

Design and Optimization of a Hydrogen Aircraft Combustor

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Design and Optimization of a Hydrogen Aircraft Combustor

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Abstract

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Abstract

The civil aviation sector faces the crucial challenge of decarbonization, with hydrogen emerging as a key energy carrier for the future of sustainable propulsion. Although hydrogen combustion eliminates CO₂ emissions, it introduces new criticalities, particularly the management of high flame temperatures which favor the production of nitrogen oxides (NO_x).

This thesis work aims to design and optimize a hydrogen-fueled annular combustor for a future-generation turbofan engine, with the primary objective of minimizing pollutant emissions while maintaining high operational performance.

The developed methodology integrates parametric geometric modeling, Computational Fluid Dynamics (CFD) simulation (RANS), and advanced numerical optimization. A hybrid simulation strategy (*Decoupled Detailed Chemistry*) was defined and validated on the Sandia Hydrogen Flame experimental test case, combining the computational efficiency of the *Flamelet* model for the thermal field with the accuracy of detailed kinetic modeling for pollutant prediction.

To explore the vast design space, an adaptive Bayesian optimization framework was implemented. The use of surrogate models based on Gaussian Processes (utilizing the Matérn 3/2 kernel) effectively guided the search for the global optimum, drastically reducing computational cost.

Results show that the identified optimal configuration achieves a reduction in NO_x emissions exceeding 60% compared to the initial reference designs. Phenomenological analysis reveals that this improvement is driven by a transition towards a "strained flame" regime, where intense aerodynamic mixing prevents the mixture from reaching adiabatic equilibrium temperatures, thereby inhibiting the thermal formation of nitrogen oxides.

Acknowledgments

The writing of this thesis marks the end of a year of intense work, concluding a troubled yet exciting academic journey. This adventure took shape two years ago with my arrival at KAIST in South Korea: there, thanks to the courses held by Professors **Dong Hyuk Shin** and **Sung Min Jo**, I had the opportunity to immerse myself in the world of reacting flow modeling and combustion, remaining fascinated by the complexity of thermoacoustic instabilities.

Upon my return to the Politecnico, I could not help but ask Professor Ferrero to link my thesis work to these topics, and fortunately, so it was.

Since then, I have had the opportunity to develop new skills, deepening my knowledge of surrogate models and Gaussian processes in particular, whose error theory immediately captivated me, and immersing myself in the Ansys software suite. My relationship with the latter was often conflicting, but overcoming every error allowed me to achieve results I never thought I would be capable of. I also discovered the Linux HPC environment, in a love/hate relationship that taught me what it means to work with resources that are as powerful as they are limited, and the importance of sharing them.

I therefore wish to thank primarily **Prof. Andrea Ferrero**, for teaching what I consider the best course taken at the Politecnico and for his constant guidance during this year of work. A special thanks goes to **Eng. Lorenzo Folcarelli**, whose technical and moral support was immense and indispensable in all phases of the project.

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Nomenclature

The following lists describe the acronyms and symbols used throughout the thesis. Symbols are grouped by category (Acronyms, Greek, Roman). Where a symbol has multiple meanings depending on the context (e.g., Combustion physics vs. Statistics), the specific domain is indicated in parentheses.

Acronyms

Acronym	Description
AMG	Algebraic Multigrid
AR	Area Ratio
BOI	Body Of Influence
CAD	Computer-Aided Design
CFD	Computational Fluid Dynamics
CFL	Courant-Friedrichs-Lewy Number
CHJU	Fuel Cells and Hydrogen 2 Joint Undertaking
CRZ	Central Recirculation Zone
CSJU	Clean Sky 2 Joint Undertaking
DDC	Decoupled Detailed Chemistry
DNS	Direct Numerical Simulation
DoE	Design of Experiments
DZ	Dilution Zone
EARSM	Explicit Algebraic Reynolds Stress Model
EDC	Eddy Dissipation Concept
EI	Expected Improvement
EINO _x	Emission Index of NO _x
FVM	Finite Volume Method
GP	Gaussian Process
GPR	Gaussian Process Regression
HPC	High Performance Computing
LHS	Latin Hypercube Sampling
LIF	Laser Induced Fluorescence
LOOCV	Leave-One-Out Cross Validation
MPI	Message Passing Interface
MUSCL	Monotone Upstream-Centered Schemes for Conservation Laws
NPF	Normalized Pattern Factor

Acronym	Description
OOM	Out Of Memory
OPF	Overall Pattern Factor
OQ	Orthogonal Quality
PDE	Partial Differential Equation
PDF	Probability Density Function
PLF	Pressure Loss Factor
PRESTO!	PREssure STaggering Option
PSD	Power Spectral Density
PSR	Perfectly Stirred Reactor
PZ	Primary Zone
RAM	Random Access Memory
RANS	Reynolds-Averaged Navier-Stokes
RMS	Root Mean Square
RSM	Reynolds Stress Model
RTE	Radiative Transfer Equation
SAF	Sustainable Aviation Fuel
SFM	Steady Laminar Flamelet Model
SPDE	Stochastic Partial Differential Equation
SST	Shear Stress Transport (Turbulence Model)
SZ	Secondary Zone (Intermediate)
TCI	Turbulence-Chemistry Interaction

Greek Symbols

Symbol	Description
Γ	Radiative diffusion parameter
δ_{LOO}	Actual absolute error (LOOCV)
ΔP	Total Pressure Drop
ε	Turbulent Dissipation Rate
η	Parallel Efficiency
η_b	Combustion Efficiency
μ	Dynamic Viscosity
$\mu(\mathbf{x})$	Mean Function of the Gaussian Process
μ_t	Turbulent (Eddy) Viscosity
μ_Z	Mean of residuals (Statistics)
ν	Kinematic Viscosity
ν	Smoothness parameter (Matérn kernel)
ρ	Density
σ	Standard Deviation
σ_{LOO}	Predicted uncertainty (LOOCV)
τ_{res}	Residence Time
Φ	Equivalence Ratio
$\Phi(\cdot)$	Cumulative distribution function (Standard Normal)
$\phi(\cdot)$	Probability density function (Standard Normal)
χ	Scalar Dissipation Rate

Symbol	Description
ω	Specific Dissipation Rate (Turbulence)
$\dot{\omega}_k$	Chemical reaction rate of species k

Roman Symbols

Symbol	Description
a	Absorption coefficient
A_{ref}	Reference Area
C_d	Discharge Coefficient
Da	Damköhler Number
d	Internal burner diameter
G	Incident Irradiance
h_{ft}	Flame Tube Height
H	Total Enthalpy
k	Turbulent Kinetic Energy
$k(\mathbf{x}, \mathbf{x}')$	Kernel (Covariance) Function
$\mathbf{K}$	Covariance Matrix
Ka	Karlovitz Number
L_{vis}	Visible flame length
l	Length-scale parameter (Kernel)
$\dot{m}$	Mass flow rate
M_{req}	Required Memory Estimation
N_{cells}	Total number of cells
N_{core}	Number of cores (partitions)
N_{sect}	Number of angular sectors (also referred to as N_{st}, N_{slices})
p	Pressure
Q	Generic conserved scalar quantity
R_{dil}	Radial position / Radius of dilution holes (r_{dil})
Re	Reynolds Number
R^ϕ	Residual for variable ϕ
S	Speedup
Sc_t	Turbulent Schmidt Number
S_N	Swirl Number
T	Temperature
$\mathbf{u}, U$	Velocity vector / Magnitude
U_{ft}	Flame Tube Velocity
V	Volume
V_{ref}	Reference Velocity
y^+	Dimensionless wall distance
Y_k	Mass fraction of species k
$Y(\mathbf{x})$	Stochastic Process
$\hat{y}$	Predicted Mean (Kriging)
Z	Mixture Fraction (Combustion Physics)
Z	Standardized Residual (Statistics)

Chemical Species

Formula	Name
CO ₂	Carbon Dioxide
H ₂	Hydrogen (Molecular)
H ₂ O	Water Vapor
NO _x	Nitrogen Oxides (generic)
NO	Nitric Oxide (Nitrogen Monoxide)
OH	Hydroxyl Radical

Introduction

Introduction

The path toward aviation decarbonization: challenges, opportunities, and the role of hydrogen in future propulsion.

ABSTRACT

Over the last few years, increasing attention has been directed toward the civil aviation sector by policymakers, industry leaders, and public opinion regarding the climate impact for which it is responsible. Although this represents a relatively minor share of total global CO₂ emissions, driven by the ever-growing demand for air transport, an urgent need for solutions to minimize them has emerged.

Technological, Political, and Environmental Context

The goal of “net neutrality” throughout the entire aircraft life cycle (production, operational use, fuel production, and disposal) is currently very complex to achieve. The strategic direction considered among the most promising is the adoption of alternative and low-impact fuels, in a manner compatible with the high levels of safety, efficiency, and sustainability required by the sector.

In this context, a leading candidate is **hydrogen** (H_2). The combustion (or potential use within fuel cells) of carbon-free hydrogen would allow for the elimination of direct CO_2 emissions during flight, while maintaining only the indirect emissions from production. Furthermore, if hydrogen were derived from low-impact production processes, for example, via electrolysis powered by renewable or nuclear energy, the entire fuel life cycle could be significantly more sustainable compared to the traditional fossil fuels currently in use or “drop-in” Sustainable Aviation Fuels (SAF), i.e., fuels chemically compatible with Jet-A.

On the political and institutional level, European projects and studies identify hydrogen as one of the main levers to decarbonize air transport [1, 2, 3, 4]. In particular, the study promoted by the *Clean Sky 2 Joint Undertaking* (CSJU) and the *Fuel Cells and Hydrogen 2 Joint Undertaking* (CHJU) considers scenarios where hydrogen-powered aircraft could enter service as early as 2035 for short- and medium-haul routes [1].

Environmental Criticalities of Hydrogen

However, hydrogen combustion is not exempt from environmental criticalities. While eliminating CO_2 emissions and carbon particulate matter, the use of air as an oxidizer introduces atmospheric nitrogen: due to high combustion temperatures, nitrogen oxides (NO_x) can be generated [5, 6].

Moreover, the emission of water vapor (H_2O) at altitude can increase the formation of condensation trails (contrails) and cirrus clouds, phenomena recognized as non-negligible from a climate-altering perspective [7].

These issues make it evident that the simple adoption of hydrogen is not enough: it is necessary to develop innovative combustors and propulsion systems capable of minimizing residual emissions and integrating new methods for fuel storage, distribution, and usage.

Contrails: In addition to NO_x , water vapor is a potent greenhouse gas at high altitudes. Contrails can persist and form cirrus clouds that trap terrestrial heat.

Hydrogen: Energy vs. Volume

It is interesting to analyze the properties of hydrogen compared to traditional fuels. From an energetic standpoint, hydrogen is the substance with the highest energy per unit of mass, which is fundamental for flight.

The flip side of the coin is its extremely low volumetric density. To provide the same energy as Kerosene, a much larger volume of hydrogen (cryogenic liquid) must be stored, requiring voluminous tanks that radically impact the aircraft structure.

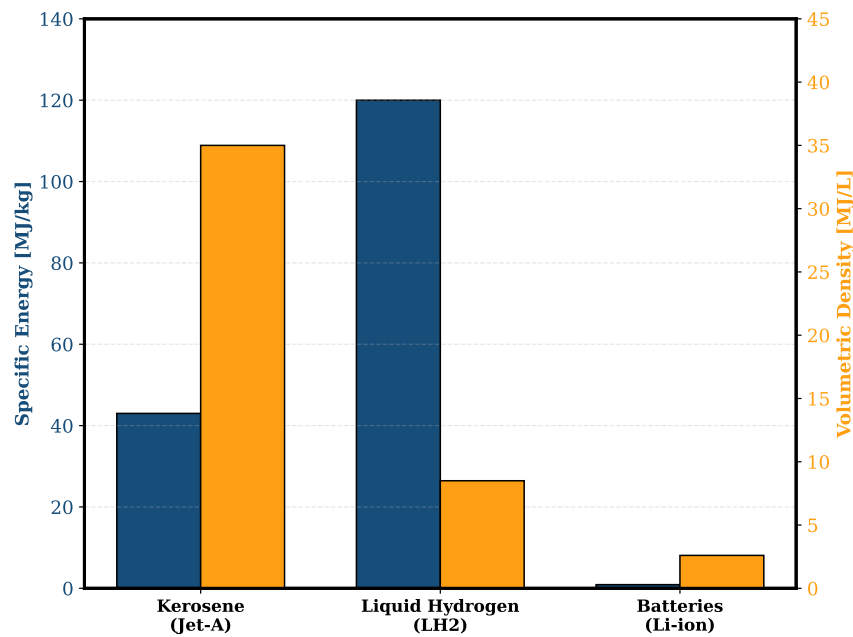


Figure 1: Comparison between Specific Energy (mass advantage) and Energy Density (volume disadvantage): hydrogen wins on weight but loses on volume.

The Challenge of Nitrogen Oxides (NO_x)

A strictly relevant issue in the design of hydrogen-fueled combustors is the reduction of nitrogen oxide production. Indeed, even hydrogen combustion in air entails the formation of these substances, which are responsible for acid rain and ozone alteration, with climate-altering effects.

However, recent studies [8] have shown that through adequate combustor design (use of lean mixtures, correct air dilution) and the use of specific geometric optimization strategies (turbulence control), it is possible to drastically reduce NO_x emissions compared to traditional kerosene flames. The latter, in fact, must simultaneously comply with constraints on CO_2 and NO_x emissions, two requirements that are chemically conflicting.

Trade-off: Less NO_x , More Water

By way of example, a study [7] conducted on a model of an A320-type aircraft powered by liquid hydrogen showed an 86 % reduction in NO_x compared to traditional fuel, accompanied, however, by a 430 % increase in water vapor emissions.

The decrease in NO_x would have a positive impact on the medium-term climate balance, net of the increase in water vapor at altitude.

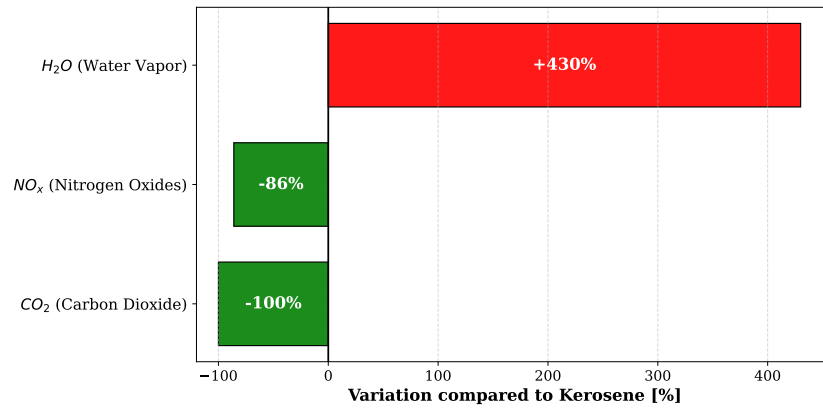


Figure 2: Percentage variation of emissions: hydrogen eliminates CO₂ and cuts NO_x but drastically increases water vapor.

Scope of the Thesis Work

In light of the potential and challenges outlined, this thesis work intends to contribute to the development of hydrogen-fueled aircraft combustors optimized to minimize NO_x emissions.

The work stands as an extension and development of the hydrogen turbofan model presented in the article: “*Integrated Numerical Modeling of a Hydrogen Turbofan Engine and Fuel System With Alternative Thermodynamic Cycles*” [9], focusing specifically on the combustor subsystem.

Specifically, the following activities were carried out:

- **Preliminary design** of an annular combustor, built based on expected cruise conditions.
- **Geometric optimization** (parametric) of the combustion chamber, with the main objective of minimizing nitrogen oxide production while maintaining compatible performance and sustainable computational costs.
- **Definition of a methodological procedure** that balances physical accuracy, computational efficiency, and adequate use of available resources.

