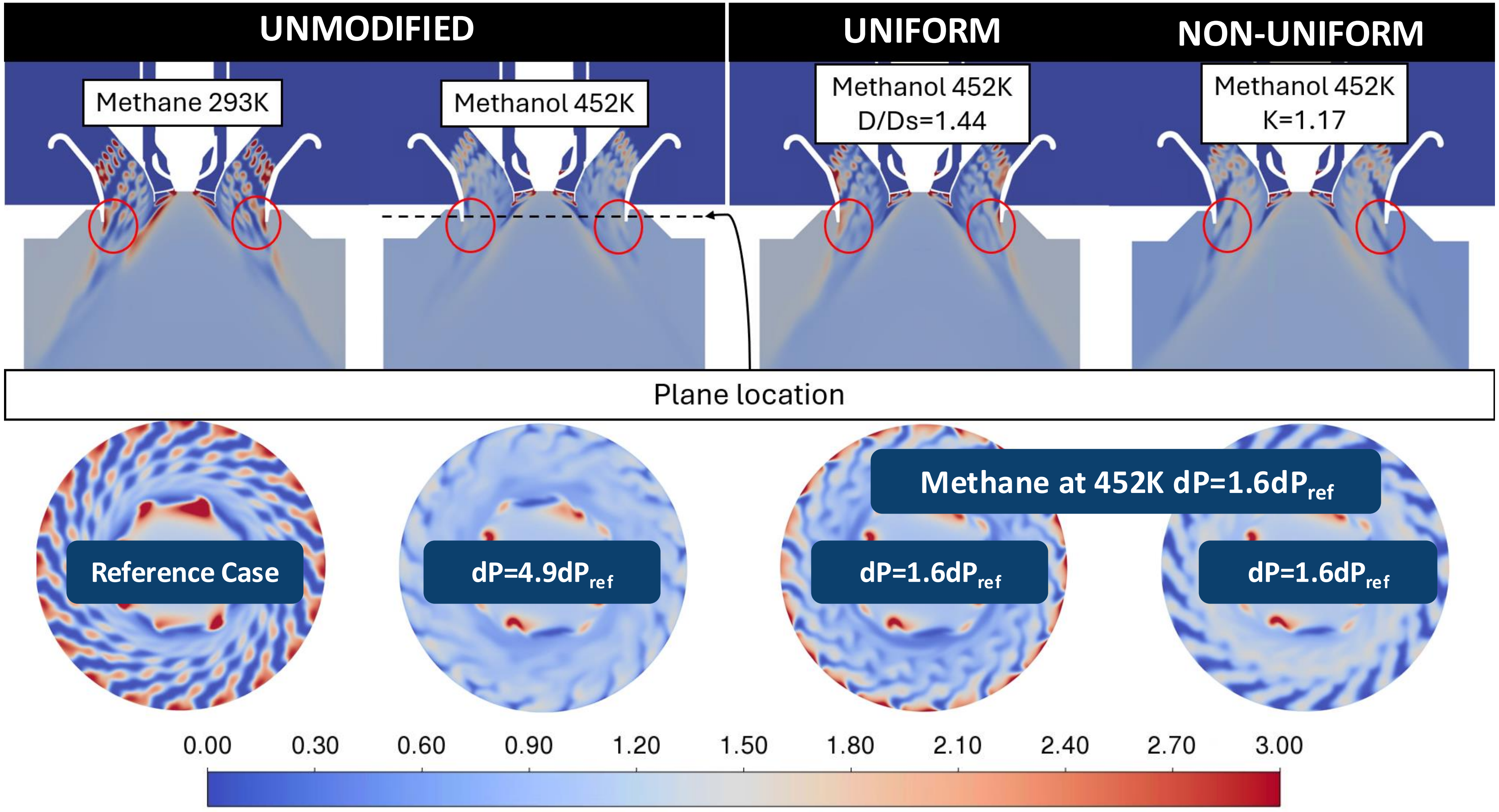
CFD – Mixing Quality Study

$$\phi_{norm} = \frac{A/F_{local}}{A/F_{BC}}$$

- A/F_{BC}- boundary conditions air to fuel ratio by mass
- A/F_{local}- local air to fuel ratio by mass

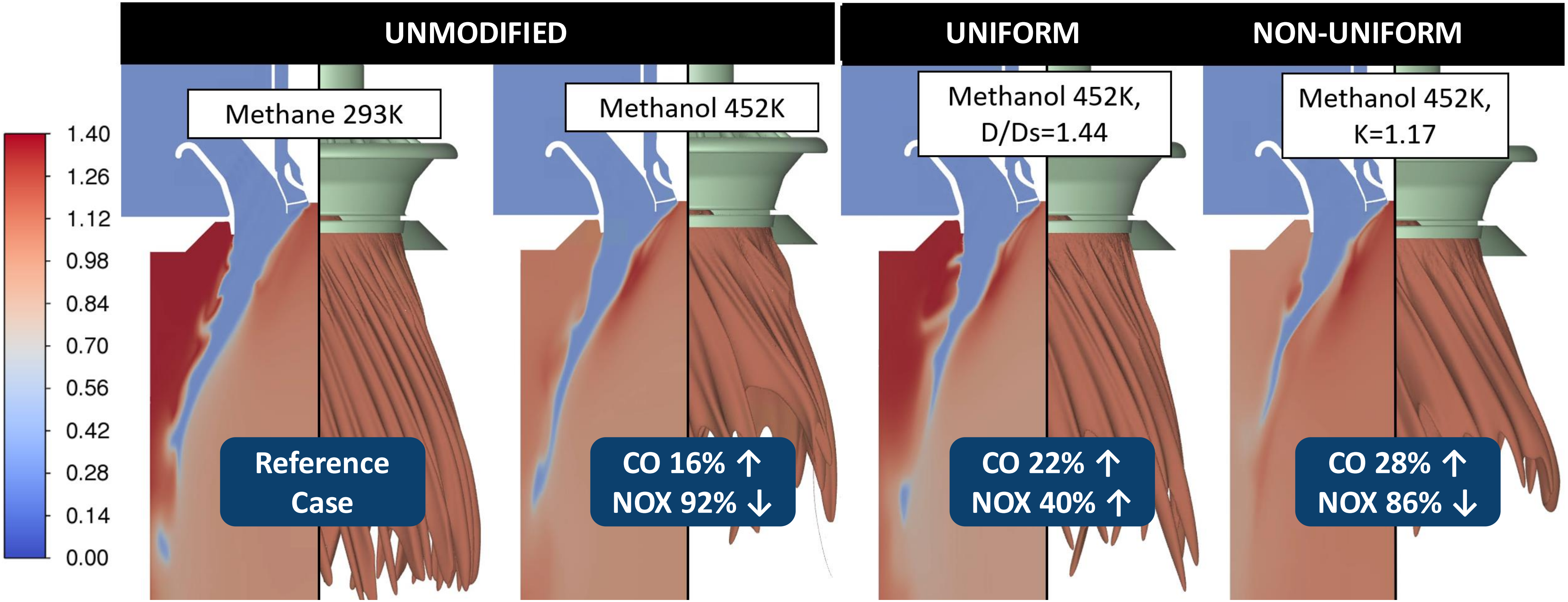
dP – pressure drop through the injection vane

Normalized Equivalence Ratio Contour (ϕ_{norm})



CFD – Combustion

$T_{norm} = \frac{T_{local}}{T_{mean\ flame}}$ contour and Progress Variable Iso-Surface c=0.8



Conclusions

Dual phase concept is likely **to be viable** and **worth further analytical and experimental investigation** based on **presented results**

Liquid and vapor methanol firing is possible for the **analysed burner**; however, it **requires increased injector capacity**

Due to **waste heat recovery, evaporated methanol** could potentially **lower fuel consumption by 5-6%**

Flashback risk increases with **methanol**

PSR (perfectly stirred reactor) analysis predicts **a 10% reduction in NOx emissions** for **methanol compared to methane**

Non-uniform injector diameter increase (K=1.17) **reduces NOx emissions by 86%** compared to **methane** and **lowers flashback risk** compared to uniform diameter increase in **methanol-fired burner**

References

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[2] T. Clifford, C. Booth, M. Houde, R. Fowler, C. Maclean, M. Basu, B. Witzel, G. Bulat, Green methanol demonstrated as an alternative fuel to decarbonise gas turbines. in Proceedings of ASME Turbo Expo 2024: Turbomachinery Technical Conference and Exposition, London, United Kingdom, June 24-28, (2024), https://doi.org/10.1115/GT2024-122266

[3] H. Kliemke and T. Johnke, Gas turbine modernization – fuel conversion and special fuel applications for the Asian Market, in Proceedings of POWER-GEN Asia 2012, Bangkok, Thailand, October 3-5, (2012), https://www.scribd.com/document/344941324/Siemens-Technical-Paper-Gas-Turbine-Modernization

[4] A.H. Lefebvre and V.G. McDonell, Atomization and sprays, 2nd edition (Taylor & Francis, CRC Press, Boca Raton, 2017)

[5] The CRECK Modelling Group. Detailed kinetic mechanisms (Internet). visited on 2025-05-07, https://creckmodeling.chem.polimi.it/menu-kinetics/menukinetics-detailed-mechanisms/

[6] C.A. Caputo, Evaporated ethanol for industrial gas turbines, Master Thesis, Cranfield University, School of Aerospace Transportation and Manufacturing (2024)

[7] B. Prade, H. Streb, P. Berenbrink, B. Schetter, G. Pyka, Development of an improved hybrid burner-initial operating experience in a gas turbine. in Proceedings of ASME 1996 International Gas Turbine and Aeroengine Congress and Exhibition, Birmingham, United Kingdom, June 10-13, (1996), https://doi.org/10.1115/96-GT-045

Thank you. Questions?

This work has been supported by Uniper but the results, analysis, conclusions and views expressed in this presentation are those of the author and his research supervisors and do not necessarily reflect those of Uniper.