In this context, industrial software was used (Ansys suite: SpaceClaim, Fluent Meshing, Fluent Solver, PyFluent), Python code was created for CAD process automation and simulation preparation (mesh generation and definition of the reference Journal), and HPC computing resources provided by the Politecnico di Torino were exploited.

The **expected contribution** is to outline a standardizable preliminary design procedure that is effective and efficient within the context of limited computational resources and capable of contributing to the development of lower-impact hydrogen aircraft combustors.

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Theoretical Basis of Turbulent Combustion

Mathematical modeling of reactive fluid dynamics: from Navier-Stokes equations to turbulence and combustion models for hydrogen.

ABSTRACT

Before delving into the operational activities, it is fundamental to recall the theoretical elements underlying the study of combustion phenomena and their treatment in computational analysis. This chapter provides the mathematical and physical framework necessary to understand the modeling choices adopted, starting from the governing equations up to advanced turbulence-chemistry interaction models for hydrogen.

1.1 Governing Equations of Fluid Motion

The mathematical description of fluid motion relies on the three conservation laws of classical mechanics and thermodynamics: conservation of mass, momentum (Newton's Second Law), and energy (First Law of Thermodynamics) [10, 11]. To derive these equations, the Eulerian approach is adopted, considering an infinitesimal control volume $dV = dx dy dz$ fixed in space and traversed by a fluid. The balance of physical properties is calculated by analyzing what enters, what exits, and what accumulates within this volume.

In the context of this work, resolving the physics of the considered fluid will require additional equations—discussed in a subsequent section—that specifically describe the evolution of chemical species within the combustor.

Although the flow regime in a classic combustor is subsonic and therefore treated in simulation with a *pressure-based* solver, density variations due to strong thermal gradients and changes in chemical composition are significant. Therefore, the equations are presented in their form for variable-density flows.

1.1.1 Conservation of Mass (Continuity)

The principle establishes that the temporal variation of mass in the control volume must equal the net flux through the surfaces:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \quad (1.1)$$

where ρ is the density and $\mathbf{u}$ is the velocity vector. The first term represents mass accumulation (zero for stationary flows), while the second is the divergence of the mass flux, describing the balance between incoming and outgoing mass.

1.1.2 Conservation of Momentum (Navier–Stokes)

This equation is the application of Newton's second law ($\mathbf{F} = m\mathbf{a}$) to the fluid volume [11]. Forces are divided into surface forces (pressure p and viscous stresses $\boldsymbol{\tau}$) and body forces (neglected in this treatment).

$$\frac{\partial(\rho \mathbf{u})}{\partial t} + \nabla \cdot (\rho \mathbf{u} \mathbf{u}) = -\nabla p + \nabla \cdot \boldsymbol{\tau} \quad (1.2)$$

Assuming the fluid is Newtonian, we can mathematically model the viscous stress tensor $\boldsymbol{\tau}$, which is linearly related to the strain rate via the dynamic viscosity μ :

$$\tau_{ij} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} \right) - \frac{2}{3} \mu \delta_{ij} (\nabla \cdot \mathbf{u}) \quad (1.3)$$

1.1.3 Conservation of Energy

For reactive flows, the energy equation is fundamental as it couples fluid dynamics with chemistry, which governs the reactions between species within the flow. Using the total enthalpy $H = h + \frac{1}{2}|\mathbf{u}|^2$, the equation takes the form [10]:

$$\frac{\partial(\rho H)}{\partial t} + \nabla \cdot (\rho \mathbf{u} H) = \frac{\partial p}{\partial t} + \nabla \cdot (\boldsymbol{\tau} \cdot \mathbf{u}) - \nabla \cdot \mathbf{q} \quad (1.4)$$

The heat flux vector $\mathbf{q}$ includes thermal conduction (Fourier) and species diffusion:

$$\mathbf{q} = -\lambda \nabla T - \sum_{k=1}^N h_k \mathbf{J}_k \quad (1.5)$$

where λ is the thermal conductivity, h_k is the enthalpy of species k , and $\mathbf{J}_k$ is the relative diffusive flux. The term $\sum h_k \mathbf{J}_k$ describes the chemical heat release due to combustion.

1.1.4 RANS Equations and the Closure Problem

The Navier–Stokes equations are valid instantaneously, but turbulent flows exhibit chaotic fluctuations that are too rapid and distributed over a spectrum of scales too broad to be directly resolved in complex domains like that of a combustor [11].

Even with the use of supercomputers, **DNS** (*Direct Numerical Simulation*) would be computationally unsustainable for Reynolds numbers typical of industrial applications, especially considering the objective of this treatment, namely the geometric optimization of a combustor, which requires running a high number of simulations in reasonable times.

To overcome this problem, knowledge of the flow evolution in its minutest details (both spatial and temporal) is forgone in favor of deriving a mean field, which is certainly less detailed but decidedly faster to solve. To do this, the Navier–Stokes equations are altered through an averaging operator, thus obtaining a new system of equations known as **RANS** (*Reynolds Averaged Navier–Stokes*).

Favre Averaging

In flows with strong density variations, Favre averaging (density-weighted) is introduced to avoid complex correlation terms [10]:

$$\tilde{\phi} = \frac{\overline{\rho \phi}}{\bar{\rho}}, \quad \phi = \tilde{\phi} + \phi'' \quad (1.6)$$

where $(\bar{\cdot})$ indicates the classical Reynolds average and $(\cdot)''$ the Favre fluctuation.

1.1.5 Favre-Averaged Continuity Equation

Starting from the instantaneous continuity equation (mass conservation):

$$\frac{\partial \rho}{\partial t} + \frac{\partial(\rho u_i)}{\partial x_i} = 0 \quad (1.7)$$

Substituting the Reynolds decomposition for density ($\rho = \bar{\rho} + \rho'$) and Favre decomposition for velocity ($u_i = \tilde{u}_i + u_i''$), and applying the averaging operator:

$$\frac{\partial(\bar{\rho} + \rho')}{\partial t} + \frac{\partial[(\bar{\rho} + \rho')(\tilde{u}_i + u_i'')]}{\partial x_i} = 0 \quad (1.8)$$

Using the fundamental property of Favre averaging, i.e., that the average of density-weighted fluctuations is zero ($\overline{\rho u_i''} = 0$), the averaged equation reduces to:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial(\bar{\rho} \tilde{u}_i)}{\partial x_i} = 0 \quad (1.9)$$

*The DNS approach to resolving turbulent flows consists of **directly** solving all turbulent phenomena through the use of extremely refined computational MESHES. By doing so, the use of turbulence models—which would require introducing additional hypotheses—is not required; the **trade-off** is the unsustainably high computational cost derived from calculation grids of such dimensions.*

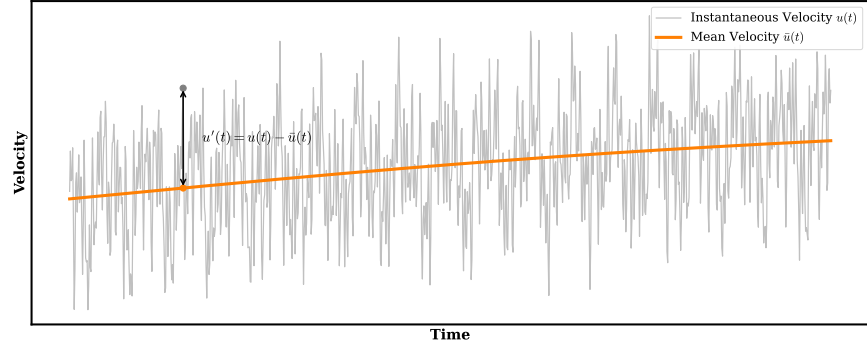


Figure 1.1: Graphical representation of Reynolds decomposition: the instantaneous velocity signal is separated into a mean component (orange line) and an instantaneous turbulent fluctuation (gray line), highlighting the relationship $u'(t) = u(t) - \bar{u}(t)$.

1.1.6 Favre-Averaged Energy Equation

Applying the average to the total enthalpy equation H , the non-linearity of the convective part generates an unclosed term. The averaged equation takes the form (simplified to highlight the transport term):

$$\frac{\partial(\bar{\rho}\tilde{H})}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j\tilde{H})}{\partial x_j} = \dots - \frac{\partial}{\partial x_j}(\overline{\rho u_j'' h''}) + \dots \quad (1.10)$$

The new term is the turbulent heat flux $q_t = \overline{\rho u_j'' h''}$. This describes the transport of enthalpy by velocity fluctuations. It requires modeling, typically done via an analogy with Fourier's law and using a turbulent thermal conductivity (λ_t):

$$-\overline{\rho u_j'' h''} \approx \lambda_t \frac{\partial \tilde{T}}{\partial x_j} \quad (1.11)$$

1.1.7 Favre-Averaged Momentum Equation

The instantaneous momentum equation, in Einstein notation, is:

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial(\rho u_i u_j)}{\partial x_j} = -\frac{\partial p}{\partial x_i} + \frac{\partial \tau_{ij}}{\partial x_j} \quad (1.12)$$

The most critical term is the convective one. Expanding the product of velocities with Favre decomposition:

$$\overline{\rho u_i u_j} = \overline{\rho(\tilde{u}_i + u_i'')(\tilde{u}_j + u_j'')} \quad (1.13)$$

Since the mixed terms vanish (given that $\overline{\rho u_i''} = 0$), we are left with:

$$\overline{\rho u_i u_j} = \bar{\rho} \tilde{u}_i \tilde{u}_j + \overline{\rho u_i'' u_j''} \quad (1.14)$$

Substituting into the overall equation yields the RANS equation for momentum:

$$\frac{\partial(\bar{\rho}\tilde{u}_i)}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_i\tilde{u}_j)}{\partial x_j} = -\frac{\partial \bar{p}}{\partial x_i} + \frac{\partial}{\partial x_j}(\bar{\tau}_{ij} - \overline{\rho u_i'' u_j''}) \quad (1.15)$$

The new term, born from the non-linearity of the convective term, is the Reynolds Stress Tensor:

$$\tau_{ij}^R = -\overline{\rho u_i'' u_j''} \quad (1.16)$$

Physical interpretation of Reynolds stresses

Although mathematically derived from the non-linearity of the convective term, Reynolds stresses are interpreted as an additional stress [11]. This tensor is physically justified as the mathematical term describing the effect of momentum transport due to turbulent fluctuations. Although velocity oscillations seem random, they continuously move portions of fluid from one zone to another; this movement produces mean momentum contributions that manifest as actual stresses. These considerations allow us to visualize turbulence as a very efficient mixing mechanism: vortices transport momentum from the core of the flow towards the wall and vice versa, generating non-zero mean exchanges over time. However, since new unknowns (the tensor components) appear without introducing new equations, the problem of system closure arises, necessitating the formulation of a turbulence model.

1.2 Turbulence Modeling

The RANS equation closure problem, highlighted in the previous section, materializes in the need to model the Reynolds stress tensor:

$$\tau_{ij}^R = -\overline{\rho u_i'' u_j''} \quad (1.17)$$

as a function of mean flow quantities.

Physically, this term represents the momentum transport operated by turbulent fluctuations. In a turbulent flow such as that inside a combustor, energy is transferred from large vortical scales (generated by geometry) to small dissipative scales (where kinetic energy is converted into heat by molecular viscosity) through the mechanism of the *energy cascade* introduced by **Kolmogorov**.

Since it is impossible to directly resolve all these scales, turbulence models introduce equations to calculate the statistical properties of vortices (typically an energy and a temporal or spatial scale) and model their effect on the mean flow.

1.2.1 Boussinesq Hypothesis and Eddy Viscosity

The most widespread approach (Boussinesq, 1877) is based on an analogy with the kinetic theory of gases: just as molecular viscosity derives from molecular collisions, it is assumed that turbulent vortices generate a stress proportional to the mean velocity gradient.

The eddy (or turbulent) viscosity μ_t is thus introduced, defining the linear constitutive relation:

$$-\overline{\rho u_i'' u_j''} = \mu_t \left(\frac{\partial \tilde{u}_i}{\partial x_j} + \frac{\partial \tilde{u}_j}{\partial x_i} \right) - \frac{2}{3} \delta_{ij} \left(\mu_t \frac{\partial \tilde{u}_k}{\partial x_k} + \bar{\rho} k \right) \quad (1.18)$$

The isotropy hypothesis fails in swirling flows because the strong curvature of streamlines induces high anisotropy in the Reynolds stress tensor. The Boussinesq approximation fails to capture the energy redistribution among directional components caused by centrifugal and Coriolis forces.

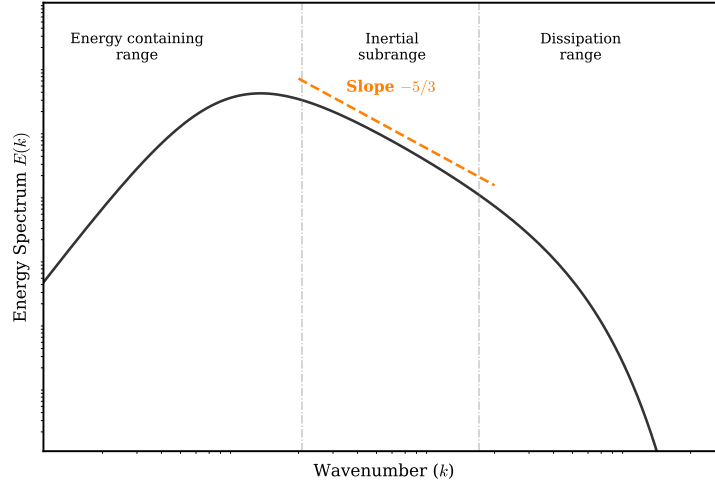


Figure 1.2: Kolmogorov energy cascade. Kinetic energy is produced at large scales (Energy containing range), transferred through the inertial sub-range (characterized by the $-5/3$ slope), and finally dissipated into heat by viscous forces at small scales (Dissipation range).

This hypothesis drastically simplifies the problem: instead of determining 6 independent components of the stress tensor, only the scalar μ_t must be calculated. However, it requires a limiting hypothesis: turbulence isotropy. Assuming μ_t is a scalar means assuming that the turbulent response is identical in all directions, a condition not always verified in flows of engineering interest, such as swirling flows.

1.2.2 The k - ω SST Model (Menter)

To determine the eddy viscosity μ_t , it is necessary to calculate the characteristic scales of turbulence. Historically, the most well-known two-equation models are k - ε , valid in free flows but weak near walls, and k - ω (Wilcox), which excels in resolving the boundary layer down to the wall but is extremely sensitive to free-stream ω values specified at the computational domain inlet, making results dependent on arbitrary boundary conditions. The *Shear Stress Transport* (SST) model, proposed by Menter (1994) [[12]], combines the two approaches, using Wilcox's formulation near the wall, where it is qualitatively superior, and gradually switching to the k - ε model as one moves towards the free stream. The model formulation uses the k - ω transport equations, adapting them with blending functions: F_1 and F_2 (which depend on distance from the wall and local variables), to implement the transition to k - ε .

The transport equations obtained are:

Turbulent Kinetic Energy equation (k):

$$\frac{\partial(\rho k)}{\partial t} + \frac{\partial(\rho u_i k)}{\partial x_i} = \tilde{P}_k - \beta^* \rho k \omega + \frac{\partial}{\partial x_i} \left[(\mu + \sigma_k \mu_t) \frac{\partial k}{\partial x_i} \right] \quad (1.19)$$

Specific Dissipation Rate equation (ω):

$$\begin{aligned} \frac{\partial(\rho\omega)}{\partial t} + \frac{\partial(\rho u_i \omega)}{\partial x_i} = & \frac{\gamma}{\nu_t} \tilde{P}_k - \beta \rho \omega^2 + \frac{\partial}{\partial x_i} \left[(\mu + \sigma_\omega \mu_t) \frac{\partial \omega}{\partial x_i} \right] + \\ & + 2(1 - F_1) \rho \sigma_{\omega 2} \frac{1}{\omega} \frac{\partial k}{\partial x_i} \frac{\partial \omega}{\partial x_i} \end{aligned} \quad (1.20)$$

The last term is the Cross-Diffusion term. It emerges from the mathematical transformation of the ε equation into the ω equation. The blending function F_1 equals 1 near the wall (nullifying cross-diffusion and recovering the standard k - ω model) and 0 far from it (activating cross-diffusion and recovering k - ε behavior).

Bradshaw Limiter In classical models, μ_t is proportional to the strain rate S . However, Bradshaw showed that in the presence of adverse pressure gradients, turbulent stress is proportional to ρk , not S . The SST model incorporates this limit by calculating viscosity as [13]:

$$\mu_t = \frac{\rho a_1 k}{\max(a_1 \omega, S F_2)} \quad (1.21)$$

where a_1 is Bradshaw's constant, S is the strain rate magnitude (or the derivative of velocity with respect to wall distance), and F_2 is a blending function with boundary values analogous to F_1 ; thus, it equals 1 near walls and 0 in the free stream. This variation in eddy viscosity calculation prevents μ_t from growing artificially in stagnation or separation regions, significantly improving the prediction of the detachment point.

1.2.3 The WJ-BSL-EARSM Model

As known in the literature [11], the linear eddy viscosity hypothesis upon which the SST model relies is inadequate in the presence of strong streamline curvature, conditions characterizing the Central Recirculation Zone (CRZ) induced by *swirlers*. Although *Reynolds Stress Models* (RSM) would be capable of resolving anisotropy by solving transport equations for individual stress tensor components, their use would entail high computational cost (7 additional equations) and potential numerical instabilities [13].

In this context, the EARSM (*Explicit Algebraic Reynolds Stress Model*) proposed by Wallin and Johansson [14] emerges as an ideal compromise solution, extending the validity of two-equation modeling to flows with strong anisotropy through an explicit non-linear constitutive relation, while keeping computational costs for system resolution contained.

The basic idea is to extend the Boussinesq relation by assuming a “weak equilibrium” condition for anisotropic stresses: the stress transport equation is thus transformed into an algebraic equation. The anisotropy tensor is defined as:

$$a_{ij} = \frac{\overline{u'_i u'_j}}{k} - \frac{2}{3} \delta_{ij} \quad (1.22)$$

And it is expressed as a tensor expansion (polynomial series in deformation

and rotation tensors):

$$\begin{aligned}
 a_{ij} = & \beta_1 S_{ij} + \beta_2 (S_{ik} \Omega_{kj} - \Omega_{ik} S_{kj}) \\
 & + \beta_3 \left(S_{ik} S_{kj} - \frac{1}{3} S_{mn} S_{nm} \delta_{ij} \right) \\
 & + \beta_4 \left(\Omega_{ik} \Omega_{kj} - \frac{1}{3} \Omega_{mn} \Omega_{nm} \delta_{ij} \right) + \dots
 \end{aligned} \tag{1.23}$$

with dimensionless tensors defined as:

$$S_{ij} = \tau \bar{S}_{ij}, \quad \Omega_{ij} = \tau \bar{\Omega}_{ij} \quad \text{and} \quad \tau \approx \frac{1}{\omega} \tag{1.24}$$

The coefficients β_n are not constant but non-linear functions of the tensor invariants (i.e., local deformation and rotation intensity), allowing the model to adapt the turbulent response by taking rotation into account.

1.3 Equations for Reactive Flows and Hydrogen Specifics

In the previous paragraphs, the fluid was treated as a homogeneous mixture whose thermodynamic properties varied only as a function of temperature and pressure. However, in an aircraft combustor, the physics of the problem is dominated by the chemical transformation of reactants (Hydrogen and air in our case) into combustion products (water vapor and, to a lesser extent, nitrogen oxides). To describe the evolution of chemical composition in space and time, it is necessary to extend the Navier–Stokes system by introducing transport equations for chemical species.

1.3.1 Chemical Species Transport Equations

The mixture composition is described through mass fractions. If the mixture is composed of N chemical species, we define the mass fraction of the k -th species, Y_k , as the ratio of the mass of species k to the total mass in an elementary volume. By definition, the sum of mass fractions must be unity:

$$\sum_{k=1}^N Y_k = 1 \tag{1.25}$$

Applying the principle of mass conservation to the single species k , the transport and reaction equation is obtained:

$$\frac{\partial(\rho Y_k)}{\partial t} + \frac{\partial(\rho u_j Y_k)}{\partial x_j} = -\frac{\partial J_{k,j}}{\partial x_j} + \dot{\omega}_k \tag{1.26}$$

By doing so, $N - 1$ new equations are introduced into the system; the solution for the N -th species will indeed be found as the complement to one of the summation of the mass fractions of the directly calculated species.

Meaning of terms in the transport equation:

In numerical codes, to avoid rounding errors, the species present in the largest quantity (in our case Nitrogen, N_2) is calculated as $Y_N = 1 - \sum_{k=1}^{N-1} Y_k$.

Diffusive term (J_k) This is the transport of species k due to molecular diffusion, i.e., the relative movement of molecules of species k with respect to the mean mixture velocity. Generally, this term is modeled with Fick's law:

$$J_{k,j} = -\rho D_{k,m} \frac{\partial Y_k}{\partial x_j} \quad (1.27)$$

where $D_{k,m}$ is the diffusion coefficient of species k in the mixture. Alternatively, the Hirschfelder and Curtiss approximation is also implemented in numerical calculation codes, used in contexts where Fick's law loses validity (in the presence of strong pressure gradients and significant body forces).

Source term ($\dot{\omega}_k$) This represents the net production/destruction rate of the species due to chemical reactions modeled via Arrhenius kinetics. Source terms are highly non-linear functions of temperature.

1.3.2 RANS Formulation and Turbulent Closure

Applying Favre averaging ($\phi = \tilde{\phi} + \phi''$), the averaged equation is obtained:

$$\frac{\partial(\bar{\rho}\tilde{Y}_k)}{\partial t} + \frac{\partial(\bar{\rho}\tilde{u}_j\tilde{Y}_k)}{\partial x_j} = \frac{\partial}{\partial x_j} \left(\bar{J}_{k,j} - \overline{\rho u_j'' Y_k''} \right) + \bar{\dot{\omega}}_k \quad (1.28)$$

Averaging introduces two main closure problems. The first concerns the modeling of the **turbulent scalar flux** $\overline{\rho u_j'' Y_k''}$, which is treated via the gradient diffusion hypothesis:

$$-\overline{\rho u_j'' Y_k''} = \frac{\mu_t}{Sc_t} \frac{\partial \tilde{Y}_k}{\partial x_j} \quad (1.29)$$

with μ_t being the eddy viscosity (calculated by SST, EARSM models, etc.) and Sc_t the turbulent Schmidt number (typically constant, ≈ 0.7).

The second problem concerns the modeling of the **mean source term** $\bar{\dot{\omega}}_k$. Due to the strong non-linearity of chemical kinetics (exponential Arrhenius law):

$$\overline{\dot{\omega}_k(\rho, T, Y_k)} \neq \dot{\omega}_k(\bar{\rho}, \bar{T}, \bar{Y}_k) \quad (1.30)$$

Simply using averaged quantities (the term on the right of the inequality) would result in significant prediction errors regarding reaction rate and temperature. It will therefore be necessary to study specific turbulence-combustion interaction models (such as EDC, Flamelet, etc., which we will see in the following section) to proceed with an adequate calculation of these terms.

The Schmidt number ($Sc = \nu/D$) expresses the ratio between momentum diffusivity and mass diffusivity. Its turbulent analogue, $Sc_t = \nu_t/D_t$, regulates turbulent species diffusion. For gases, it is typically set to 0.7.

1.4 Turbulence–Chemistry Interaction (TCI) Models

Before analyzing specific numerical models, it is fundamental to physically understand how turbulence interacts with the flame front. This interaction is not unique but depends on the ratio between the energetic and temporal scales of the turbulent flow and those of the chemical reaction. To classify these phenomena, the Borghi–Peters diagram is used [15].

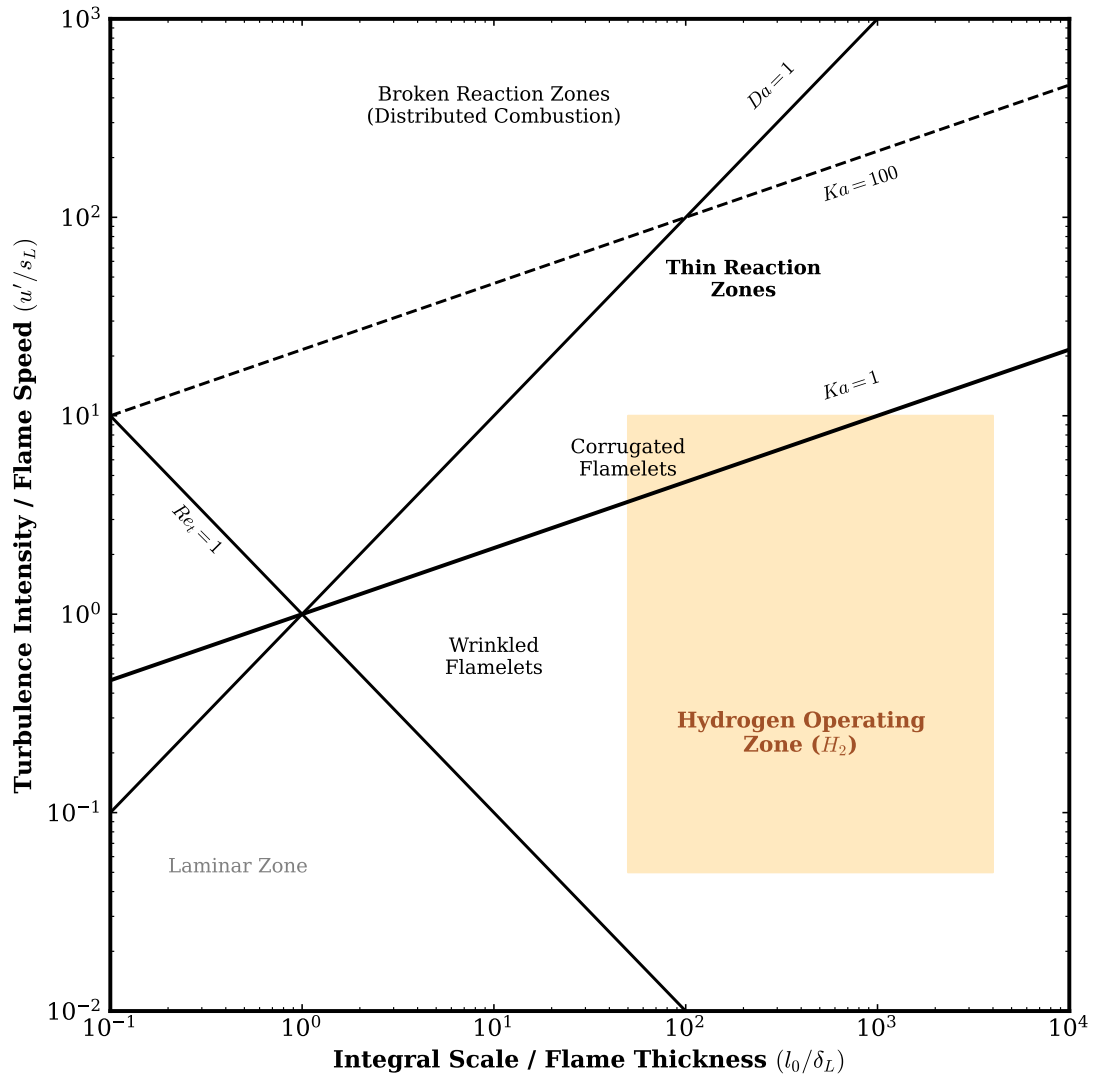


Figure 1.3: Borghi-Peters diagram for the classification of turbulent combustion regimes. The typical operating zone for hydrogen is highlighted (bottom right), characterized by high Damköhler numbers thanks to the high laminar flame speed.

1.4.1 Turbulent Combustion Regimes

The structure of a turbulent flame is determined by the competition between two processes: **Chemical kinetics**, which tends to propagate the flame at the laminar speed S_L with a characteristic thickness δ_L , and **turbulence**, characterized by RMS velocity fluctuation u' and a spectrum of length scales ranging from the integral scale l_0 to the Kolmogorov scale η_k . To map the regimes, two fundamental dimensionless numbers are introduced:

Damköhler Number (Da) Measures the ratio between the integral turbulent time scale (τ_t) and the chemical time scale (τ_c):

$$Da = \frac{\tau_t}{\tau_c} = \frac{l_0/u'}{\delta_L/S_L} \quad (1.31)$$

A value of $Da \gg 1$ indicates that chemistry is much faster than macroscopic turbulence.

Karlovitz Number (Ka) Measures the ratio between the chemical time scale and the turbulent time scale related to the Kolmogorov length (τ_η):

$$Ka = \frac{\tau_c}{\tau_\eta} = \left(\frac{\delta_L}{\eta_k} \right)^2 \quad (1.32)$$

The Karlovitz number thus indicates whether the smallest turbulent vortices can penetrate the flame thickness.

Constructing the Borghi-Peters diagram, plotted on logarithmic coordinates (with u'/S_L on the ordinate and l_0/δ_L on the abscissa), three main regimes are distinguished:

Flamelet Regime ($Ka < 1$) In this zone, even the smallest vortices (η_k) are larger than the flame thickness (δ_L). Turbulence does not penetrate the internal structure of the reaction zone but deforms the laminar front. Combustion occurs in thin layers (*flamelets*) that are locally laminar. For high-turbulence phenomena, we distinguish the *Corrugated Flamelets* zone; otherwise, for phenomena characterized by less intense turbulence, we have *Wrinkled Flamelets*.

Thin Reaction Zones Regime ($1 < Ka < 100$) Kolmogorov vortices are smaller than the total flame thickness ($\eta_k < \delta_L$) and penetrate the preheating zone, increasing heat and mass transport. However, such vortices are not energetic enough to disturb the *Inner Reaction Zone*, which remains thin and intact.

Broken Reaction Zones Regime ($Ka > 100$) Turbulence is so intense ($Ka \gg 1$) and scales are so small that they destroy the flame structure. Mixing is so rapid compared to chemistry ($Da < 1$) that a defined front no longer exists: the reaction occurs throughout the volume in a distributed manner. This shifts towards a *stirred reactor* type model.

The Flamelet Regime for Hydrogen

Hydrogen possesses an exceptionally high laminar flame speed s_L (up to 7–8 times that of methane). From the definitions of Da and Ka , a high s_L implies a high Damköhler number.

Consequently, hydrogen flames tend to remain in the **Flamelet** regime even in the presence of very intense turbulence levels, conditions under which a traditional hydrocarbon would enter the distributed regime or undergo quenching.

1.4.2 The Chemical Averaging Problem

The instantaneous chemical reaction rate $\dot{\omega}$ is governed by the Arrhenius law, which depends exponentially on temperature T :

$$\dot{\omega} = A \exp\left(-\frac{E_a}{RT}\right) \quad (1.33)$$

where E_a is the activation energy, A the pre-exponential factor, and R the universal gas constant. In a turbulent flow, temperature and concentrations fluctuate around their mean values ($T = \tilde{T} + T''$, $Y_k = \tilde{Y}_k + Y_k''$). As previously anticipated, due to the strong non-linearity of the exponential, calculating the mean reaction rate using the mean temperature leads to serious errors:

$$\overline{A \exp\left(-\frac{E_a}{RT}\right)} \neq A \exp\left(-\frac{E_a}{R\tilde{T}}\right) \quad (1.34)$$

Since the Arrhenius curve is strongly convex, using the mean temperature drastically underestimates the effective reaction rate (the mean rate is dominated by temperature peaks, which are lost by averaging before the exponential).

Furthermore, turbulence causes **segregation** between fuel and oxidizer: despite having macroscopic means compatible with reaction within a cell, reactants may be locally separated (unmixed), preventing reaction. Ignoring these effects means ignoring the mutual interaction between thermo-chemical phenomena and turbulent phenomena, resulting in unacceptable discrepancies between numerical results and experimental evidence.