Appendix

Further work

CFD Modelling Enhancements - to more accurately predict the flame front behaviour based on LES (Large Eddy Simulation) or utilizing Hybrid Methods like DES or SBES

Thermoacoustic Modelling and Analysis

Fuel System Design and Optimization

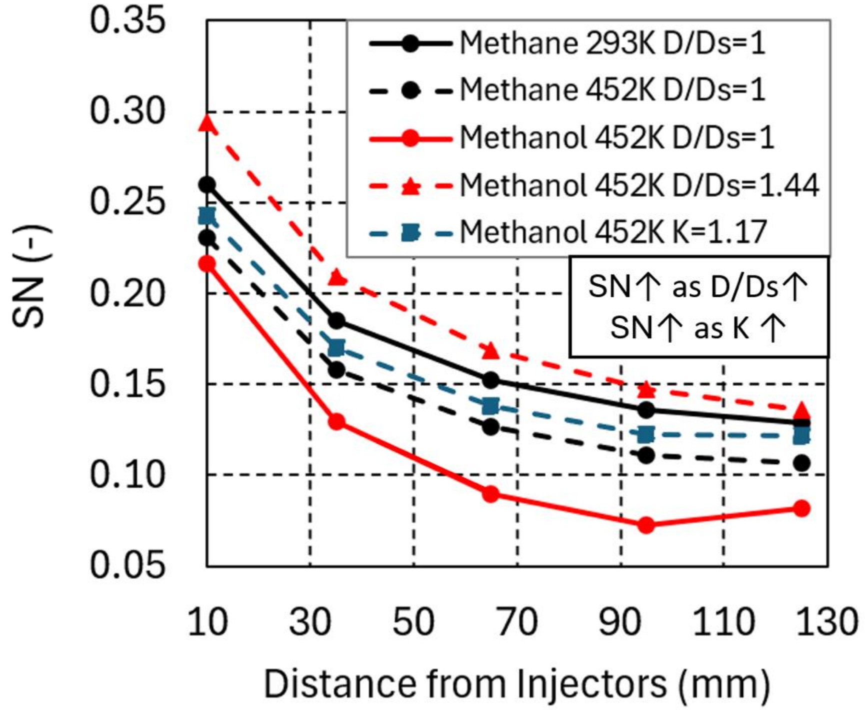
Performance Modelling of the Gas Turbine

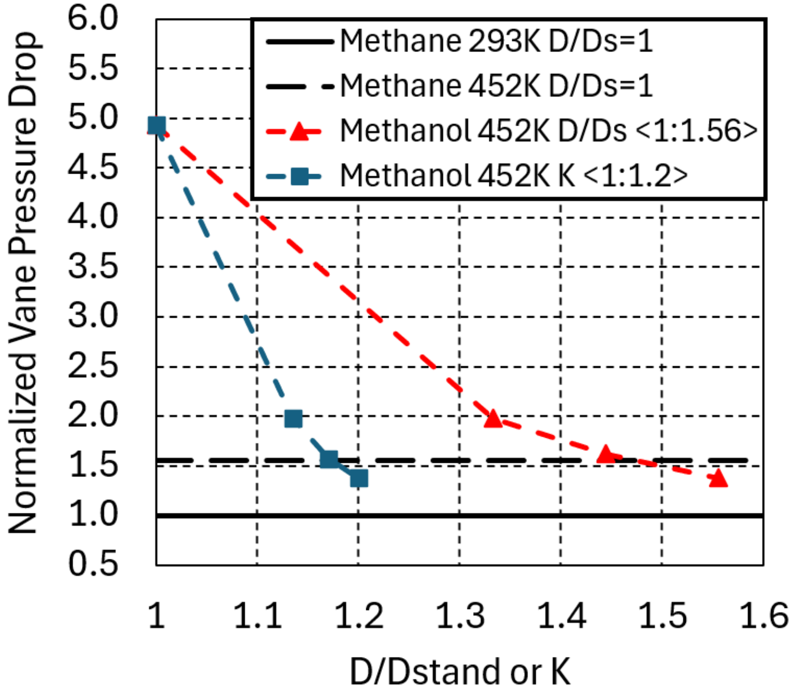
Start-up Procedures Design for Methanol Firing

Further Experimental Work on Spray Characteristics

Unmixedness Parameter

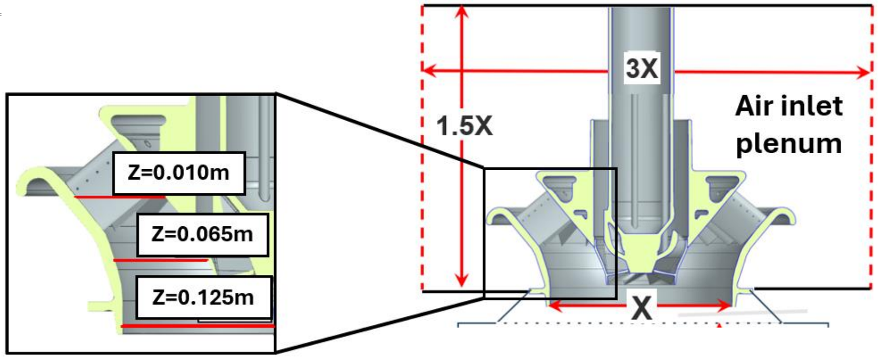
CFD – Mixing Quality Study (Unmixedness Parameter)





From: Hornsby et. al [8] and Sun et. al [9]

Location of "unmixedness" measuring planes



$$S_N = \frac{\sqrt{\left(\frac{\sum C_i^2 M_i}{\sum M_j}\right) - \left(\frac{\sum C_i M_i}{\sum M_j}\right)^2}}{\sqrt{\left(\frac{1}{\frac{A}{F}+1}\right) - \left(\frac{1}{\frac{A}{F}+1}\right)^2}}$$

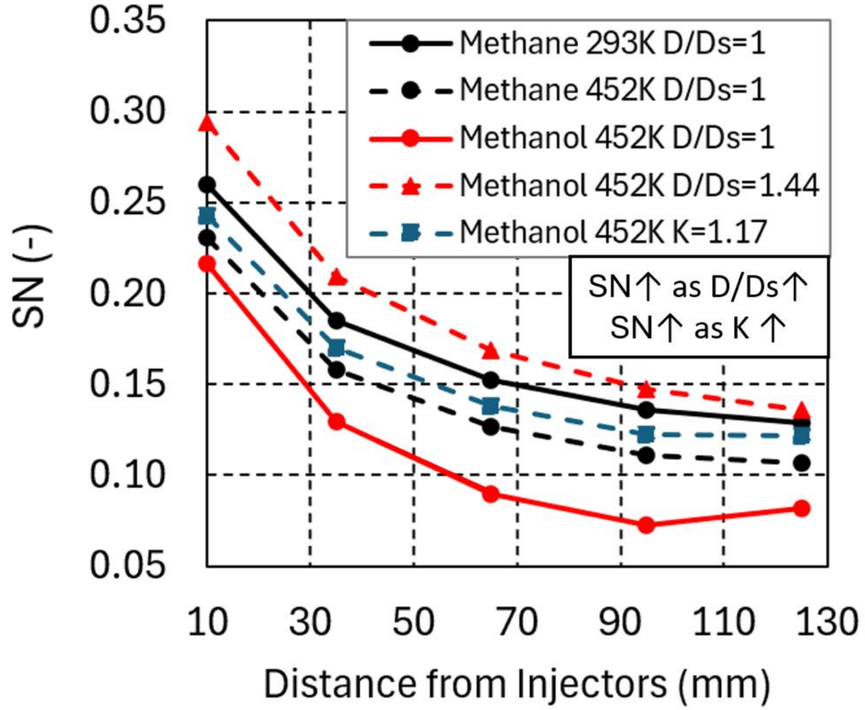
S_N - normalized unmixedness parameter

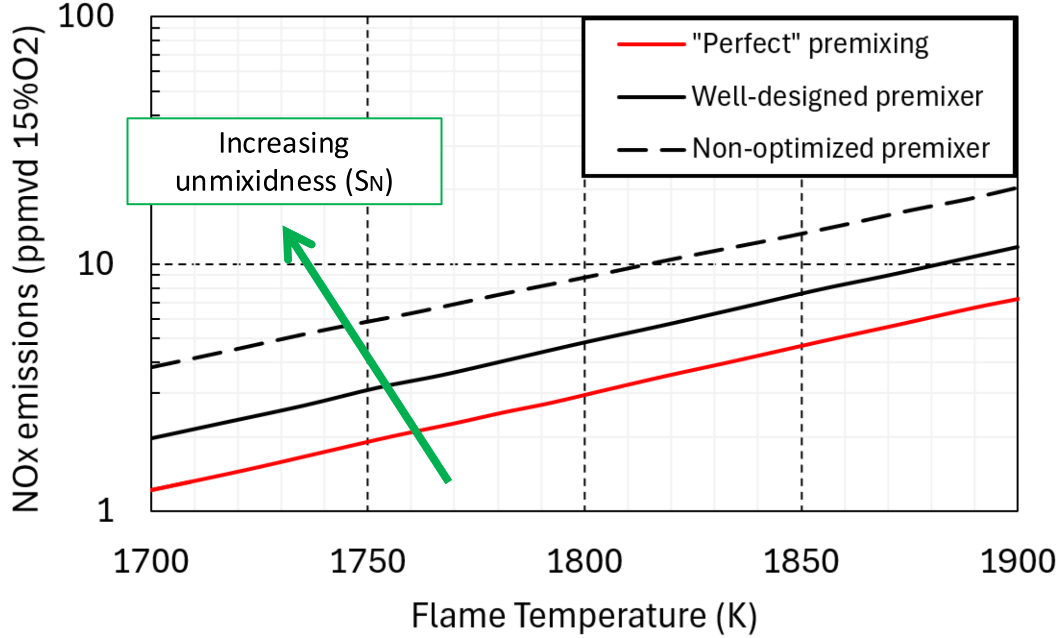
C_i- cell mass fraction

M_i - mass flow through the cell

$\frac{A}{F}$ - air to fuel ratio by mass

CFD – Mixing Quality Study (Unmixedness Parameter)





From: Hornsby et. al [8] and Sun et. al [9]

Reference Values For Power Generation Gas Turbine with DLN System

$$S_N = \frac{\sqrt{\left(\frac{\sum C_i^2 M_i}{\sum M_j}\right) - \left(\frac{\sum C_i M_i}{\sum M_j}\right)^2}}{\sqrt{\left(\frac{1}{\frac{A}{F}+1}\right) - \left(\frac{1}{\frac{A}{F}+1}\right)^2}}$$

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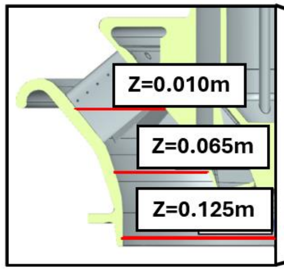
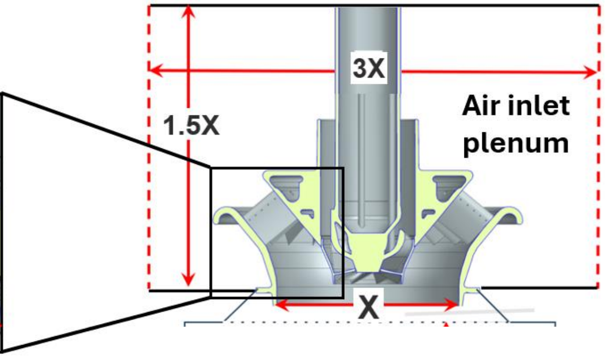




Unmixdness Parameter References

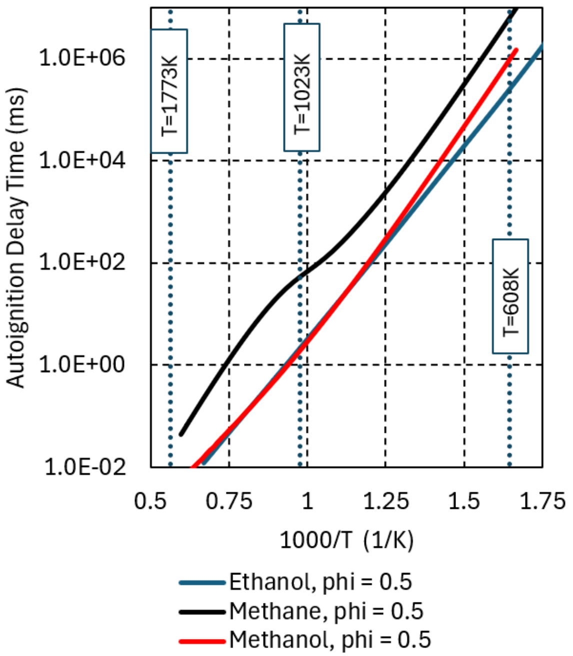
[8] C. Hornsby and E.R. Norster, Application of CFD to DLN combustion. in Proceedings of ASME 1997 International Gas Turbine and Aeroengine Congress and Exhibition, Orlando, FL, United States Jone 2-5, (1997), https://doi.org/10.1115/97-GT-371