1.4.3 Finite Rate Model (Decoupled / No TCI)

The simplest approach, widely used in commercial codes (such as the *Finite-Rate/No TCI* option in Ansys Fluent), consists of completely neglecting the effect of turbulent fluctuations on chemical kinetics. It is assumed that the mean reaction rate can be calculated directly from averaged variables, ignoring fluctuation terms:

$$\overline{\dot{\omega}(T, Y_k)} \approx \dot{\omega}(\tilde{T}, \tilde{Y}_k) = A \exp\left(-\frac{E_a}{R\tilde{T}}\right) \prod (\tilde{Y}_k)^{\nu_k} \quad (1.35)$$

Chemistry is resolved via the detailed kinetic mechanism, but acting as if the flow were laminar or perfectly mixed within the control volume. This approach is theoretically valid only in the limit of very small Damköhler numbers ($Da \ll 1$), i.e., in conditions of very slow chemistry compared

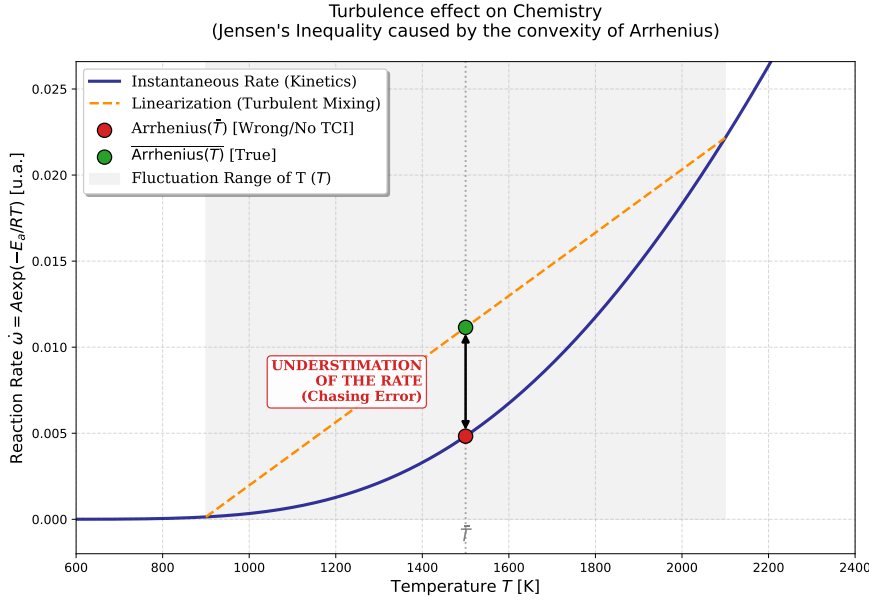


Figure 1.4: Graphical illustration of the impact of turbulent fluctuations on chemical kinetics (Jensen's Inequality). The solid curve represents the instantaneous Arrhenius law. Due to the strong convexity of the exponential function, the reaction rate calculated using the mean temperature ($\dot{\omega}(\bar{T})$, red dot) systematically underestimates the effective mean rate ($\dot{\omega}(T)$, green dot), introducing a closure error that necessitates turbulence-chemistry interaction (TCI) models.

to turbulent mixing. In the case considered in this work, it was chosen to simulate only the *pollutant chemistry* (e.g., NO_x) with this approach. The formation reactions of pollutants are indeed significantly slower compared to the main oxidation reactions releasing heat within the combustor, making the approximation acceptable for these specific sub-mechanisms.

1.4.4 Steady Laminar Flamelet Model (SFM)

For high Damköhler number regimes ($Da \gg 1$), as in stable hydrogen flames, the *Steady Laminar Flamelet* model represents one of the most used models at the industrial level. The basic idea is to visualize the turbulent flame as a collection of thin 1D laminar structures (*flamelets*), corrugated by turbulence but with internal structure unchanged compared to the laminar counterpart. The problem is thus mapped from physical space to the space of the **mixture fraction**, denoted by Z , which assumes a unitary value ($Z = 1$) in zones of space where only fuel is present, while in zones where only oxidant is present, it equals zero ($Z = 0$). If chemistry is sufficiently fast, chemical species Y_k and temperature T depend uniquely on the mixture fraction and a second term, called the “scalar dissipation rate”, defined as:

$$\chi = 2D \left(\frac{\partial Z}{\partial x_j} \frac{\partial Z}{\partial x_j} \right) \quad (1.36)$$

where D is the molecular diffusivity. χ measures the deformation and stretching of the flame: high values of this parameter lead to local extinction

(*quenching*). In operationally implementing this method, one begins by creating a **flamelet library** (solutions of chemistry at given values of mixture fraction and scalar dissipation rate, $Y_k^{lam}(Z, \chi)$) by solving simplified 1-D counterflow simulations. Subsequently, during the actual CFD calculation, only two transport equations are solved: one for the *mean mixture fraction* $\tilde{Z}$ (Favre averaged value), and a second equation for the mixture fraction variance $\tilde{Z}''^2$. Once the values allowing the definition of the statistical distribution shape are obtained from numerical integration of the transport equations, a PDF $P(Z)$ (typically a presumed Beta function) is used to integrate the mean mass fraction of the species of interest:

$$\tilde{Y}_k = \int_0^1 Y_k^{lam}(Z, \tilde{\chi}_{st}) P(Z) dZ \quad (1.37)$$

This approach decouples kinetics (used to create the flamelet library in pre-processing) from hydrodynamics (solved in CFD), making the model extremely efficient from a computational standpoint.

1.4.5 Eddy Dissipation Concept (EDC)

When the fast chemistry hypothesis of *flamelets* fails (as in the case of slow chemistry characteristic of nitrogen oxides, NO_x), a model is needed that treats chemistry and turbulence together without assuming immediate equilibrium. The *Eddy Dissipation Concept* (EDC) model (Magnussen, 1981) [16] is the advanced extension of *Eddy Break-Up* models and, unlike the flamelet model, integrates detailed chemical kinetics directly into the simulation.

The reaction is considered as a phenomenon occurring mainly within so-called “*fine structures*”, regions of turbulent dissipation typically on the order of Kolmogorov scales. The rest of the fluid (the “surrounding”) is evaluated as chemically inert. The length fraction of the *fine structures* (ξ^* , related to the volume fraction $\gamma_\lambda = (\xi^*)^3$) and the residence time (τ^*) depend on turbulent kinetic energy k and its dissipation ε (or ω):

$$\xi^* = C_\xi \left(\frac{\nu \varepsilon}{k^2} \right)^{1/4}, \quad \tau^* = C_\tau \left(\frac{\nu}{\varepsilon} \right)^{1/2} \quad (1.38)$$

where $C_\xi = 2.1377$ and $C_\tau = 0.4082$ are the model constants. The source term of the species equations is then calculated by modeling combustion as a PSR (*Perfectly Stirred Reactor*) within the *fine structures* reacting for a time τ^* . The mean reaction rate returned to the RANS solver is expressed as the mass transfer between fine structures and the surrounding environment:

$$\bar{\dot{\omega}}_k = \frac{\bar{\rho}(\xi^*)^2}{\tau^* [1 - (\xi^*)^3]} (Y_k^* - \tilde{Y}_k) \quad (1.39)$$

where Y_k^* is the concentration of species k inside the *fine structures* after reacting (integrating detailed chemical kinetics for time τ^*) and $\tilde{Y}_k$ is the mean concentration in the cell.

Since it requires numerical integration of *stiff* kinetics (often hundreds of reactions) in every cell at every iteration, EDC is very expensive (10–100 times the computational cost of flamelets), but it is indispensable when the Damköhler number is low ($Da \sim 1$), i.e., when chemical times are comparable to turbulent mixing times.

In chemical kinetics, a system is said to be stiff when processes with extremely different time scales coexist (e.g., radicals reacting in nanoseconds vs. stable species in milliseconds). This forces the numerical solver to use infinitesimal integration steps to maintain stability, drastically increasing computational cost.

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Numerical Methodology and Computational Strategies

From finite volume to HPC: analysis of the solver, discretization techniques, and computing resource management for complex CFD simulations.

ABSTRACT

After introducing the theoretical bases underpinning the mathematical models used to describe the flow of interest, it is interesting and useful to understand the functioning of the numerical solver and the particularities of the environment in which it will operate (the High Performance Computing ecosystem). This chapter serves to justify many of the choices made during the thesis activities.

2.1 Numerical Solver Theory and Discretization

The governing equations (Navier-Stokes, Energy, Species, and Turbulence) constitute a system of non-linear and strongly coupled partial differential equations (PDEs). For this type of system, no general analytical solution exists; to solve it, it is necessary to adopt a numerical strategy that approximates the continuous solution in a discrete domain [17, 18].

The calculation code used, ANSYS Fluent, is based on the **Finite Volume Method (FVM)** [19]. This algorithm approximates the value of the quantity of interest by weighing it over the cell volume, according to the formula:

$$Q_j^n = \frac{1}{V} \int_V Q dV \quad (2.1)$$

defined for the quantity Q in cell j at time step n . The computational domain is thus subdivided into a finite number of non-overlapping control volumes (cells). The differential equations are integrated over each control volume, converting the PDEs into a system of linear algebraic equations. The distinctive feature of FVM is its intrinsic conservativeness: fluxes exiting a volume are, by definition, identical to fluxes entering the adjacent volume.

2.1.1 The Pressure-Based Solver

ANSYS Fluent offers two numerical architectures for solving transport equations: the *Pressure-Based* solver and the *Density-Based* solver [19].

The *Density-Based* solver, originally developed for high-speed aerospace applications (flows where Mach number effects become relevant), uses the continuity equation to directly derive fluid density, while pressure is then obtained using the thermodynamic equation of state.

In applications where the Mach number remains contained, as in the case of internal flows in a civil aviation engine combustor, the Pressure-Based solver is preferred over the Density-Based one. This type of solver does not exploit the equation of state to relate density and pressure; rather, it dynamically modifies pressure to ensure compliance with the continuity equation. Consequently, the pressure field is calculated by solving a specific pressure correction equation, obtained by algebraically manipulating the continuity and momentum equations.

The advantage of this second approach is greater stability and the creation of a system that is decidedly less ‘stiff’ compared to that obtained with the Density-Based solver [13].

2.1.2 Pressure-Velocity Coupling: The Coupled Algorithm

The discretization of the Navier-Stokes equations on a “cell-centered” grid poses two fundamental problems:

Checkerboarding The possibility of having unphysical oscillating pressure fields that mathematically satisfy the discrete equation [18]. This issue is resolved via Rhie-Chow interpolation for the calculation of mass fluxes on cell faces [13].

P-V Coupling Velocity depends on the pressure gradient, but pressure must be such as to guarantee the continuity of the velocity field.

While segregated algorithms (SIMPLE, PISO) solve equations sequentially (decoupling pressure and velocity), the *Coupled Pressure-Based* algorithm solves the momentum equations system and the pressure-based continuity equation simultaneously.

Structure of the Linear System

For each cell in the domain, the algorithm constructs a vector of unknown variables:

$$\mathbf{Q} = \{u, v, w, p\}^T \quad (2.2)$$

The discretized system takes the form of a block matrix:

$$\sum_{nb} \begin{bmatrix} A_{uu} & A_{uv} & A_{uw} & A_{up} \\ A_{vu} & A_{vv} & A_{vw} & A_{vp} \\ A_{wu} & A_{wv} & A_{ww} & A_{wp} \\ A_{pu} & A_{pv} & A_{pw} & A_{pp} \end{bmatrix}_{nb} \begin{bmatrix} \Delta u \\ \Delta v \\ \Delta w \\ \Delta p \end{bmatrix}_{nb} = \begin{bmatrix} R_u \\ R_v \\ R_w \\ R_p \end{bmatrix} \quad (2.3)$$

Where the summation extends to all neighboring cells (nb).

- The diagonal terms (A_{uu}, A_{pp}) represent the equation's own coefficients.
- The off-diagonal terms (A_{up}, A_{pu}) represent the implicit coupling: the influence of pressure on velocity (pressure gradient) and of velocity on pressure (mass flux).

Solving this coupled system requires more RAM memory (1.5–2 times compared to segregated methods) but offers particular robustness for flows with strong body forces or adverse pressure gradients, avoiding the instabilities typical of segregated methods in the early stages of combustion [13, 19].

2.1.3 Resolution Order and Spatial Discretization

Before analyzing specific schemes, it is useful to clarify the concept of “order of accuracy” or resolution. In numerical analysis, the order of a scheme indicates how rapidly the truncation error (the difference between the exact differential equation and the discretized one) decreases as the grid is refined. A scheme of order n produces a local error proportional to Δx^n , where Δx is the cell size.

First Order Very stable but introduces strong “numerical diffusion” (or artificial viscosity) that tends to smooth out physical gradients, often making results unreliable for turbulent flows.

Higher Order (Second or Third) Drastically reduces discretization error, allowing sharper fronts and fine vortical structures to be captured. However, it requires a wider *stencil* and can introduce numerical instabilities (unphysical oscillations) that need limiter algorithms to be controlled [18].

The stencil is the set comprising the cell under consideration and its neighboring cells considered in the calculation.

Gradient Reconstruction: Least Squares Cell-Based

Many discretized terms (diffusion, second-order derivatives) require knowledge of the gradient ∇Q at the cell center. Fluent uses the Least Squares method by default. It is assumed that the variation of the variable between the cell center C_0 and neighbors C_i is linear.

The gradient ∇Q_{C_0} is the vector that minimizes the weighted sum of squared errors:

$$E = \sum_{i=1}^{N_{faces}} w_i (Q_{C_i} - (Q_{C_0} + \nabla Q_{C_0} \cdot \vec{r}_i))^2 \quad (2.4)$$

Where $\vec{r}_i$ is the distance vector between C_0 and C_i . This method is mathematically more robust than the Green–Gauss method on unstructured grids, maintaining second-order accuracy even in the presence of cells with high skewness.

Convective Scheme: Second Order Upwind with Limiters

To calculate the value of a scalar variable Q_f on a cell face, the *Upwind* scheme is used. Writing it at the first order, this results in:

$$Q_f = Q_{C_0} \quad (2.5)$$

The scheme thus outlined is stable and monotonous but introduces a first-order truncation error ($O(\Delta x)$) that acts as excessive numerical diffusivity [17, 18]. To derive the second-order scheme, a truncated Taylor series expansion is used:

$$Q_f = Q_{C_0} + \Psi \cdot (\nabla Q_{C_0} \cdot \vec{r}_f) \quad (2.6)$$

Where Ψ is a gradient limiter (such as Barth–Jespersen). The function of the limiter ($0 \leq \Psi \leq 1$) is to prevent the creation of new local maxima or minima (*overshoots/undershoots*) in zones of strong gradients (such as flame fronts). The use of the second order is strongly recommended and almost mandatory in combustion to avoid underestimating temperature peaks [13, 18].

Notes on Higher-Order Schemes (MUSCL)

For complex flows, Fluent also offers the possibility of using the third-order MUSCL (*Monotone Upstream-Centered Schemes for Conservation Laws*) scheme. This scheme calculates the face value by combining a central interpolation (second order) with a second-order upwind scheme [13]. Although theoretically offering superior spatial resolution by further reducing numerical diffusion for vortical flows on arbitrary grids, the accuracy increase compared to *Second Order Upwind* is often marginal against a potential increase in numerical instability (greater risk of unphysical overshoots).

Pressure Interpolation: The PRESTO! Scheme

Particular attention must be paid to pressure discretization on cell faces. Fluent's Standard scheme calculates pressure on the face by interpolating momentum equation coefficients. This approach works well as long as the

pressure gradient effectively balances convective terms. However, in flows with strong *swirl* (as in the combustor under examination), strong radial pressure gradients and significant centrifugal forces exist near the center of the recirculation zone. In these conditions, the equilibrium hypothesis of the Standard scheme fails, leading to erroneous or unstable pressure fields. For this thesis, the PRESTO! (*PREssure STaggering Option*) scheme was therefore adopted [13]. This algorithm uses a technique similar to staggered grids to calculate pressure directly on the face, guaranteeing the stability and physical conservation necessary to correctly capture the complex fluid dynamics induced by the *swirler*.

2.2 Implementation of Boundary Conditions

Boundary conditions close the mathematical system. The specific types that will be used are:

Velocity Inlet Used to impose the inlet vector velocity; static pressure is not fixed, but its gradient is blocked on the inlet surface. This allows pressure to adapt to the internal field.

Pressure Outlet Static pressure p_{out} is fixed. Outlet scalar variables are extrapolated from the interior exploiting the zero-gradient condition.

Periodic Boundary (Rotational) Condition used to simulate a single angular sector. The software creates a virtual node-to-node correspondence between periodic faces:

$$Q(r, \theta, z) = Q(r, \theta + \Delta\theta, z) \quad (2.7)$$

For vectors (e.g., velocity), the software applies a rotation matrix $R_z(\Delta\theta)$ to values calculated on the *shadow* face before imposing equality with the *master* face. This strictly conserves angular momentum.

2.2.1 Stability Control: Pseudo-Transient Method

In steady simulations, the temporal term $\partial/\partial t$ is physically eliminated. However, to stabilize the iterative process, Fluent reintroduces a fictitious temporal evolution term, known as *Pseudo-Transient Under-Relaxation*. The algebraic equation for cell P assumes the form:

$$\left(\frac{\rho \Delta V}{\Delta t_{\text{pseudo}}} + A_{PP} \right) \Delta Q_P + \sum_{nb} A_{nb} \Delta Q_{nb} = R_\phi \quad (2.8)$$

The term $\rho \Delta V / \Delta t_{\text{pseudo}}$ acts as an additional diagonal term that “brakes” the variation of the solution $\Delta\phi$, increasing stability. The pseudo-physical time step is calculated locally in each cell as a function of a user-defined Courant Number (CFL):

$$\Delta t_{\text{pseudo}} = \frac{\text{CFL} \cdot \Delta V}{\lambda_{\max}} \quad (2.9)$$

where $\lambda_{\max}$ is the local characteristic velocity (sum of convective velocity and speed of sound). A low CFL (< 10) makes the system diagonally dominant

and stable, which is useful in initial phases; conversely, a high CFL (50–200) accelerates convergence when the flow is stabilized. These CFL values are reported not only for explanatory purposes but also to reflect on the difference of this parameter compared to the effective CFL. Furthermore, for each equation, specific time-step scaling coefficients (less than one) are used to prevent local instabilities, chemical or otherwise, from destabilizing the global flow field [19].

2.2.2 Convergence Criteria and Calculation

Convergence evaluation is based on Residual analysis [19]. The residual R^ϕ for a variable ϕ in a cell P is defined as the imbalance of the discretized equation:

$$R_P^\phi = \left| \sum_{nb} A_{nb} \phi_{nb} + b - A_P \phi_P \right| \quad (2.10)$$

Where A_{nb} are the matrix coefficients, b the source term, and ϕ the values of the quantity considered at the current iteration. Ideally, at convergence, R_P^ϕ should be zero; however, with finite-precision arithmetic, this is impossible, so the global sum of residuals is monitored to evaluate solution progress. The absolute value of the residual depends on the physical quantity (e.g., pressure in Pascal vs. energy in Joule). To make them comparable, Fluent calculates scaled residuals:

$$R_{\text{scaled}}^\phi = \frac{\sum_{\text{cells}} R_P^\phi}{F_{\text{norm}}} \quad (2.11)$$

Where the normalization factor F_{norm} varies depending on the equation: for momentum, species, and energy equations, the factor considered is given by the sum of fluxes (of the respective quantity) over the computational domain; for the continuity equation, the value of F_{norm} is given by the maximum absolute residual observed in the first 5 iterations performed.

Since low residuals do not guarantee the absence of macroscopic physical oscillations, and given that the *flamelet* method (to be seen later) is difficult to converge according to criteria used by Fluent, the definitive convergence of the calculation to be performed is decreed via *Surface Monitors*. Therefore, surface integrals at the combustor outlet are defined:

$$Q_{\text{out}} = \frac{\int Q \rho \vec{u} \cdot d\vec{A}}{\int \rho \vec{u} \cdot d\vec{A}} \quad (2.12)$$

The solution is considered ‘converged’ when the percentage variation of these monitored parameters, over a moving window of N iterations (a parameter set by the user), falls below a pre-set relative tolerance threshold, indicating the achievement of a stable steady state.

2.3 Computational Grid Generation

The generation of the calculation grid (*mesh*) is not merely a geometric operation of domain subdivision, but represents the first step of the numerical discretization process. Grid quality directly influences solution accuracy: discretization error scales as a power of the characteristic cell dimension,

with the exponent depending on the order of the scheme used. Moreover, the grid typology also influences solver stability; low-quality cells induce errors in gradient calculation, which can lead to high residuals or even calculation divergence. Last but not least is the computational cost factor: a higher number of cells (which is not necessarily synonymous with better overall grid quality) causes a corresponding increase in both calculation time per single iteration and required RAM memory [18].

2.3.1 Theoretical Fundamentals: Element Topology

Ideally, to minimize numerical error, cell faces should be aligned with the flow direction and orthogonal to variable gradients. Several volumetric element topologies exist:

- **Hexahedra (Hex):** These are the “perfect” element for numerical efficiency. They possess maximum orthogonality (faces perpendicular to each other) and fill the volume with the lowest possible number of elements. However, generating a purely hexahedral grid on complex geometries is an extremely onerous operation and requires much time to complete [18].
- **Tetrahedra (Tet):** These are extremely flexible and can adapt to any geometry automatically. However, for the same volume, they require many more cells than hexahedra and suffer from greater numerical diffusion (flow is almost never aligned with triangular faces).
- **Polyhedra (Poly):** These represent the state of the art for modern FVM solvers. A polyhedral cell has many neighbors (typically 10–20, versus 4 for tetrahedra) [13, 19].

According to the Green-Gauss theorem or Least Squares, having more neighbors allows for a much more accurate reconstruction of the solution gradient at the cell center. Furthermore, polyhedra are less sensitive to *stretching* (elongation) compared to tetrahedra.

2.3.2 Ansys Fluent Meshing: Watertight Geometry Workflow

For this work, the Ansys Fluent Meshing *Watertight Geometry* workflow was used [19]. Unlike traditional methods that required manual surface cleaning to close holes or correct intersections, this automated workflow handles raw geometries by wrapping them in a continuous surface mesh based on local sizing logic. The fundamental steps of the workflow are:

1. **Local Sizing:** Definition of “Bodies of Influence” (BOI) to refine the grid in critical zones (flame zone, swirler wake) independently of CAD geometry.
2. **Surface Mesh:** Generation of a high-quality triangular surface tessellation.
3. **Boundary Condition Definition:** Starting from the specification of periodic walls up to a first definition of the BC type assigned to each wall.

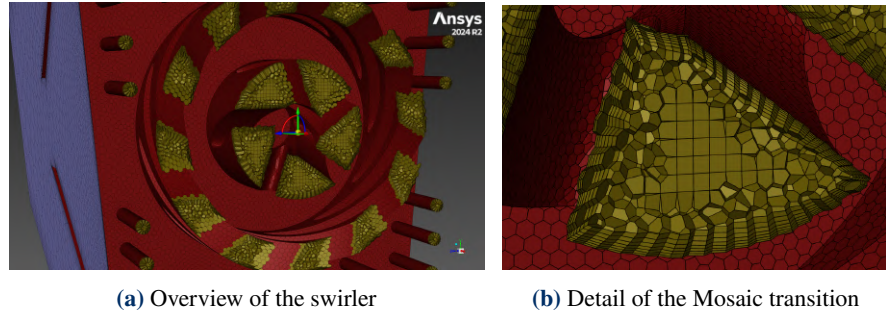
4. **Boundary Layer (Inflation):** Generation of prism layers aligned to the wall to resolve viscous gradients.
5. **Volume Mesh:** Filling the fluid volume.

Poly-Hexcore Technology (Mosaic)

The grid topology chosen for this thesis is **Poly-Hexcore**. This hybrid technology structures the grid into three zones:

1. **Boundary Layer (Inflation):** Prismatic/polyhedral cells to resolve viscous wall gradients.
2. **Bulk Region (Core):** The heart of the domain is filled with Cartesian hexahedral cells (octree cubes). This maximizes orthogonality and reduces the number of cells (1 hexahedron replaces ≈ 5 tetrahedra).
3. **Mosaic Transition:** A special layer of polyhedra that conformally connects (node-on-node) the core hexahedra to the wall prisms, avoiding non-conformal interfaces.

Importance of y^+ : The SST $k-\omega$ turbulence model is a Low-Reynolds model. To correctly resolve the viscous sublayer and capture wall shear stresses and heat flux, the first grid prism must be located at $y^+ \approx 1$. Values of $y^+ > 30$ would activate Wall Functions, reducing accuracy in thermal load prediction.



(a) Overview of the swirler

(b) Detail of the Mosaic transition

Figure 2.1: Cross-section of the calculation grid. On the left (a), the overview highlighting Mosaic technology with the hexahedral core (yellow) and the polyhedral transition (red). On the right (b), a magnified detail of the conformal interface between different element types.

2.3.3 Grid Quality Metrics

In a Finite Volume solver like Fluent, the geometric quality of the cell is defined by its capacity to correctly approximate diffusive and convective fluxes without introducing errors. The metrics monitored are [13]:

1. Orthogonal Quality (OQ)

This is the most critical metric. For each face f , it is defined based on the alignment between:

- the area vector normal to the face $\vec{A}_f$,
- the vector connecting the centers of adjacent cells $\vec{r}_{ij}$,
- the vector from the cell center to the face center $\vec{c}_f$.

The formula is defined as:

$$OQ = \min \left(\frac{\vec{A}_f \cdot \vec{r}_{ij}}{|\vec{A}_f| |\vec{r}_{ij}|}, \frac{\vec{A}_f \cdot \vec{c}_f}{|\vec{A}_f| |\vec{c}_f|} \right) \quad (2.13)$$

The value varies between 0 (worst) and 1 (perfect). If $OQ \approx 0$, the diffusive term (which depends on $\partial\phi/\partial n$) cannot be calculated correctly. For hydrogen combustion simulations, Ansys recommends not dropping below 0.1 for OQ [20].

2. Skewness

Measures how much the cell shape deviates from an ideal cell (equilateral/equiangular):

$$\text{Skewness} = \frac{\text{Optimal Cell Size} - \text{Cell Size}}{\text{Optimal Cell Size}} \quad (2.14)$$

High values indicate excessive distortion:

- > 0.85 for hexahedra,
- > 0.9 for polyhedra.

Cells with high skewness can drastically slow down convergence.

3. Aspect Ratio

This is the ratio between the maximum and minimum dimensions of the cell. In the boundary layer, high *aspect ratio* values (> 50) are acceptable if elongation is aligned with flow direction. Conversely, in the mesh core zone, an attempt is made to keep a controlled *aspect ratio* value (< 20) to avoid excessive numerical dissipation.

2.4 HPC (High Performance Computing) Architecture

CFD simulations of aeronautical combustors require solving systems with tens of millions of degrees of freedom (fine *meshes*, multiple chemical species, adequate chemistry-turbulence interaction models). Such requirements exceed the capabilities of a single *workstation*, necessitating the use of High Performance Computing (HPC) resources. An HPC cluster is not a single monolithic “supercomputer”, but a distributed system composed of hundreds or thousands of independent calculation units, called nodes, interconnected by a high-speed network [21]. The typical architecture (such as the one in use at Politecnico di Torino) is structured in levels:

Login Nodes These are access points for the user. Here data is prepared, codes are compiled, and jobs are submitted. They are never used for intensive calculation.

Compute Nodes These are the system nodes with which calculations are performed. Each node is a server containing:

- **Multi-Core CPU:** x86 architectures usually configured in *dual-socket*, offering from 24 to 128 physical *cores* per node; for the Legion cluster at Politecnico di Torino, depending on the partition chosen, from 32 to 48.
- **RAM Memory:** A critical and finite resource. Nodes are classified based on available memory. In the case of Politecnico di Torino, a standard RAM quantity is assigned per node (1 GB/core equivalent or similar per node policy), but it is possible to request up to specific high-memory configurations. In an HPC system, memory is not virtualizable (no *swap*): exceeding the physical limit entails immediate process termination (*OOM Kill*) to avoid node lockup.
- **Interconnection (InfiniBand):** Unlike a standard Ethernet network (high latency), nodes communicate via ultra-low latency protocols (e.g., InfiniBand HDR/NDR). This is vital for parallel CFD, where *cores* must continuously exchange partition boundary data.

Access to computing resources is not interactive but mediated by a scheduler (Slurm). The user defines a *Job Script* specifying the calculation partition, a queue of nodes with homogeneous characteristics, and parallelism, i.e., the number of MPI *tasks* (processes) required.

2.4.1 Memory Management and Computational Requirement Estimation

RAM (*Random Access Memory*) management represents the main operational constraint in high-performance CFD simulations on cluster architectures. Unlike computation time, which is a relatively elastic resource, memory is a rigid resource: exceeding the allocated physical capacity on the node leads to the immediate intervention of the operating system (*OOM Killer*) and irreversible process termination, regardless of whether it happens after twelve hours of actual work preceded by fifteen hours of waiting in the queue.

Understanding how ANSYS Fluent allocates memory is therefore indispensable for correctly sizing the ‘job submission’. Allocation is not static but results from the sum of three non-linear contributions: the basic data structure (heaviness of the *mesh*), solution variables (physical models, how many equations they entail), and parallelization *overhead* (depending on the number of *cores* provided to Fluent to execute the simulation).

Fluent’s parallel solver, based on the MPI standard [21], does not share memory between processes but distributes the load by subdividing the computational grid into N partitions, where N corresponds to the number of physical *cores* required. Each process loads cells belonging to its own partition (*Local Cells*) into memory. However, numerical integration of fluxes on boundary faces requires access to data from adjacent cells managed by neighboring processors. To minimize communication latency, Fluent duplicates these boundary cells in the local memory of each process. These duplicated cells, called *Halo Cells* (or *Ghost Cells*), occupy physical memory despite not contributing to the resolved degrees of freedom [13, 19].

The impact of *Halo Cells* on total RAM is not constant but grows with the degree of parallelism. Since the surface/volume ratio of a partition increases as its size decreases, increasing the number of *cores* leads to domain fragmentation that increases the percentage of ghost cells relative to real cells. This phenomenon is particularly critical with the *Pressure-Based Coupled* algorithm. Unlike segregated solvers, which store single scalars, the *Coupled* solver maintains a coupled dense block matrix for each cell (including *Halo Cells*). Therefore, duplicating a cell in *Coupled* mode is energetically much more expensive in terms of RAM compared to *Segregated* mode.

To prevent *job* failures, it is possible to estimate the necessary peak memory M_{req} through a semi-empirical relationship considering grid size, physical complexity, and parallelization factor. To approximately size the required RAM requirement, the following conservative formulation is proposed based on user guide indications [19]:

$$M_{req} \approx N_{cells} (C_{base} + C_{chem} N_{eq}) \left(1 + \alpha N_{core}^{1/3}\right) f_{safe} \quad (2.15)$$

Where:

- N_{cells} is the total number of mesh cells (in millions).
- C_{base} is the base memory cost per cell in *Double Precision* with *Coupled* solver. A prudential reference value is 2.5 GB–3.0 GB per million cells.
- C_{chem} is the additional cost for each transported chemical species (about 0.1 GB per million cells per species).
- N_{eq} is the number of equations that are part of the system.
- $\left(1 + \alpha N_{core}^{1/3}\right)$ represents the inflation factor due to parallelism (MPI overhead). The coefficient α can be estimated as 0.2 – 0.3.
- f_{safe} is the safety margin to consider eventual usage peaks, such as writing simulation results to file; a value of 1.4 – 1.5 is adequate for a conservative estimate.