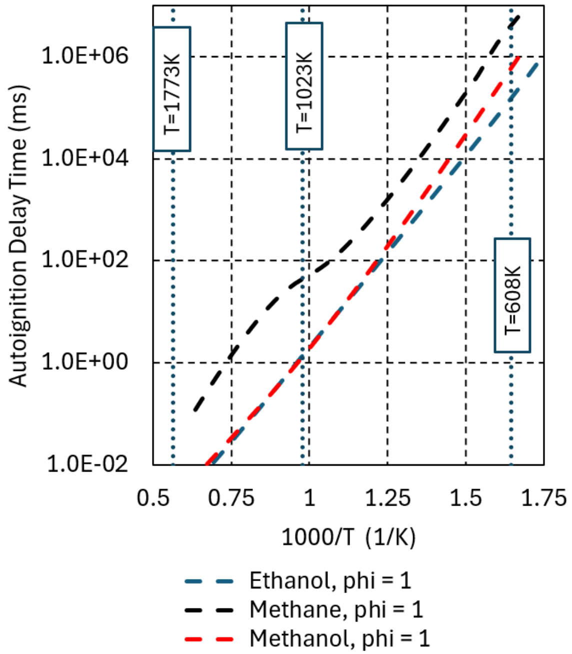
[9] X. Sun, P. Agarwal, F. Carbonara, D. Abbott, P. Gauthier, B. Sethi, Numerical investigation into the impact of injector geometrical design parameters on hydrogen micromix combustion characteristics. in Proceedings of ASME Turbo Expo 2020: Turbomachinery Technical Conference and Exposition, Virtual, Online, September 21-25, (2020), https://doi.org/10.1115/GT2020-16084

Chemical Kinetics – Autoignition Time Delay

www.cranfield.ac.uk

Chemical Kinetic – Autoignition Time Delay





Market temperatures represents:

- Temperature 608K represents the compressor discharge temperature
- Temperature 1023K represents potential corner recirculation zones temperature where periodic flashes may lead to flashback [10]
- Temperature 1773K represents mean flame temperature [7]

[7] B. Prade, H. Streb, P. Berenbrink, B. Schetter, G. Pyka, Development of an improved hybrid burner-initial operating experience in a gas turbine. in Proceedings of ASME 1996 International Gas Turbine and Aeroengine Congress and Exhibition, Birmingham, United Kingdom, June 10-13, (1996), https://doi.org/10.1115/96-GT-045
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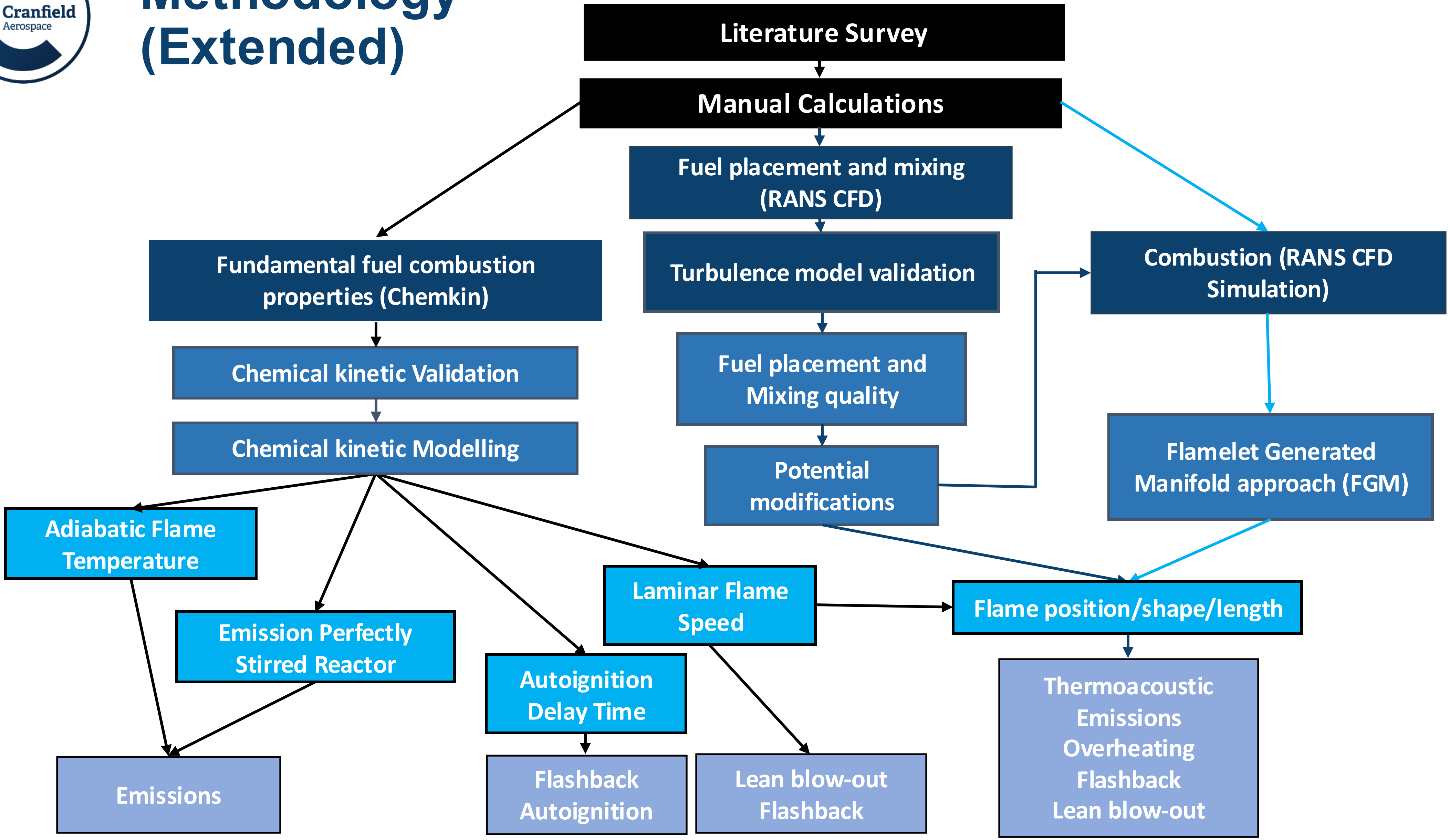
Methodology (Extended)



Aims and Objectives

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Aims

- Feasibility study of the usage of **alcohols as potential "green" fuels** in **existing units**.
- **Identification of changes** that can be implemented in the **existing combustor**.

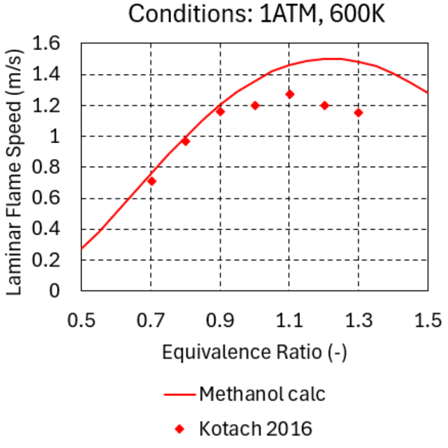
Objectives

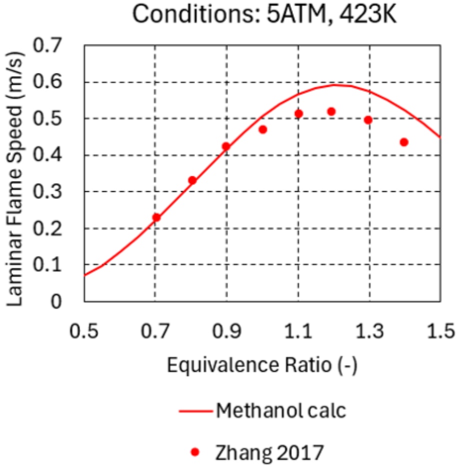
- **Liquid firing investigation** based on **manual calculations**.
- Make comparison between **methane** and **methanol** to assess the impact of **switching fuel on combustion performance**.
- Create **chemical kinetic model** to analyse parameters such as: **flame temperature**, **laminar flame speed**, **autoignition time delay**, and **estimated NOx emissions**.
- Create **CFD model** to explore: **fuel mixing characteristics**, **flame front behaviour**, **emissions**, and **temperature distribution.**