This formula highlights how the addition of chemical species and the increase in calculation *mesh* size act predominantly on the amount of RAM required; conversely, increasing parallelization *cores* generates a less consistent increase.

2.4.2 Scalability and Parallel Efficiency Limits

Using an HPC cluster does not automatically guarantee a linear reduction in calculation times as resources increase. The performance of a parallel CFD code is governed by the scalability law, evaluated through two fundamental metrics: *Speedup* (S) and Parallel Efficiency (η).

Defining T_1 as the computation time on a single *core* (serial) and T_N as the

computation time on N cores, *speedup* is defined as:

$$S_N = \frac{T_1}{T_N} \quad (2.16)$$

In an ideal scenario (*Linear Scaling*), doubling the *cores* would halve the time, leading to $S_N = N$. In reality, this asymptotic limit is never reachable. Parallel efficiency measures the deviation from ideality [21]:

$$\eta_N = \frac{S_N}{N} \times 100\% \quad (2.17)$$

Efficiency degradation ($\eta_N < 100\%$) is caused by communication *overhead*. Each solver iteration consists of two phases: the computational phase, which involves solving equations on the partition's internal cells; the time required in this phase scales linearly with the number of local cells:

$$t_{\text{comp}} \propto \frac{N_{\text{cells}}}{N_{\text{core}}}$$

And the communication phase, in which the exchange of updated values on boundary cells between adjacent processors takes place via the MPI network.

As the number of *cores* N increases, for a fixed grid size, the local partition size decreases. Consequently, the time spent on useful calculation (t_{comp}) reduces, but the ratio between interface surface and partition volume increases. A critical point is defined, called the **saturation point**, where the time necessary to exchange data across the network (latency and bandwidth) becomes comparable to or greater than the time gained by parallelizing the calculation. Beyond this limit, adding further *cores* produces no benefits or, alternatively, the simulation could even slow down, wasting computational resources [21].

Efficiency Criterion for ANSYS Fluent

For the *Pressure-Based Coupled* solver, which requires intensive data exchanges for the coupled matrix and the AMG (*Algebraic Multigrid*) algorithm, parallel efficiency collapses rapidly if partitions become too small. HPC *best practices* identify an optimal workload to maintain efficiency $\eta > 80\%$:

- **Recommended Minimum Limit:** 100 000 cells per *core* [19].
- **Inefficiency Threshold:** < 50 000 cells per *core*.

Therefore, for a *mesh* of 7.4 M cells, the largest dimension *mesh* among those used in this work, the theoretical maximum efficient parallelism stands around:

$$\frac{7.4 \times 10^6}{100\,000} \approx 74 \text{ cores} \quad (2.18)$$

Pushing beyond (e.g., 96 or 128 *cores*) would lead to inefficient use of the architecture, where *cores* spend most of the time idle, waiting for MPI synchronization rather than calculating the physical solution.

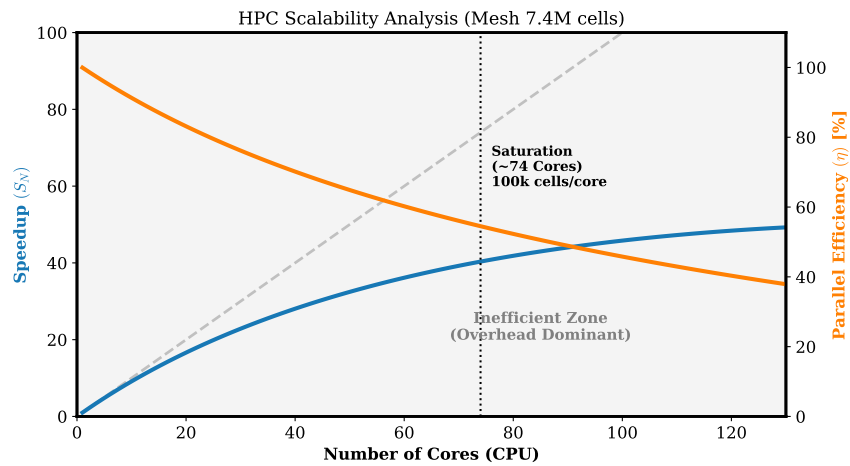


Figure 2.2: Theoretical analysis of parallel scalability (Amdahl's Law extended to communication costs). Curves were analytically calibrated considering the efficiency constraints of the Coupled solver (critical threshold at 100,000 cells/core) applied to the 7.4 million cell calculation mesh used, identifying the saturation point around 74 cores.

The phenomenon of parallel efficiency saturation is theoretically described by Amdahl's Law. This establishes that the maximum obtainable speedup (S_{max}) is limited by the fraction of code that must necessarily be executed serially, regardless of the number of processors used. In practical terms: even if only 5% ($f = 0.05$) of the simulation process is serial (e.g., node-to-node communication time), the maximum speedup can never exceed a value of 20 ($1/0.05$), even using an infinite number of processors. This explains why, beyond a certain threshold, adding hardware resources brings no tangible benefits.

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Model Validation

Analysis of the Sandia H2 Test Case

ABSTRACT

This chapter presents the validation of the numerical model through the reproduction of the "Sandia H2/He Flame" test case. The accuracy of different turbulence models ($k - \varepsilon$ vs $k - \omega$) and chemistry interaction models (Flamelet vs EDC) in predicting temperature, major species, and pollutants (NO_x) is analyzed. The results justify the choice of the hybrid *Flamelet + Decoupled Detailed Chemistry* strategy for the subsequent combustor design simulations.

3.1 The Test Case: Sandia H2 Turbulent Jet Flame

For validation purposes, it was chosen to numerically reproduce the turbulent hydrogen jet flame studied by Barlow and Carter at Sandia National Laboratories [22].

This experiment is considered a "canonical" standard for the great amount of data recorded.

This experiment represents a standard in the scientific community, providing a detailed dataset essential for isolating mixing and chemical kinetic phenomena from geometric complexities.

Although the experimental database also includes cases with hydrogen and helium mixtures to study differential diffusion, this thesis focused exclusively on the pure hydrogen case (**Sandia Flame D**), consistent with the fuel used in the combustor design project detailed in subsequent chapters [23].

3.1.1 Experimental Setup and Measurement Techniques

The experimental setup consists of a straight tube burner with an internal diameter $d = 3.75$ mm (outer diameter 4.84 mm), centered at the exit of a vertical square-section wind tunnel (30×30 cm).

The hydrogen jet is injected with an exit velocity of 296 m/s, corresponding to a Reynolds number $Re \approx 22800$, into a laminar air co-flow at ambient temperature (294 K) with a velocity of 1.0 m/s [23]. These conditions define a fully turbulent regime dominated by shear layers.

Advanced Laser Diagnostics

A crucial aspect that makes this test case unique is the combined and simultaneous use of three diagnostic techniques [24]:

- **Rayleigh Scattering:** For density and temperature measurement.
- **Raman Scattering (Spontaneous):** For the simultaneous measurement of major species concentrations (H_2 , O_2 , N_2 , H_2O).
- **LIF (Laser Induced Fluorescence):** Specific for the detection of low-concentration radicals such as OH (flame front marker) and pollutants like NO.

This combination allows obtaining not only mean values but also instantaneous correlations between temperature and composition.

3.2 Thermal Radiation Modeling (P-1 Model)

Neglecting radiation would lead to overestimating local T by as much as 100-200 K, falsifying the prediction of thermal NO_x .

In hydrogen flames, peak temperatures can exceed 2400 K. At such temperatures, heat transfer by radiation plays a fundamental role in the energy balance.

Although the hydrogen flame is non-luminous (devoid of particulate matter or soot), water vapor molecules (H_2O) produced by combustion emit and absorb significantly in the infrared spectrum.

Neglecting radiation in this context would lead to an overestimation of the

local flame temperature and, consequently, a gross error in the prediction of thermal NO_x , whose formation depends exponentially on temperature [25].

3.2.1 Fundamentals of the P-1 Model

To model this phenomenon without incurring the prohibitive costs of Ray Tracing, the P-1 model was adopted. The P-1 model is an approximation of the Spherical Harmonics (P-N) method, which allows simplifying the Radiative Transfer Equation (RTE) by transforming it into a simpler diffusion-type partial differential equation. The basic assumption is that radiation intensity varies in a "quasi-isotropic" manner in space, allowing the radiative intensity to be expanded into a series of spherical harmonics truncated at the first term ($N = 1$).

The equation solved for the incident irradiance G is:

$$\nabla \cdot \Gamma \nabla G - aG + 4a\sigma T^4 = S_G \quad (3.1)$$

Where a is the absorption coefficient of the medium (a function of H_2O concentration) and Γ is the radiative diffusion parameter.

3.2.2 Role of Radiation in Validation

The use of the P-1 model is strictly necessary in this validation phase to replicate the conditions of the Sandia experiment. In the laboratory, the flame is free (unconfined): the walls are distant and transparent, allowing the flame to radiate heat towards the cold environment without receiving it back (net energy loss).

Conversely, in the real combustor designed in subsequent chapters, the flame will be confined by reflective metal walls. For design simulations, a conservative adiabatic hypothesis will be adopted to contain calculation times, but ignoring radiative losses during validation would invalidate the comparison with experimental data.

3.3 Simulation Strategy and Model Matrix

The validation strategy was based on a systematic comparison between different combinations of models. All simulations involving detailed kinetics treatment refer to a specific reaction mechanism for hydrogen composed of **31 chemical species** and related elementary reactions.

3.3.1 Turbulence Models

Correct prediction of the flow field is a fundamental prerequisite. Two RANS models were tested [25, 14]:

- **Standard $k - \varepsilon$:** Used as a historical baseline to quantify the improvement obtained by moving to more complex models.
- **$k - \omega$ SST:** The industrial standard, combining wall robustness and free-stream accuracy. It is used to verify the ability to predict jet spreading.

3.3.2 Turbulence-Chemistry Interaction (TCI) Models

For flame modeling, two distinct approaches were compared:

- **Steady Laminar Flamelet (SFM) - Detailed Chemistry:** Laminar flamelets are pre-integrated using the full 31-species mechanism. It assumes that NO_x chemistry is also fast and parameterizable only via mixture fraction (Z) and scalar dissipation (χ).
- **Eddy Dissipation Concept (EDC) - Constant Coefficients:** The 31-species mechanism is solved directly in the CFD solver by integrating kinetics in turbulent *fine structures*. It is the most onerous approach but allows capturing non-equilibrium *finite-rate chemistry* phenomena.

3.3.3 Computational Domain and Numerical Setup

To ensure high fidelity in resolving spatial gradients, the fluid domain was discretized using a **2D axisymmetric structured grid** composed of approximately **1 million elements**.

The mesh presents targeted refinement in critical zones: near the walls, to correctly resolve the boundary layer, and along the flame axis, where maximum temperature and chemical composition gradients are concentrated.

Regarding grid independence of the solution, a preliminary convergence analysis was conducted on a simplified case at the beginning of the research activity. Results showed the achievement of asymptotic convergence already with a number of elements equal to approximately half of those employed for the final simulations (500k elements). It was therefore decided to maintain the 1 million cell grid for the validation simulations presented here, adopting a conservative approach to minimize spatial discretization error.

The solver configuration included the use of the following numerical schemes:

- **Pressure-Velocity Coupling:** PRESTO! scheme, particularly indicated for flows with strong curvature or swirl.
- **Turbulence Equations:** *Second Order Upwind* scheme.
- **Scalar Quantities:** *Third Order MUSCL* scheme, to maximize accuracy in capturing flame fronts.

3.4 Comparative Analysis of Results

The analysis of results is based on the comparison between experimental data and numerical simulations for five physical quantities: static temperature, mole fraction of molecular hydrogen (H_2), hydroxyl radical (OH), water (H_2O), and nitrogen monoxide (NO).

These quantities were evaluated along the flame axis and on radial distributions at characteristic distances: $x/L_{vis} = 0.25, 0.5$, and 1.0 (where $L_{vis} = 0.675$ m is the visible flame length [23]).

Preliminary grid-independence tests showed convergence as early as 500k cells. 1M was chosen for conservatism.

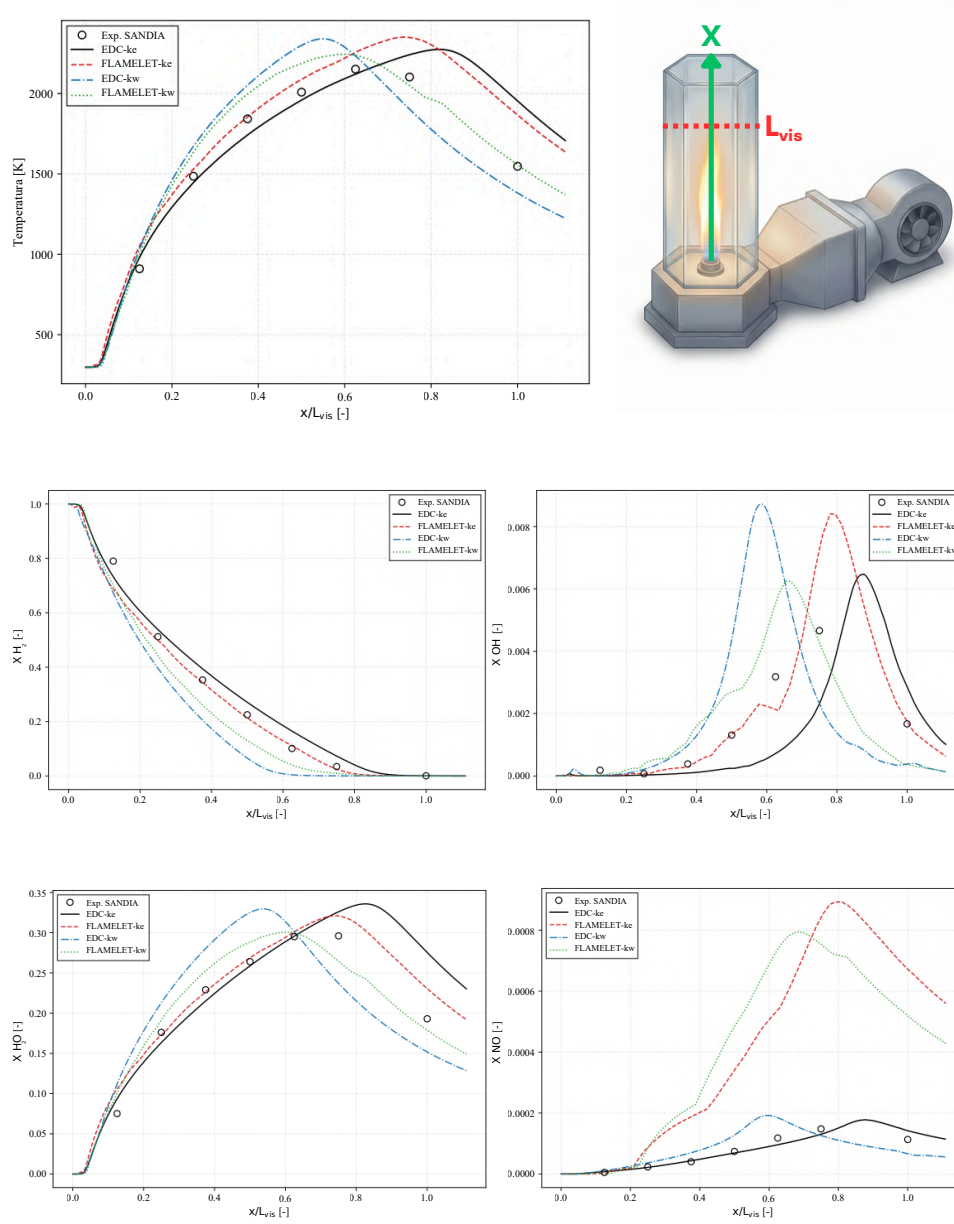


Figure 3.1: Axial profiles of Temperature and Mole Fractions (H_2 , OH, H_2O , NO). Comparison between Sandia experimental data and numerical models.

3.4.1 Axial Distribution

Observing the distributions along the axis (fig. 3.1), it is noted that, in general, all methods tend to overestimate peak temperatures. Flamelet models show greater adherence to experimental data in the first half of the flame, especially if coupled with the $k - \varepsilon$ turbulence model.

In the second half ($x/L_{vis} > 0.6$), the $k - \omega$ model appears to better follow the thermal decay. Similar considerations apply to water and hydrogen mole fractions, where the Flamelet + $k - \varepsilon$ approach guarantees the best accuracy.

Discrepancies become marked for minor species. For the hydroxyl radical (OH), no model perfectly replicates the axial profile, although Flamelet methods better capture its order of magnitude. The most critical result concerns nitrogen monoxide (NO): a **significant overestimation** is observed by Flamelet methods, which predict unrealistically high pollutant levels. Conversely, EDC (*Eddy Dissipation Concept*) models provide an estimate much closer to experimental data, with an advantage for the EDC + $k - \varepsilon$ coupling.

3.4.2 Radial Distributions

Analyzing the radial sections, further details on the flame structure emerge.

At $x = 0.25L_{vis}$ (fig. 3.2): Excellent congruence of Flamelet models with experimental data is noted for temperature and major species (H_2 , H_2O). EDC models struggle to predict radical (OH) concentration in this proximal zone. However, for NO, Flamelets massively overestimate production, while EDC is precise.

At $x = 0.5L_{vis}$ (fig. 3.3): The trend is confirmed. The Flamelet + $k - \varepsilon$ case is superior for thermodynamics and fast species. For pollutants (NO), EDC models contend for greater accuracy, likely thanks to better management of slow formation kinetics (thermal Zeldovich) which is not at equilibrium.

At $x = 1.0L_{vis}$ (fig. 3.4): In the distal zone ("flame tail"), the situation partially reverses. EDC models result more accurate for temperature and H_2O . Residual hydrogen, by now almost entirely oxidized, is not adequately modeled by any of the analyzed cases, suggesting difficulties in predicting fine mixing in the final recirculation zones.

3.5 Selected Strategy: Decoupled Detailed Chemistry

From the analysis, a clear *trade-off* emerges:

- The **Flamelet** model excels in modeling temperature and fast chemistry species (H_2 , OH, H_2O), but fails in predicting slow pollutants (NO).
- The **EDC** model is superior for pollutants, but computationally very onerous and sometimes less precise on the main thermal field in initial zones.

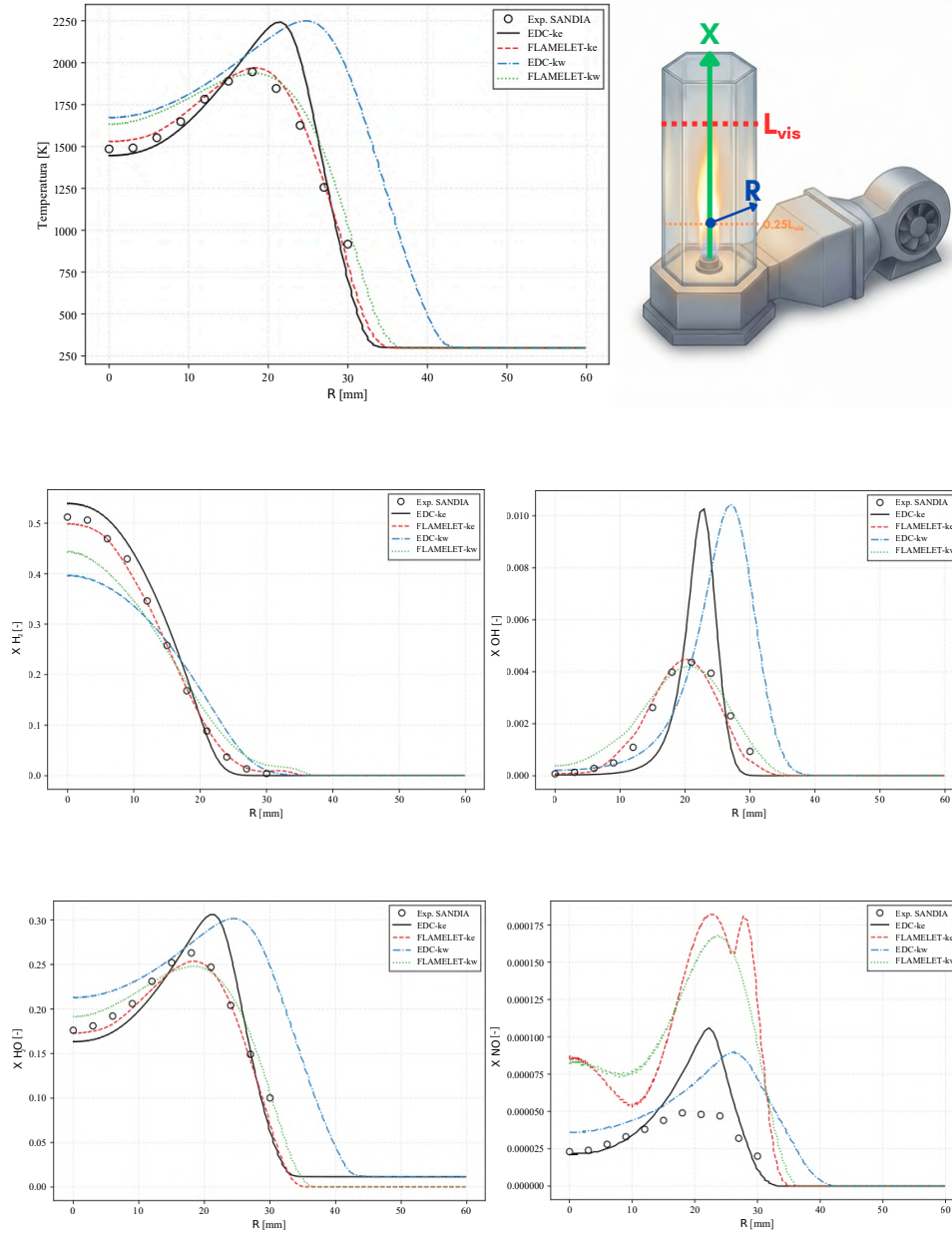


Figure 3.2: Radial profiles at $x/L_{vis} = 0.25$ (Proximal zone).

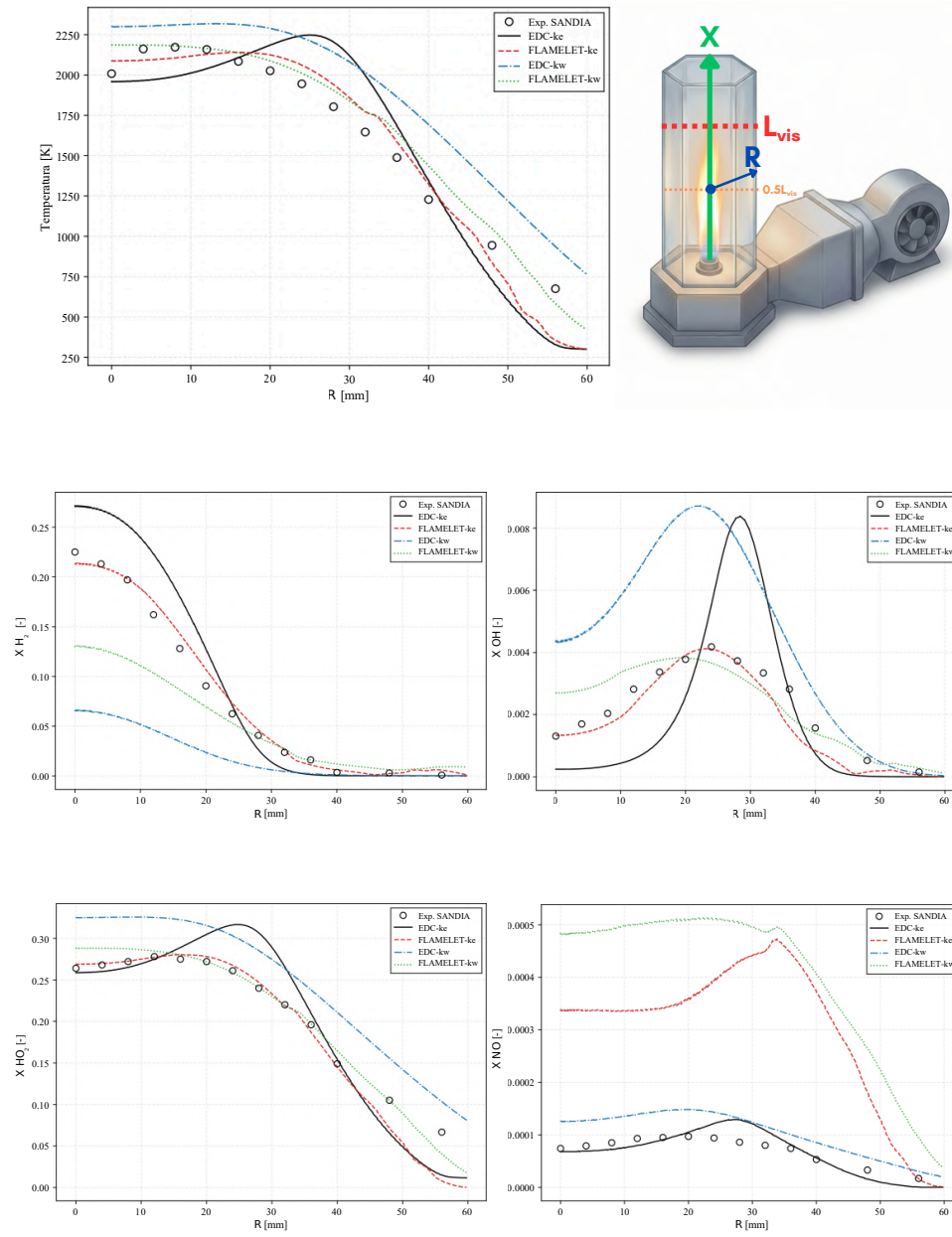


Figure 3.3: Radial profiles at $x/L_{vis} = 0.50$ (Intermediate zone).

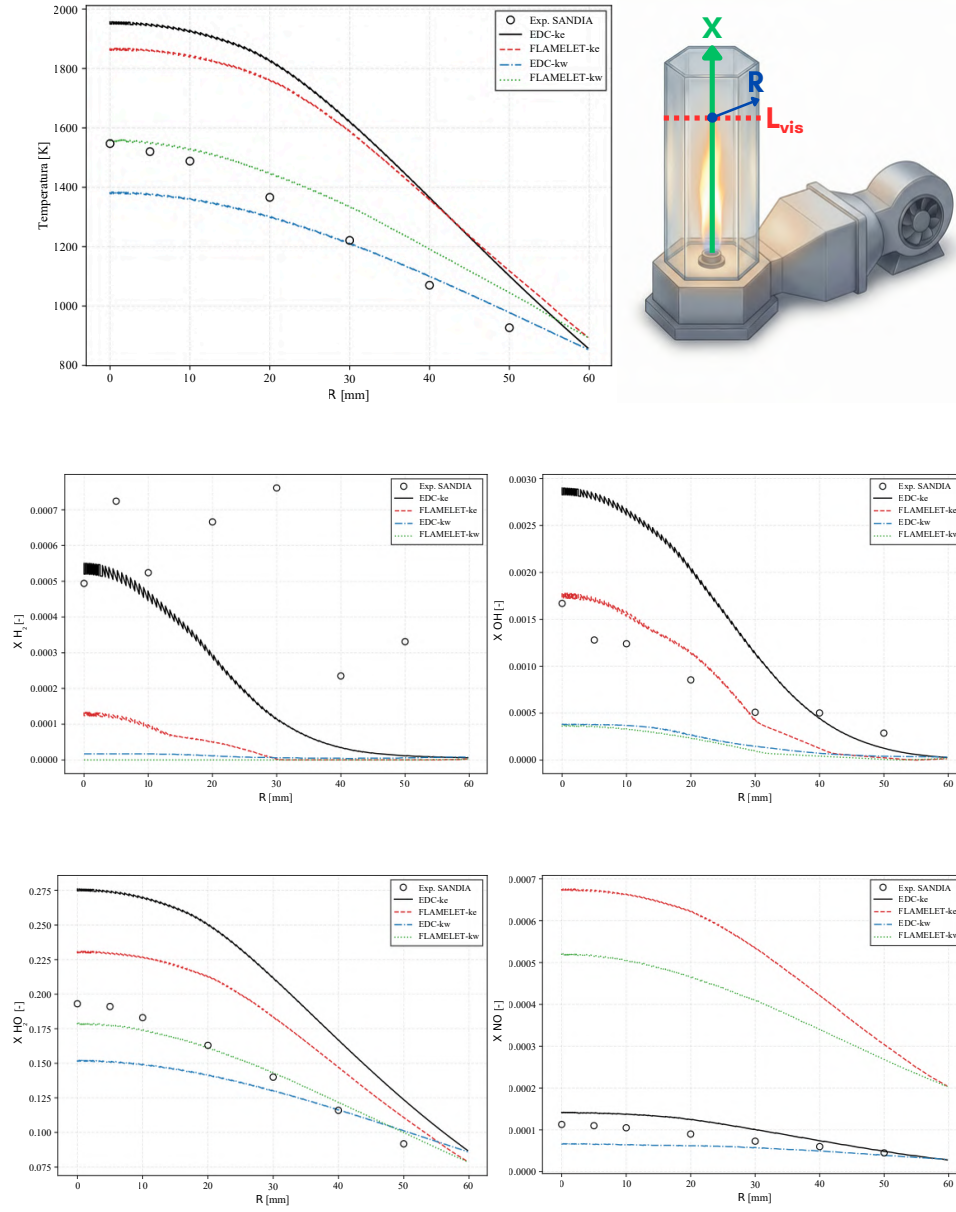


Figure 3.4: Radial profiles at $x/L_{vis} = 1.0$ (Flame tail).

To combine the advantages of both approaches in the real combustor design, it was decided to adopt a hybrid strategy based on the **Decoupled Detailed Chemistry (DDC)** method. The operational methodology will be as follows:

1. **Flow Field and Main Reaction Solution:** The Flamelet model with a simplified chemical mechanism (excluding nitrogen chemistry) will be used to efficiently calculate the temperature field and major species.
2. **Pollutant Calculation:** Subsequently, on this "frozen" flow field, transport equations for pollutants (NO_x) will be solved using the detailed 31-species mechanism.

This approach is justified by the fact that NO_x concentrations are very low and do not significantly influence the temperature field (low reverse coupling), and by the very small Damköhler number ($Da \ll 1$) for pollutant reactions.

Regarding turbulence in the real combustor, the $k - \omega$ **WJ-BSL-EARSM** model will be opted for [14]. Although $k - \varepsilon$ showed good performance in the Sandia validation, the real combustor will be dominated by strong swirl motions and confinement, where linear models fail.

3.6 Limitations of the Validation Approach

It is finally necessary to discuss the limitations of this process. The designed aeronautical combustor will operate under thermodynamic conditions different from the Sandia test case (high pressure and $T_{in} > 700$ K vs. atmospheric pressure and ambient T_{in} [9]).

This discrepancy introduces uncertainties, as chemical kinetics scales non-linearly with pressure. However, in the absence of public experimental data for hydrogen combustors at specific cycle conditions, validation on the Sandia case guarantees that the numerical model is at least capable of reproducing the fundamental physics of turbulence-chemistry interaction, offering a solid basis for subsequent comparative optimization.

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Combustor Design and Sizing

0D/1D design methodology and parametric model generation: from cycle requirements to the definition of the annular geometry.

ABSTRACT

This chapter describes the design methodology adopted for the definition of the hydrogen-fueled annular combustion chamber under study. The design process follows a hierarchical approach: starting from the thermodynamic boundary conditions defined by the engine cycle, a preliminary 0D/1D sizing was performed based on classic semi-empirical correlations, followed by the generation of a fully automated 3D parametric geometric model, suitable for integration into the optimization loop described in the next chapter.