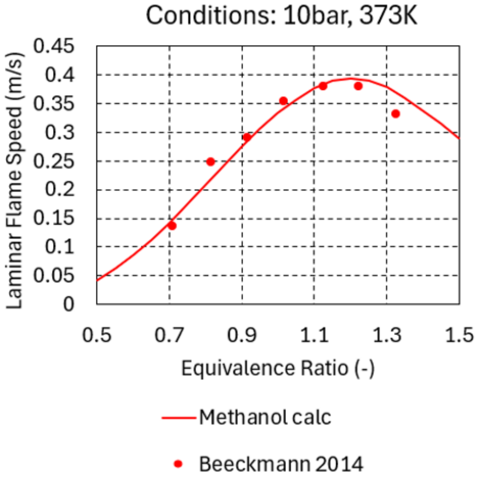
Chemical Kinetics - Validation

Chemical Kinetic Mechanism Validation - Methanol

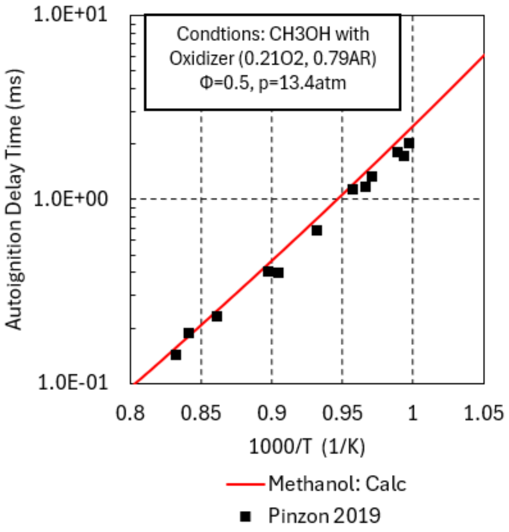
Laminar Flame speed

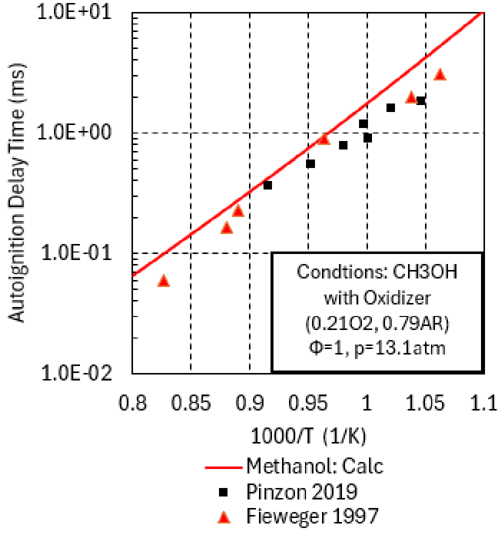


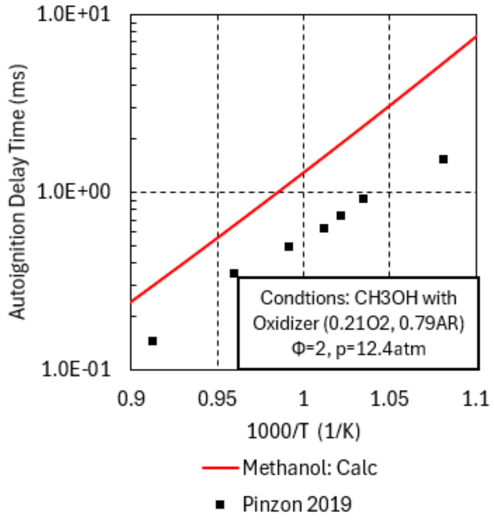




Autoignition Time Delay







Chemical Kinetic Mechanism Validation – Methanol References

- Laminar Flame Speed

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- Autoignition Delay Time

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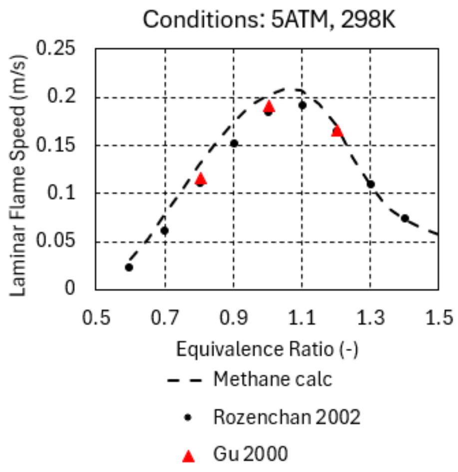
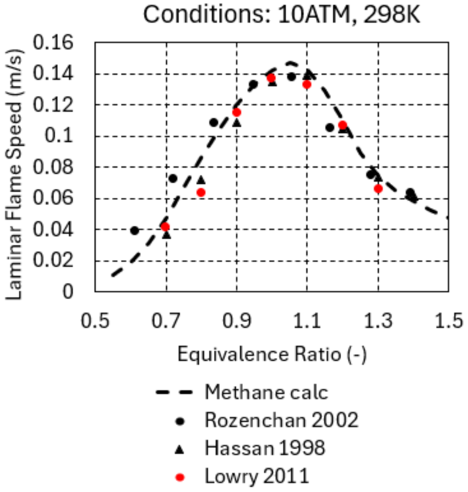
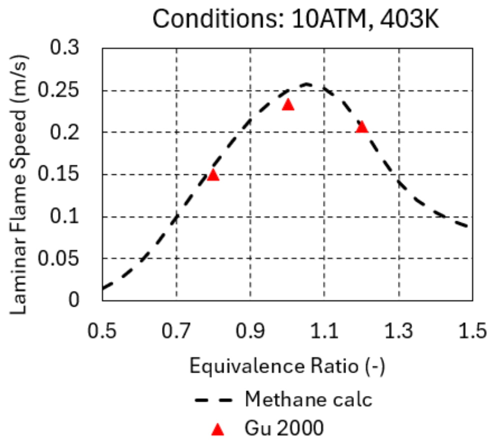
Chemical Kinetic Mechanism Validation - Methane

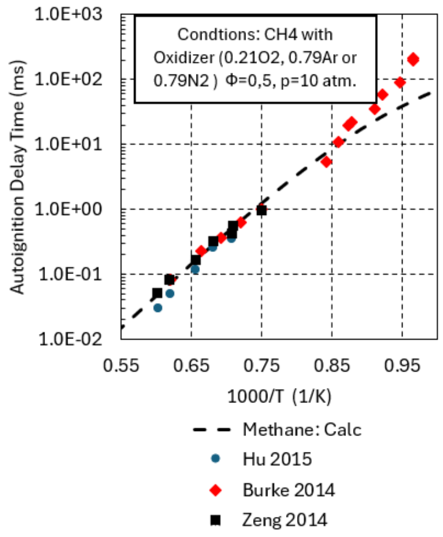
Laminar Flame speed

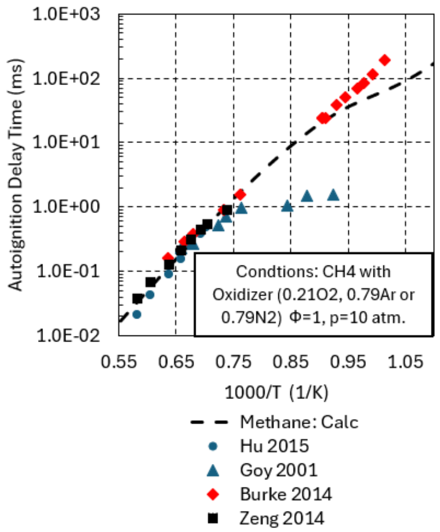


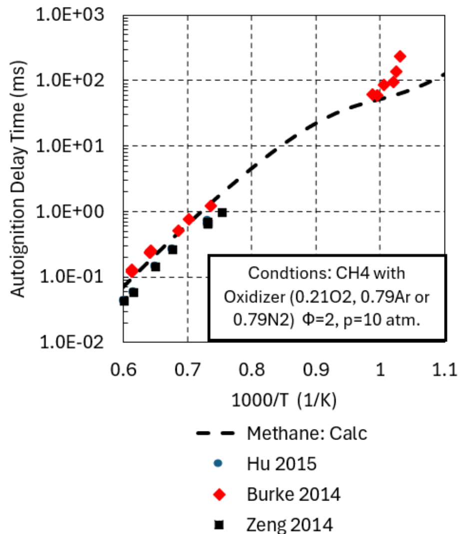




Autoignition Time Delay







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- Laminar Flame Speed
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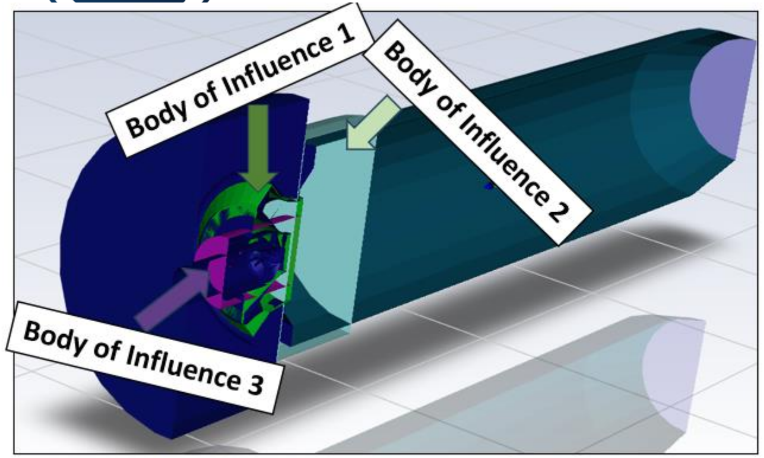
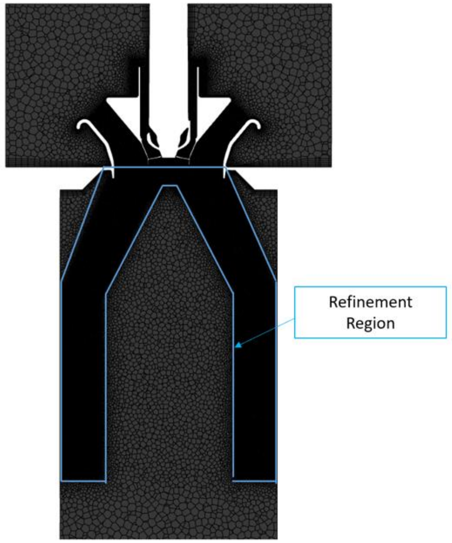
CFD – Solver Setings

CFD Solver Settings



Computational Domain And BOI Arrangement for Mixing



BOI Arrangement for Combustion

Boundary conditions for simulations:

- **Air Inlet:**
  - Mass flow: 17.71 kg/s
  - Turbulence intensity: 5%
  - Temperature: 608K
- **Fuel Main Inlet:**
  - Mass flow: 0.488 kg/s Methane, 1.220 kg/s Methanol
  - Turbulent intensity: 10%
  - Temperature: 293K Methane, 452K Methane/Methanol
- **Fuel Pilot Inlet:**
  - Mass flow: 0.054 kg/s Methane, 0.136 kg/s Methanol
  - Turbulent intensity: 5%
  - Temperature: 293K Methane, 452K Methane/Methanol
- **Outlet:**
  - Pressure outlet/Prevent reverse flow
- **Turbulence model:** Realizable k-epsilon
- **Operating pressure:** 11.2 bar
- **Up-wind Scheme:** Second order up-wind

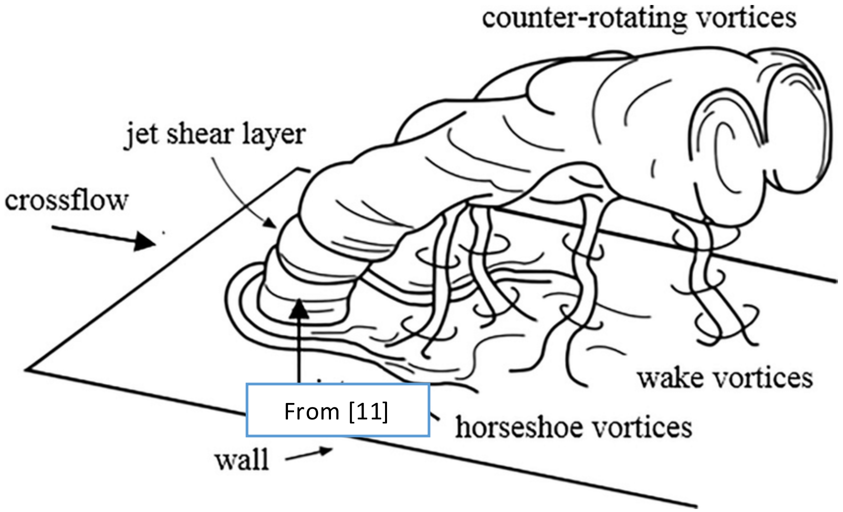
Type of elements:

- **Polyhedral (Unstructural Mesh)** – **Polyhedral cells** combine the accuracy of **hexahedrons** and the **easy generation** of **tetrahedrons**, **enhancing mesh quality** and **stability** [11]. They **reduce numerical diffusion** and **improve solution accuracy** with **fewer cells due** to better **gradient approximation** and **reduced sensitivity to stretching** [11].

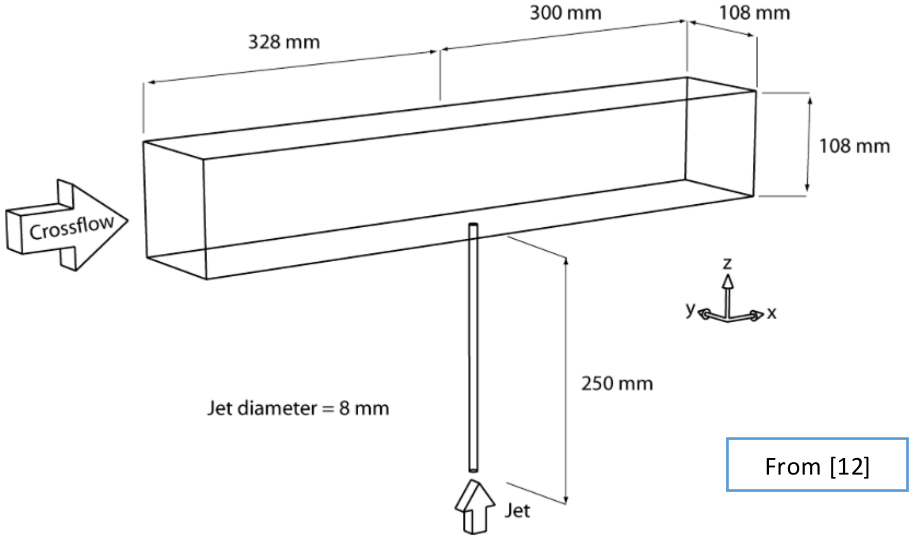
[11] M. Sosnowski, J. Krzywański, K. Grabowska, R. Gnatowska, Polyhedral meshing in numerical analysis of conjugate heat transfer, in Proceedings of EFM17 – Experimental Fluid Mechanics 2017, EPJ Web Conf., Vol. 180 (2018), https://doi.org/10.1051/epjconf/201818002096

CFD - Validation

Turbulence model selection – Validation Case



From [11]



From [12]

Case description

- For **validation of turbulence model** there has been done simulation that recreate conditions used in **Galeazzo at el.** [12].

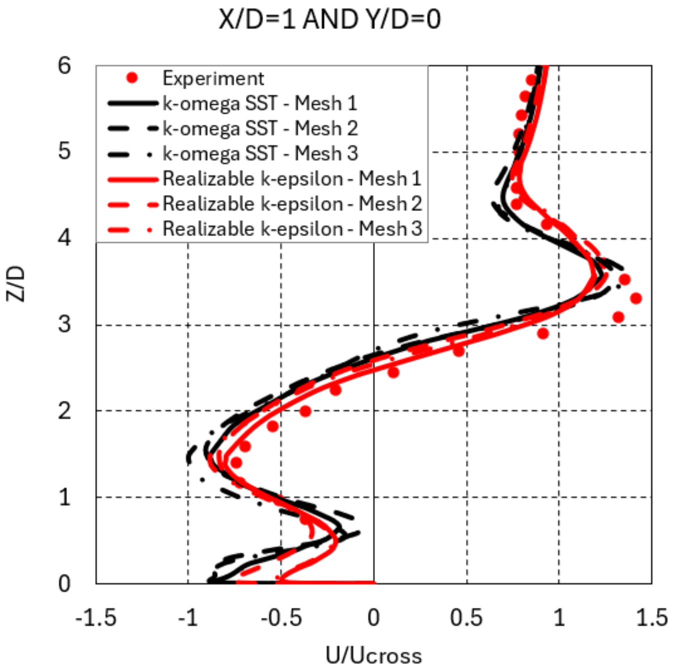
The boundary conditions for experiment and simulation:

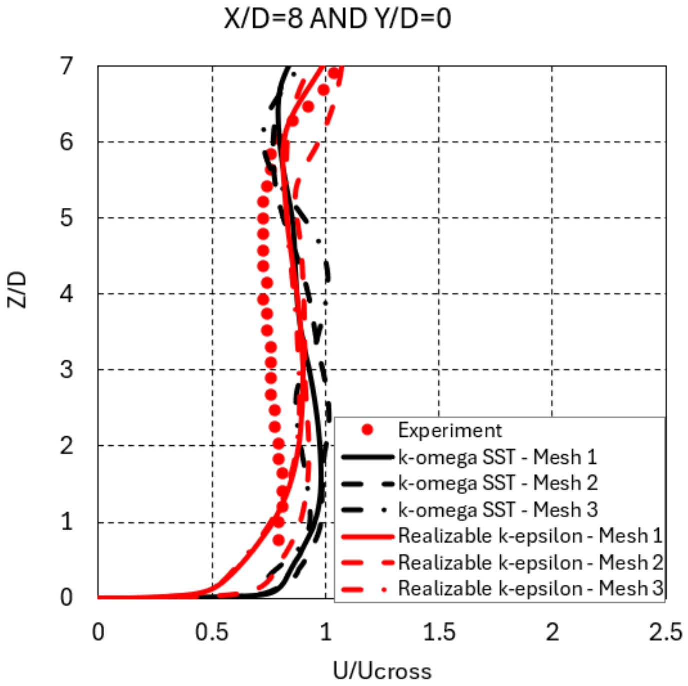
- **Crossflow:**
  - Inlet Bulk velocity: 9.08 m/s
  - Turbulence intensity: 1.5%
  - Reynolds Number 62 400
- **Jet:**
  - Inlet Bulk velocity: 37.72m/s
  - Turbulence intensity: 7%
  - Reynolds Number: 19 200
- **Mommentum ratio R:** 4.15

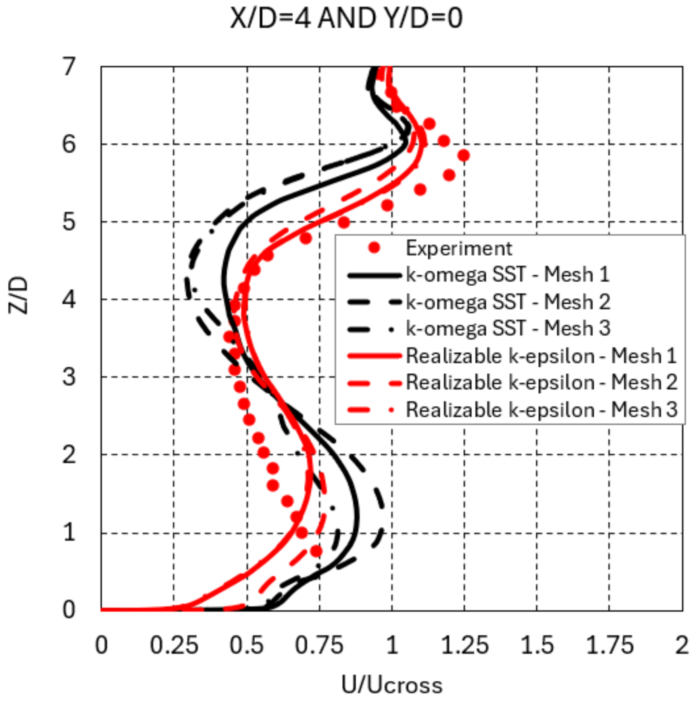
[12] F. Galeazzo, G. Donnert, C. Cárdenas, J. Sedlmaier, P. Habisreuther, N. Zarzalis, C. Beck, W. Krebs, Computational modeling of turbulent mixing in a jet in crossflow, *Int. J. Heat Fluid Flow*, 41: 55–65 (2013), https://doi.org/10.1016/j.ijheatfluidflow.2013.03.012
[13] A. Karagozian, The jet in crossflow, *Phys. Fluids*, 26(10): 101303 (2014), https://doi.org/10.1063/1.4895900

Turbulence Model Validation

Normalized Velocity Profiles on Reference Lines From Experiment



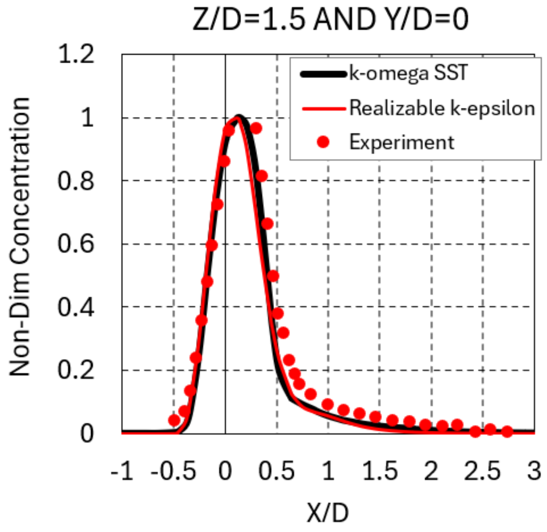


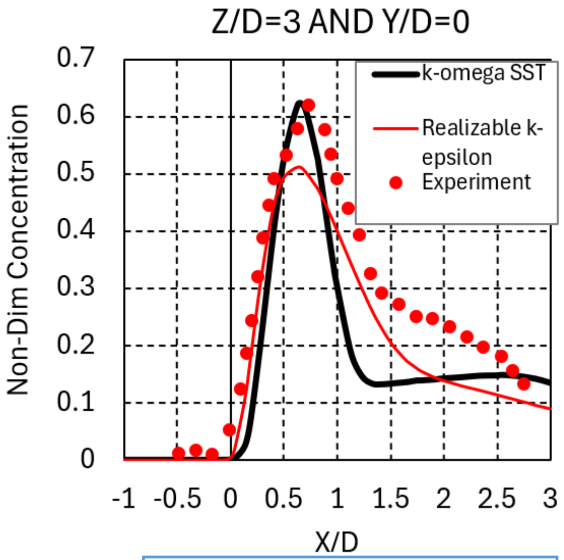


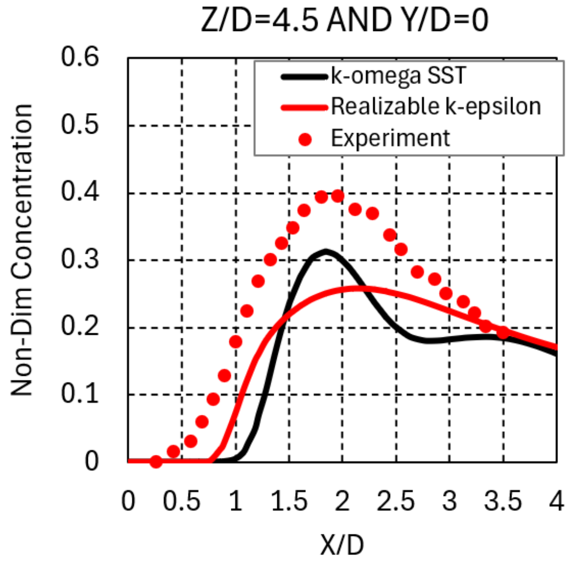
Experimental results from [12]

[12] F. Galeazzo, G. Donnert, C. Cárdenas, J. Sedlmaier, P. Habisreuther, N. Zarzalis, C. Beck, W. Krebs, Computational modeling of turbulent mixing in a jet in crossflow, *Int. J. Heat Fluid Flow*, 41: 55–65 (2013), https://doi.org/10.1016/j.ijheatfluidflow.2013.03.012

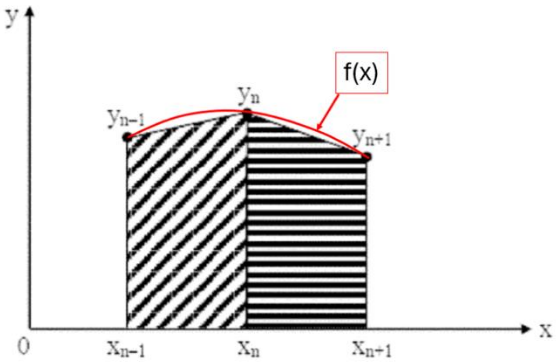
Turbulence Model Validation





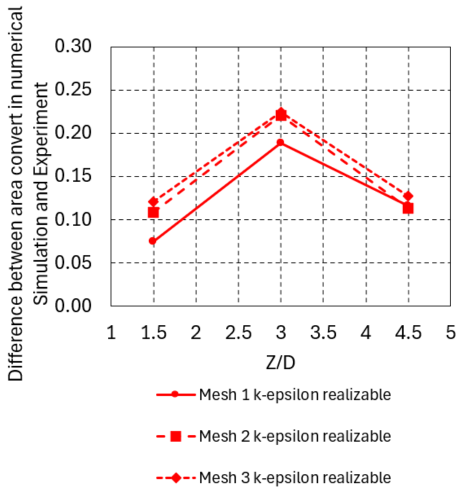


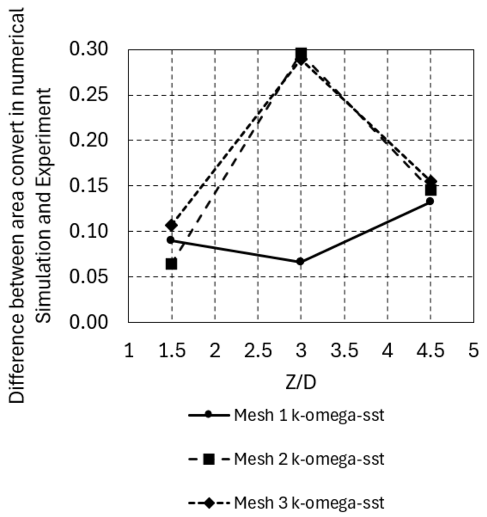
Experimental results from [12]



$$\int_a^b f(x)dx \approx \sum_{n=1}^{N} \frac{1}{2}(y_{n-1} + y_n)\Delta x_n$$

From [14]





[12] F. Galeazzo, G. Donnert, C. Cárdenas, J. Sedlmaier, P. Habisreuther, N. Zarzalis, C. Beck, W. Krebs, Computational modeling of turbulent mixing in a jet in crossflow, *Int. J. Heat Fluid Flow*, 41: 55–65 (2013), https://doi.org/10.1016/j.ijheatfluidflow.2013.03.012

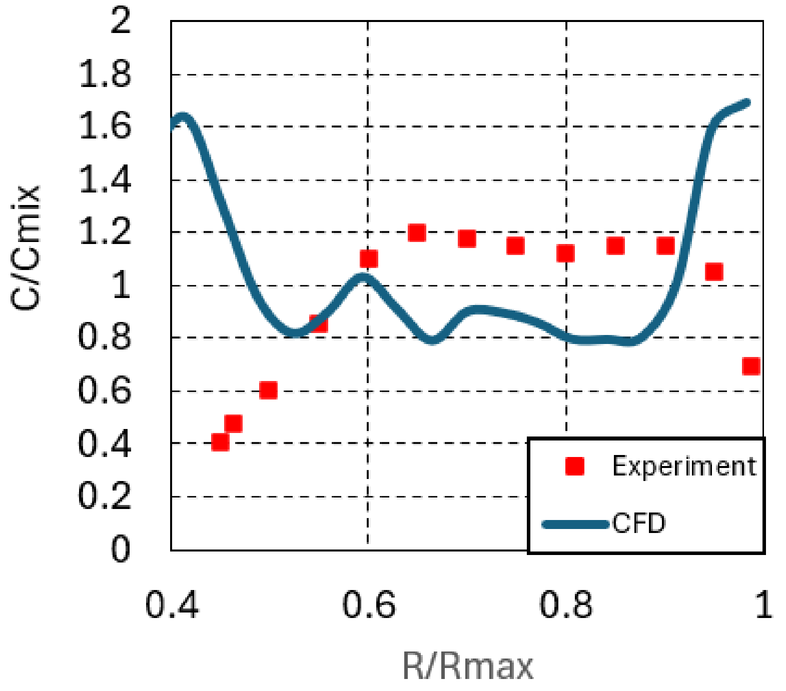
[14] Dukkipati. R V. Numerical Methods Fundamentals. MERCURY LEARNING AND INFO; 2023.

CFD - Verification

www.cranfield.ac.uk

Mixing Verification

Experimental Results From [13]

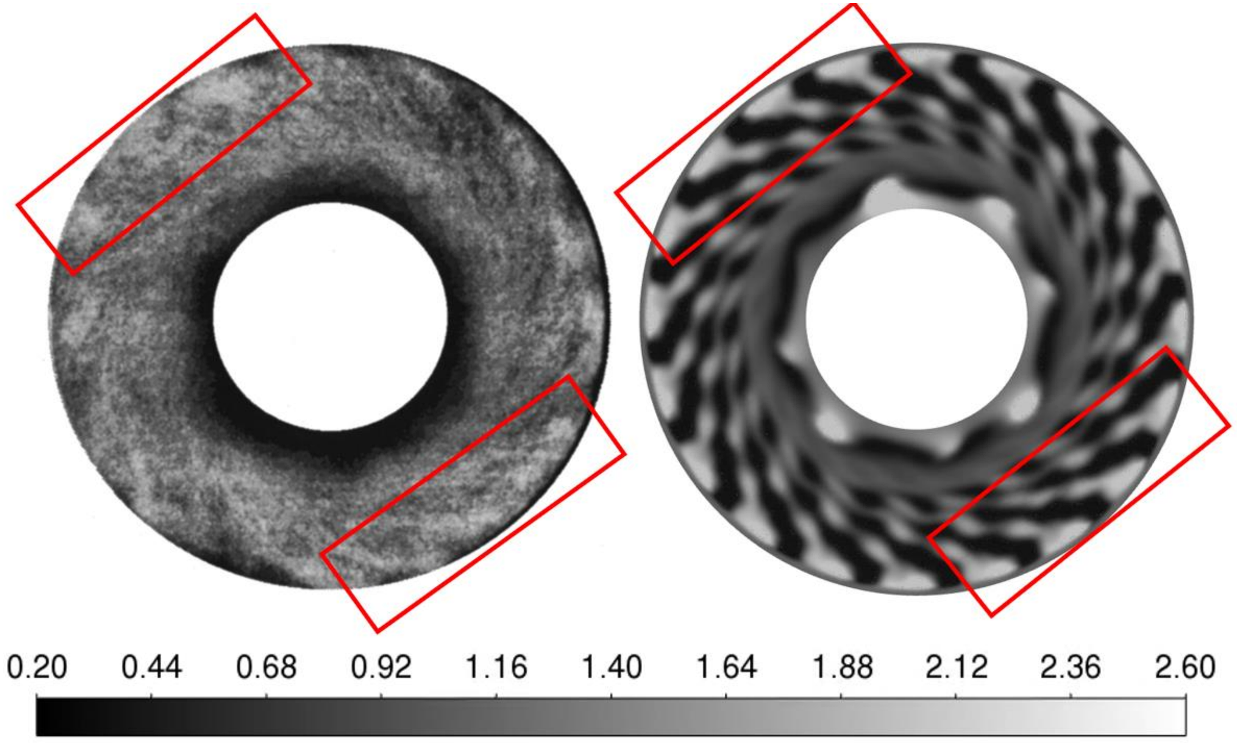


Radial Concentration Distribution

Average Normalized Local Fuel Concentration

Experiment

CFD Results

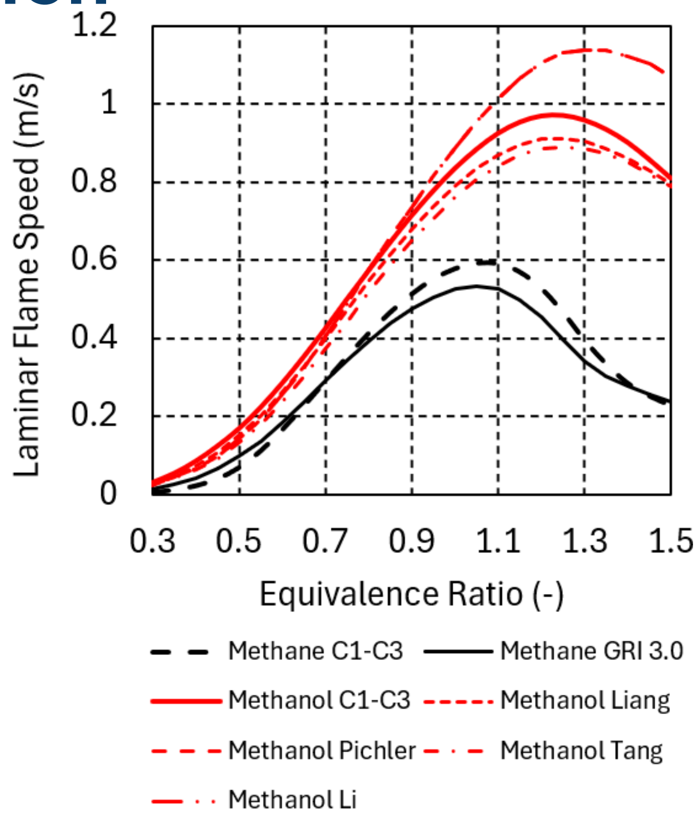


Experimental Results From [15]

[15] G. Mori, S. Razore, M. Ubaldi, P. Zunino, Integrated experimental and numerical approach for fuel-air mixing prediction in a heavy-duty gas turbine LP burner, J. Eng. Gas Turbine Power, 123(4): 803–809 (2001), https://doi.org/10.1115/1.1378297

Combustion Approach Verification

Methane			
Mechanism	**No. of Reactions**	**No. of Species**	
GRI 3.0	325	53	From [18]
Methanol			
Pichler	55	18	From [16]
Li	84	18	From [19]
Liang	74	19	From [15]
Tang	82	25	From [17]



Turbulent Schmidt Number and Prandtl Number: 0.7 and 0.85 (Default Fluent Settings) [Ansys Fluent Theory Guide]

[15] Liang J, Jia W, Sun Y, Wang Q. Skeletal chemical kinetic mechanism generation for methanol combustion and systematic analysis on the ignition characteristics. Asia-Pacific Journal of Chemical Engineering. 2020 May 25;15(3):e2434. Available from: https://doi.org/10.1002/apj.2434

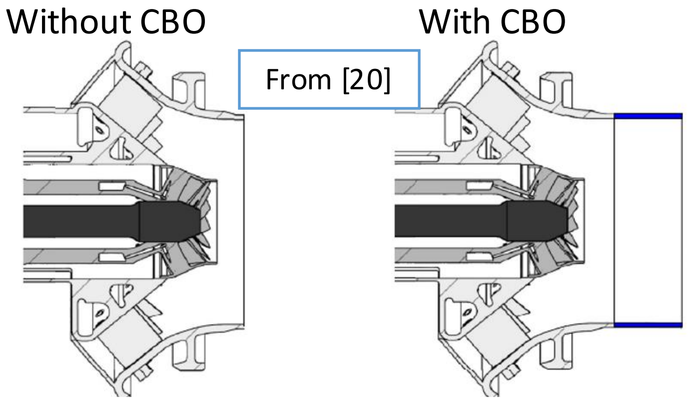
[16] Pichler C, Nilsson EJK. Reduced kinetic mechanism for methanol combustion in spark-ignition engines. Energy & Fuels. 2018 Dec 20;32(12):12805–12813. Available from: https://doi.org/10.1021/acs.energyfuels.8b02136

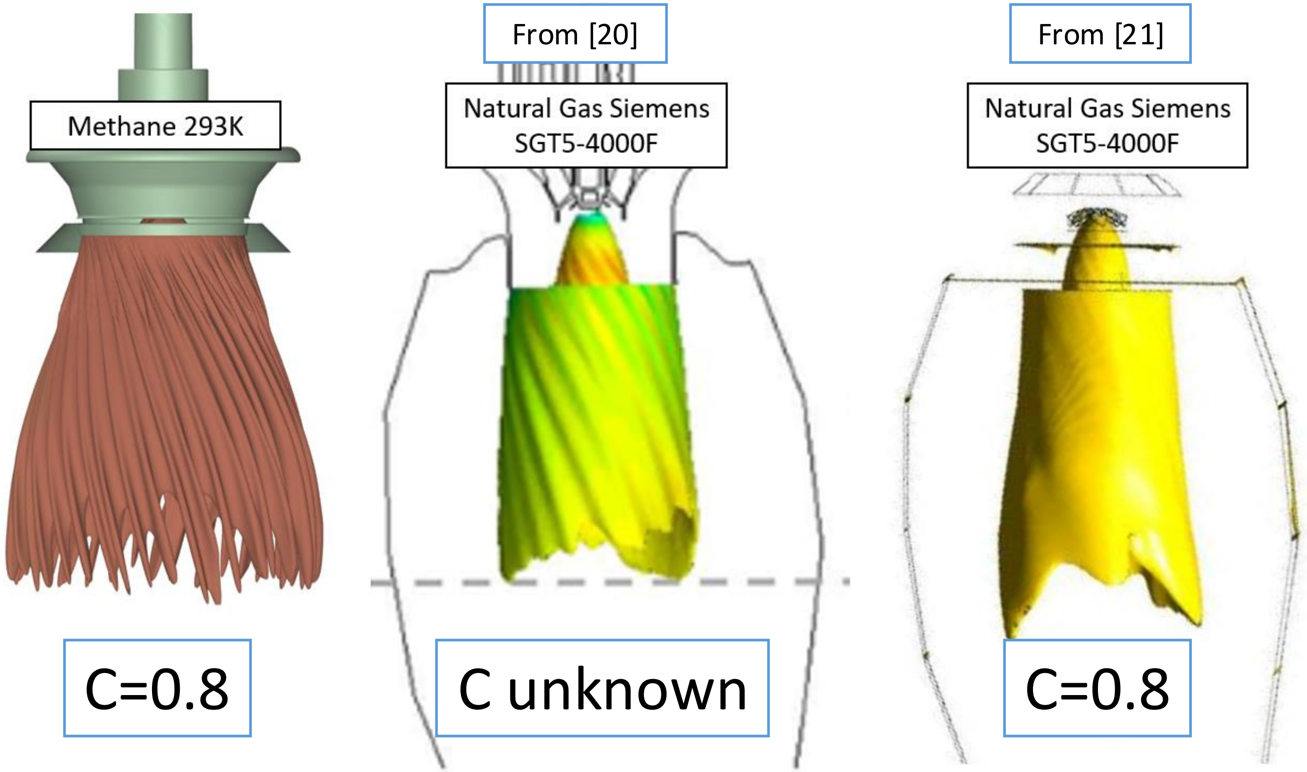
[17] Tang W, Silva M, Hakimov K, Zhang X, Hlaing P, Cenker E, AlRamadan AS, Turner JWG, Farooq A, Im HG, Sarathy SM. Skeletal CH_3OH/NO_x kinetic model for simulating spark-ignition and turbulent jet ignition engines. ACS Omega. 2024 Mar 12;9(10):11255–11265. Available from: https://doi.org/10.1021/acsomega.3c06488

[18] Tang W, Silva M, Hakimov K, Zhang X, Hlaing P, Cenker E, AlRamadan AS, Turner JWG, Farooq A, Im HG, Sarathy SM. Skeletal CH_3OH/NO_x kinetic model for simulating spark-ignition and turbulent jet ignition engines. ACS Omega. 2024 Mar 12;9(10):11255–11265. Available from: https://doi.org/10.1021/acsomega.3c06488

[19] Li J, Zhao Z, Kazakov A, Chaos M, Dryer FL, Scire JJ. A comprehensive kinetic mechanism for CO, CH_2O, and CH_3OH combustion. International Journal of Chemical Kinetics. 2007 Mar 5;39(3):109–136. Available from: https://doi.org/10.1002/kin.20218

Flame Shape Verification





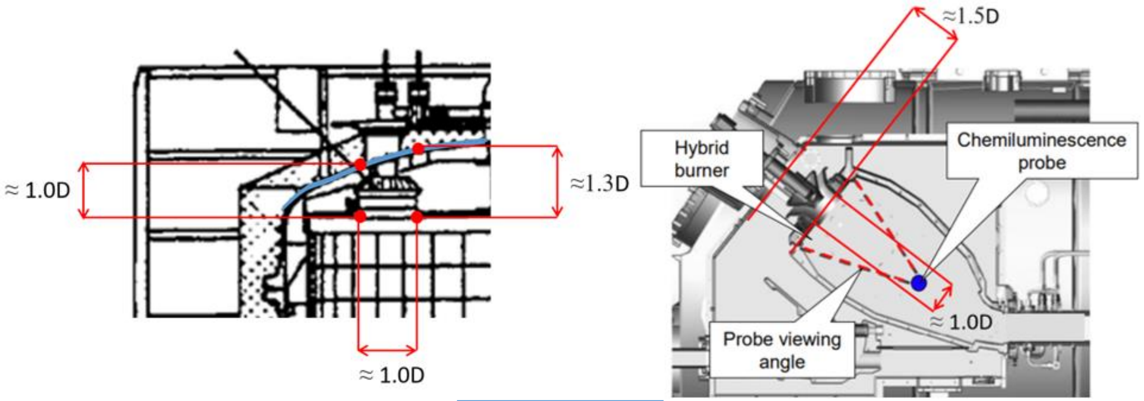
[20] L. Blaette, U. Schmitz, H. Streb, D. Vogtmann, SGT5-4000F hydrogen capability – high pressure combustion rig tests. In Proceedings of ASME Turbo Expo 2023 Turbomachinery Technical Conference and Exposition, Boston, MA, United States, June 26-30, (2023), https://doi.org/10.1115/GT2023-103574
[21] B. Witzel, Application of optical diagnostics to support the development of industrial gas turbine combustors, Ph.D. Thesis, The University of Duisburg-Essen, Faculty of Engineering (2015)

Boundary Conditions – Sensitivity Study for Mixing

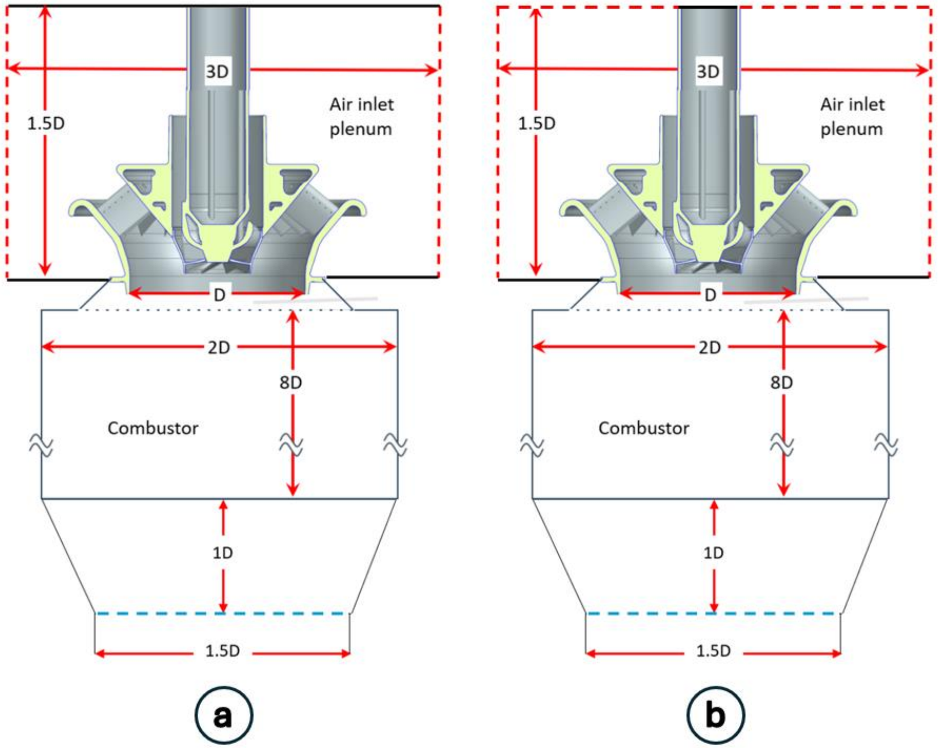
Boundary Conditions – Sensitivity Study for Mixing

Red dash line represents the mass inlet BC

Blue dash line represents the pressure outlet BC



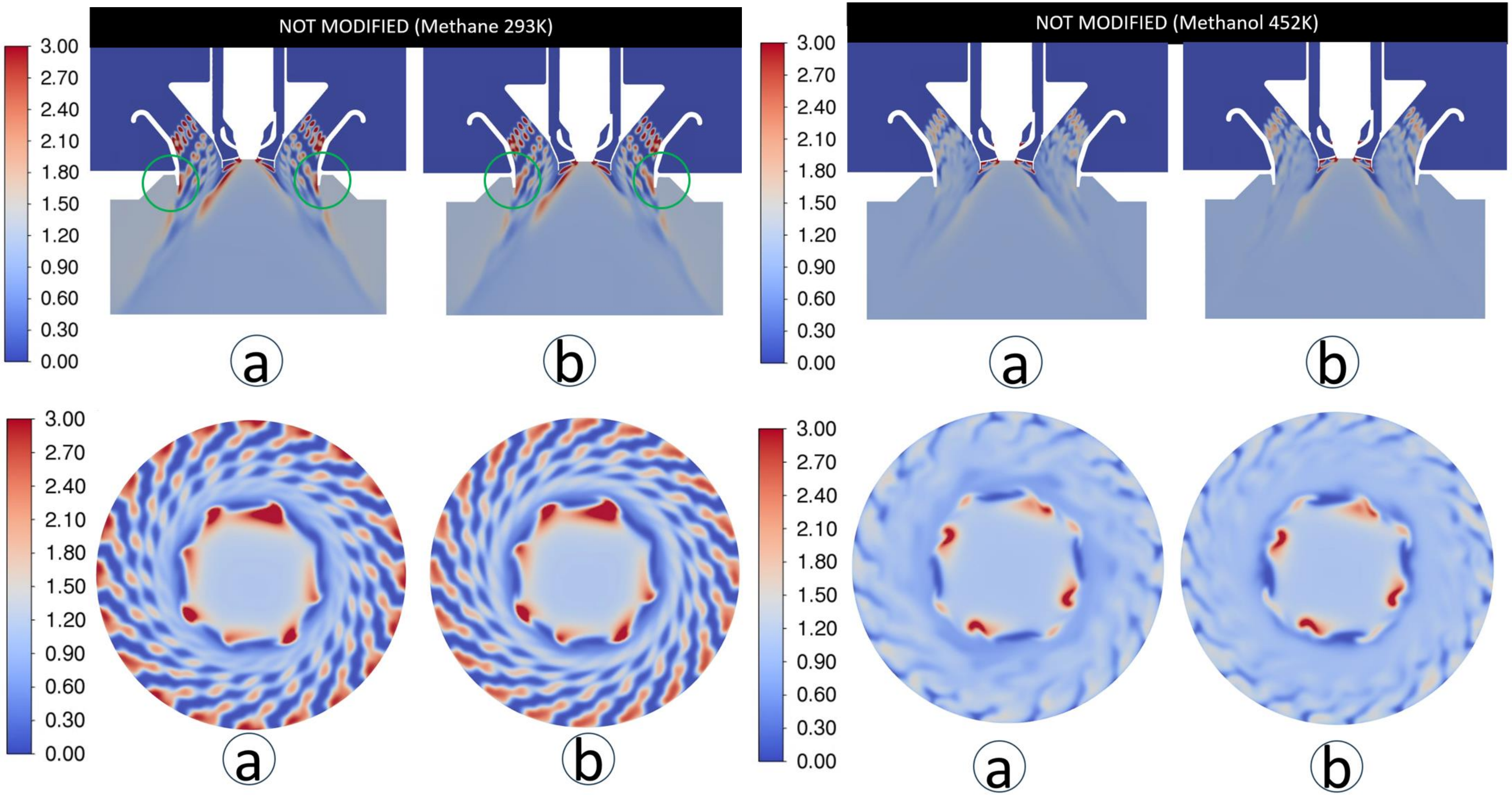
From [22, 23]



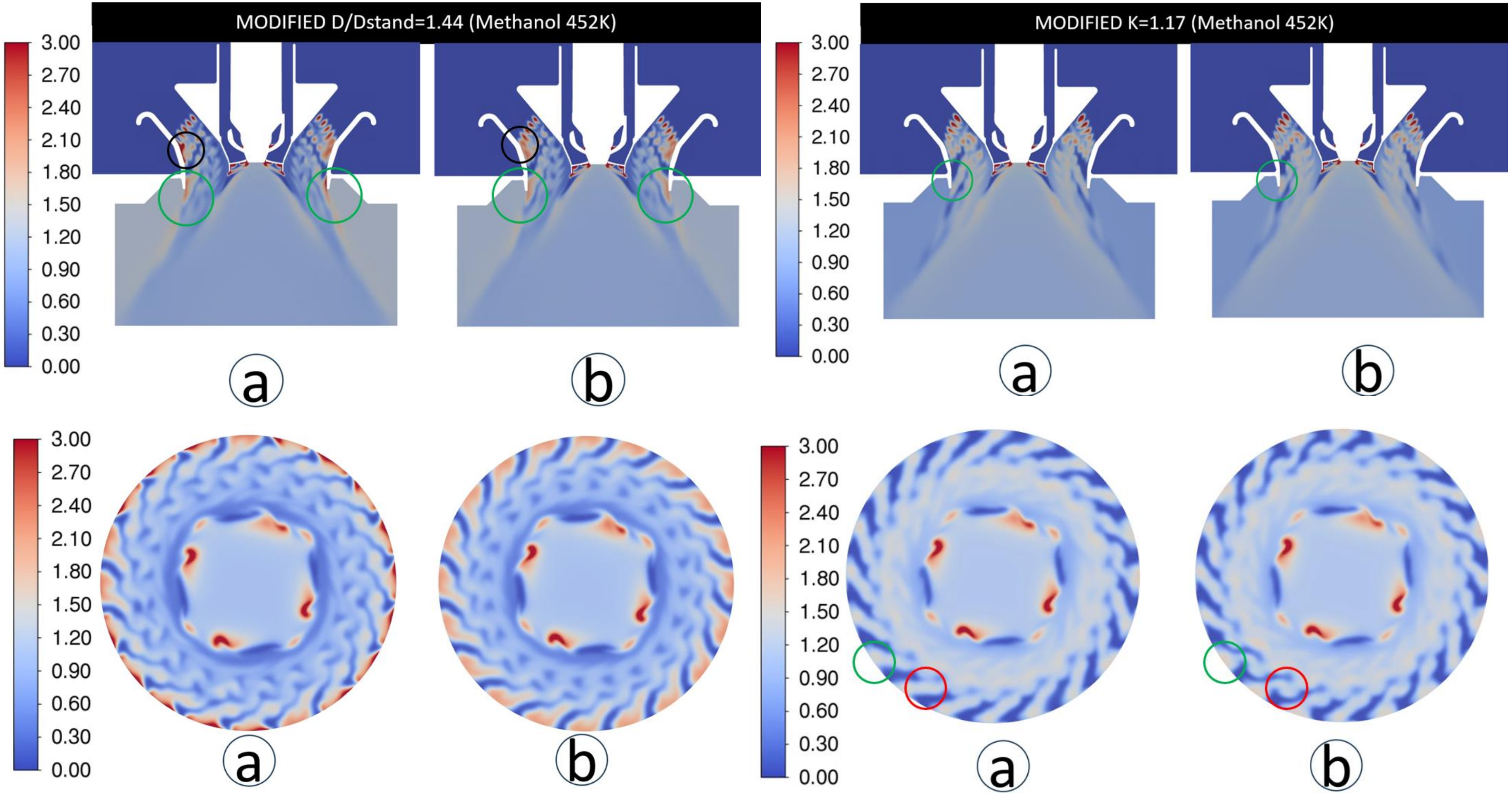
[21] B. Witzel, Application of optical diagnostics to support the development of industrial gas turbine combustors, Ph.D. Thesis, The University of Duisburg-Essen, Faculty of Engineering (2015)

[22] S Klein. On the identification of combustion instability mechanisms in Industrial Gas Turbine Combustors. In: Proceeding of the 1st Global Power and Propulsion Forum [Internet]. 2017 January 16-18; Zurich, Switzerland. [cited 2024 Aug 17]. Available from: https://gpps.global/wp-content/uploads/2021/01/GPPF_2017_paper_178.pdf

Unmodified Geometry



Modified Geometry



Overall Impact into Mixing Quality

The main difference based on this parameter is observed in **uniform increase in nozzle diameter**

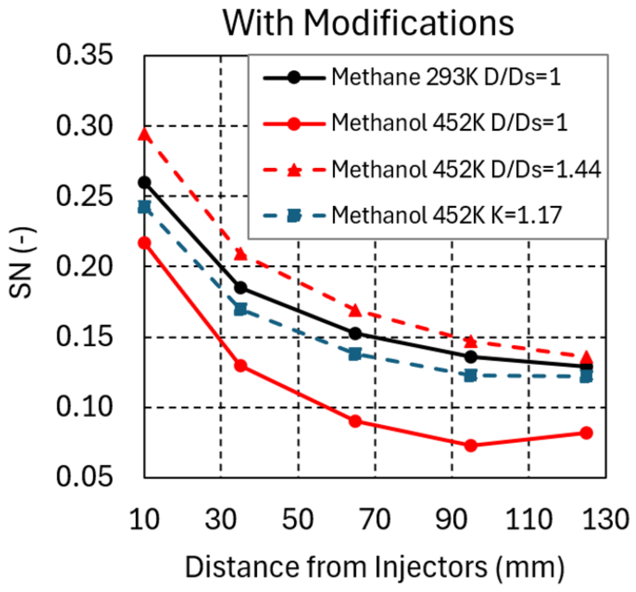
Between **both types of boundary conditions** there can be **observed some similarities in fuel placement study**

Boundary conditions (a) seems to capture better the **arrangement of the burner for** different **Siemens Gas Turbines**

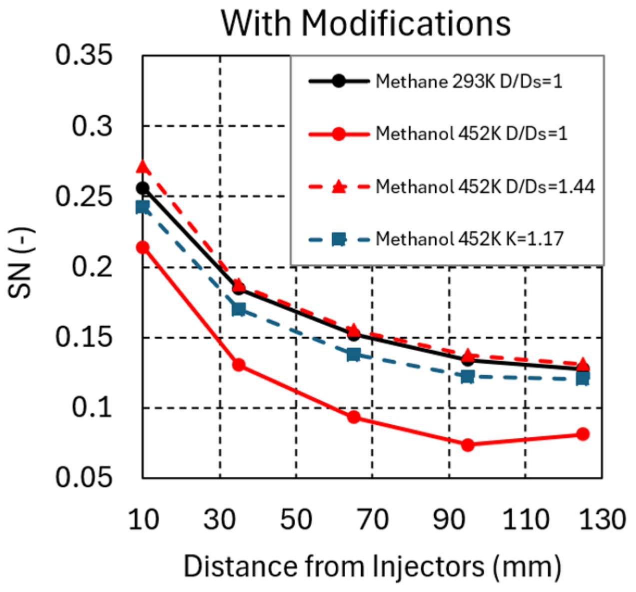
From [8, 9]

$$S_N = \frac{\sqrt{\left(\frac{\sum C_i^2 M_i}{\sum M_j}\right) - \left(\frac{\sum C_i M_i}{\sum M_j}\right)^2}}{\sqrt{\frac{1}{\left(\frac{A}{F}+1\right)} - \left(\frac{1}{\frac{A}{F}+1}\right)^2}}$$

- C_i - cell mass fraction
- M_i - mass flow through the cell
- $\frac{A}{F}$ - air to fuel ratio by mass



(a)



(b)

[8] C. Hornsby and E.R. Norster, Application of CFD to DLN combustion. in Proceedings of ASME 1997 International Gas Turbine and Aeroengine Congress and Exhibition, Orlando, FL, United States Jone 2-5, (1997), https://doi.org/10.1115/97-GT-371

[9] X. Sun, P. Agarwal, F. Carbonara, D. Abbott, P. Gauthier, B. Sethi, Numerical investigation into the impact of injector geometrical design parameters on hydrogen micromix combustion characteristics. in Proceedings of ASME Turbo Expo 2020: Turbomachinery Technical Conference and Exposition, Virtual, Online, September 21-25, (2020), https://doi.org/10.1115/GT2020-16084