4.1 Design Requirements and Operating Conditions

The combustor design point was selected in accordance with the cruise conditions of a future generation medium-to-long-range civil aircraft. Specifically, reference was made to the work of Folcarelli et al. [9], considering the turbofan propulsive configuration that provides for *Regenerative Fuel Heating*.

In this configuration, hydrogen is used as a *heat-sink* to cool bleed air or other hot components before being injected into the chamber, recovering heat and increasing the cycle's thermal efficiency. The operating conditions at the combustor inlet and the required outlet targets, used for sizing and consistent with the design spreadsheet, are summarized in table 4.1.

The choice of an **annular** architecture is dictated, primarily, by the

Table 4.1: Combustor design point (Cruise Conditions).

Parameter	Symbol	Value	Unit
Total Inlet Pressure	P_{t3}	3.60	MPa
Total Inlet Temperature	T_{t3}	962	K
Total Outlet Temperature (Target)	T_{t4}	1600	K
Total Air Mass Flow	$\dot{m}_{air}$	27.5	kg/s
Fuel	-	Gaseous H_2	-
Combustion Efficiency (Target)	η_b	≥ 0.99	-
Total Pressure Loss (Target)	$\Delta P/P_{t3}$	5.0–6.0	%

simplicity of modeling and the possibility of significantly reducing the effective combustor volume during the simulation phase (exploiting periodicity). Additionally, as noted by Lefebvre [26], this type of architecture is preferable given its ability to minimize pressure losses, reduce the wetted surface (and thus mass and cooling requirements), and guarantee a more uniform outlet temperature profile (*Pattern Factor*) compared to can-annular configurations.

4.2 Preliminary Sizing Methodology

The combustion chamber sizing was conducted following a semi-empirical procedure based on fundamental aerodynamic and chemical correlations described by Lefebvre [26] and Mattingly [27]. This approach, analogous to that recently validated by Moreno-Pacheco et al. [28], allows defining the macroscopic dimensions of the combustor (flow areas, liner heights, and reaction zone lengths) by imposing constraints on pressure drops, flame stability, and residence times.

Calculations were implemented in a dedicated calculation code (Excel) starting from the thermodynamic boundary conditions at section 3 (inlet) and 4 (outlet).

4.2.1 Definition of the Reference Section

The first fundamental step is determining the maximum cross-sectional area of the chamber, or **Reference Area** (A_{ref}), which includes both the area of the

flow inside the liner (*Flame Tube*) and that of the annular passage (*Annulus*). This dimension is constrained by the need to minimize total pressure losses (ΔP_{tot}), which reduce the thermodynamic cycle efficiency.

A target pressure drop of 5 %–6 % was set, of which a fraction (approximately 3 %–4 %) is allocated to "cold" pressure losses (through swirler and dilution holes) to promote turbulent mixing [26]. This imposes a constraint on the reference velocity (V_{ref}) of the flow in the annulus, typically limited to 20 m/s–30 m/s to limit friction losses. The reference area was calculated from mass conservation at the inlet section:

$$A_{ref} = \frac{\dot{m}_{air}}{\rho_3 V_{ref}} \quad (4.1)$$

Where ρ_3 is the density of compressed air at the inlet. Once A_{ref} is known and the mean engine radius (R_{mean}) is fixed, the reference height of the passage (h_{ref}) was determined geometrically assuming a pure annular configuration:

$$h_{ref} = \frac{A_{ref}}{2\pi R_{mean}} \quad (4.2)$$

Consistent with the design spreadsheet (see table 4.2), the calculated value ensures that the *Pressure Loss Factor* (PLF) remains within the suggested limits to guarantee sufficient authority of the dilution jets.

4.2.2 Diffuser and Faired System Sizing

Upstream of the liner lies the diffusion system, tasked with decelerating the air flow coming from the high-speed compressor ($Ma > 0.3$) to velocities compatible with stable combustor operation and low pressure losses in the annulus ($V_{ref} \approx 20$ m/s–30 m/s).

For the present project, a **Faired Diffuser** configuration was chosen. Unlike "Dump" systems that provide for a sudden expansion, this architecture uses a fairing on the combustor head to divide the flow continuously, guiding it towards the annular passages and the injector.

The sizing is articulated in two functional stages:

Aerodynamic Pre-Diffuser It is a divergent duct located immediately downstream of the compressor. Its function is to maximize static pressure recovery before flow division. The equivalent divergence angle 2θ and area ratio AR_{pre} were selected to operate near the transitory stall limit, maximizing compactness:

$$AR_{pre} = \frac{A_{exit}}{A_{in}} \approx 2.1 \div 2.5 \quad (4.3)$$

Fairing System (Snout) and Splitting At the pre-diffuser exit, the flow is not discharged into a plenum (as in the Dump), but intercepts the **Snout** (faired head of the liner). This component acts as an aerodynamic splitter that subdivides the total mass flow $\dot{m}_3$ into three distinct streams:

- Air to the injection system (Dome air flow);
- Air to the external annular passage (Outer annulus);

Faired vs Dump:

According to Lefebvre [26], faired diffusers offer the advantage of lower total pressure losses, as the flow is always guided by walls. However, they require accurate design of the "Snout" to avoid separation in case of variations in the compressor outlet velocity profile.

- Air to the internal annular passage (Inner annulus).

The Snout geometry was sized to keep the flow velocity constant or slightly decelerated during the split, avoiding parasitic recirculations in the frontal zone. This design choice is consistent with the goal of maximizing the efficiency of the regenerative thermodynamic cycle, where every percentage point of preserved total pressure (P_{t4}/P_{t3}) translates into a direct gain in specific thrust.

4.2.3 Air Distribution and Liner Sizing

The total air mass flow $\dot{m}_{air}$ was subdivided into three main contributions, each governed by specific physical needs:

Primary Air ($\dot{m}_{pz}$) Calculated to ensure a local equivalence ratio Φ in the primary zone close to stoichiometry or slightly lean, optimizing stability and avoiding excessive production of Thermal NOx.

Cooling Air ($\dot{m}_{cool}$) Estimated based on the wetted surface of the liner and the adiabatic flame temperature, using film cooling correlation curves present in Lefebvre [26]. In the current model, approximately 33 % of the air is dedicated to cooling.

Dilution Air ($\dot{m}_{dil}$) The remaining part, injected in the terminal zone to lower the temperature to the T_{t4} value.

The frontal section area of the Flame Tube A_{ft} was then derived assuming that the mean velocity inside the liner (U_{ft}) is lower than that in the annulus to prevent flame *blow-out*, maintaining a ratio V_{ref}/U_{ft} typically between 1.5 and 2.0 [27].

4.2.4 Longitudinal Zone Sizing

The total length of the combustor is the sum of the lengths of the three functional zones. The lengths were scaled as a function of the liner height h_{ft} , a parameter that governs the size of recirculation vortices.

1. **Primary Zone (L_{PZ}):** This zone must host the *Central Recirculation Zone* (CRZ) generated by the swirler for flame anchoring. The length was sized to ensure a residence time (τ_{res}) sufficient for the completion of chemical reactions. According to Lefebvre's correlations, for swirlers with high Swirl Number ($S_N > 0.6$), the optimal length is:

$$L_{PZ} \approx 0.75 \div 1.0 h_{ft} \quad (4.4)$$

2. **Secondary or Intermediate Zone (L_{SZ}):** In this region, the oxidation of radicals and unburned fuel is completed. For hydrogen combustors, which boast very rapid reaction kinetics, this zone can be reduced. A value of $L_{SZ} \approx 0.5 h_{ft}$ was adopted.

3. **Dilution Zone (L_{DZ}):** This zone is critical for the *Pattern Factor*. The length must be sufficient to allow cold air jets to penetrate to the center of the flow and mix. The empirical relation used is:

$$L_{DZ} \approx 2.0 \div 2.5 h_{ft} \quad (4.5)$$

The sum of these lengths, together with the thickness of the diffuser and pre-diffuser, defines the overall axial footprint of the machine, reported in table 4.2.

4.2.5 Dilution Hole Design

The diameter of the dilution holes d_j and their number n_j were determined by imposing the jet penetration criterion. To maximize mixing, the jet momentum (J) must be such as to penetrate to the liner mean axis. The relation used, derived from Lefebvre [26], links the total hole area to the available pressure drop:

$$A_{hole} = \frac{\dot{m}_{jet}}{C_d \sqrt{2\rho\Delta P}} \quad (4.6)$$

Where C_d is the discharge coefficient (assumed ≈ 0.6). In the optimization process described subsequently, the radius of these holes (R_{dil}) becomes a free variable, allowing the software to find the optimal compromise between penetration and circumferential coverage.

Dilution Hole Sizing Law

To ensure that the total mass flow and combustor pressure drop remain constant as the geometry varies, the constraint of conservation of total effective area was imposed. Having defined an optimal reference area A_{ref} for the base configuration with 26 sectors, the dilution area assigned to the single sector A_{sect} must vary inversely proportional to the number of sectors N_{slices} :

$$A_{sect}(N_{slices}) = A_{ref, N=26} \cdot \frac{26}{N_{slices}} \quad (4.7)$$

This physical relation implies that, as the combustor fractionation increases (increase in sectors), the area available on the single "slice" decreases proportionally to maintain the global fluid dynamic equivalence of the entire machine.

Table 4.2: Geometric parameters calculated for the combustor baseline configuration (Data from spreadsheet).

Description	Symbol	Value	Unit
<i>General Dimensions</i>			
Reference Area	A_{ref}	0.0575	m ²
Annulus Height (Ref)	h_{ref}	60.98	mm
Mean Diameter	D_{mean}	300.0	mm
Flame Tube Height	h_{ft}	40.25	mm
Flame Tube Area	A_{ft}	0.0379	m ²
<i>Characteristic Lengths</i>			
Primary Zone Length	L_{PZ}	45.73	mm
Secondary Zone Length	L_{SZ}	20.12	mm
Dilution Zone Length	L_{DZ}	91.21	mm
<i>Cooling Parameters</i>			
Number of Cooling Sectors	N_{sect}	4	-
Cooling Holes (full annulus)	N_{slot}	1560	-
Cooling Hole Diameter	D_{cool}	2.0	mm

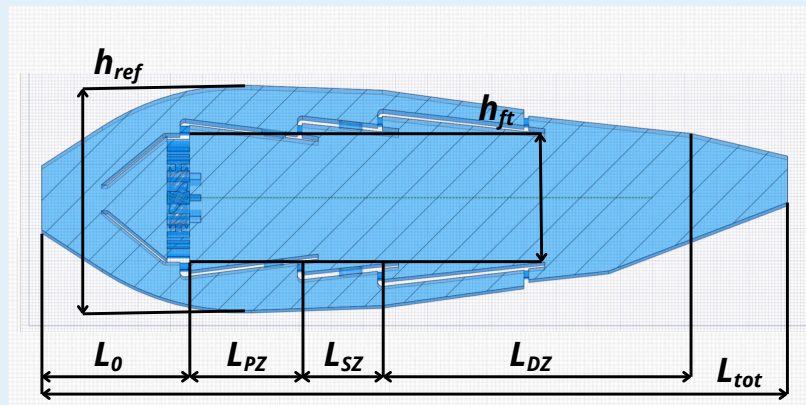


Figure 4.1: Main dimensioning of the combustor, constant as design parameters vary.

4.3 Injector Design and Swirl System Analysis

The central element for flame stabilization and combustion process management is the injection system (*Front End*), designed to ensure rapid mixing between the oxidant air and hydrogen.

4.3.1 Swirler Theory and Function

The use of *swirling flow* is the primary strategy adopted in modern gas turbines to ensure flame stability. Imposing a tangential velocity component (w) on the axial air flow (u) creates a radial pressure gradient which, when the vorticity level exceeds a critical value (typically $S_N > 0.6$), induces the phenomenon of *Vortex Breakdown*. This generates a **Central Recirculation Zone** (CRZ), i.e., a toroidal bubble of reverse flow along the axis.

4.3.2 Geometric Configuration and Justifications

For the present work, a *Flat-Vane Axial Swirler* configuration was chosen. This choice, supported by Mattingly's analysis [27], offers the best compromise between pressure losses (lower than radial swirlers) and geometric compactness. The specific geometry adopted is of the **Multi-Stage Counter-Rotating** type, composed of:

- **Inner Swirler:** Rotates clockwise and surrounds the central pilot injector.
- **Outer Swirler:** Rotates in the opposite direction, surrounding the crown of 8 main injectors.

Hydrogen vs Kerosene: Why Counter-Rotation?

In traditional Kerosene combustors, the fuel is injected as a liquid and requires time and space for atomization and evaporation. Hydrogen, being injected already gaseous and at high temperature, does not have these physical latencies.

Consequently, the design goal is not to guarantee vaporization, but to obtain immediate **Micromixing** at the molecular scale. The *Counter-Rotating* configuration is ideal for this purpose: the interaction between the two opposing vortices generates extremely high shear stress at the nozzle exit, shattering turbulent structures and allowing for extremely short and compact flames, reducing the risk of *Flashback*.

4.3.3 Swirl Number Calculation

The Swirl Number S_N is defined as the ratio between the axial flux of tangential momentum and the axial flux of axial momentum. For a flat-vane swirler, Lefebvre [26] provides the following approximate analytical expression:

$$S_N \approx \frac{2}{3} \left[\frac{1 - (R_h/R_n)^3}{1 - (R_h/R_n)^2} \right] \tan \theta \quad (4.8)$$

Where R_h and R_n are respectively the hub and nozzle radii, and θ is the vane angle. Since these radii vary during geometric optimization, the exact value of S_N changes for each tested configuration.

4.4 3D Parametric Modeling and Automation

In order to explore the design space and conduct the optimization objective of this thesis, it was necessary to overcome the traditional static CAD approach. A fully automated procedure was developed that integrates geometric modeling with mesh generation, using tools from the ANSYS suite [19].

4.4.1 Geometry Generation and Variable Parameters

The geometric model was created in ANSYS SpaceClaim via IronPython scripts. The computational domain represents a single rotational periodicity. The script manages two main design variables:

Number of Sectors (N_{sect}) Varies the angular opening of the domain (from a minimum corresponding to 36 sectors to a maximum corresponding to 16 sectors). As the angle varies, the cooling hole distribution is automatically adapted.

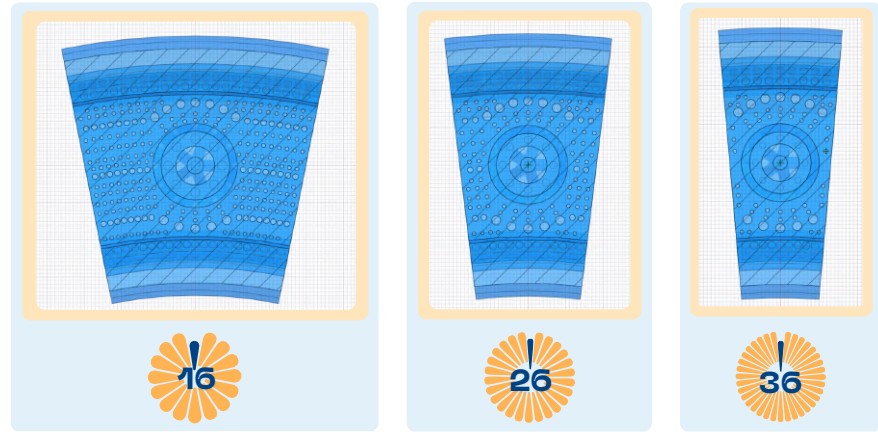


Figure 4.2: Variation of sector geometry: comparison of mixing sections as angular partitioning varies.

Dilution Hole Radius (R_{dil}) The liner features two main rows of dilution holes. The optimizer directly controls the radius of the first row of holes $R_{dil,1}$. The script automatically calculates the radius of the second row $R_{dil,2}$ imposing the conservation of total area:

$$A_{tot,dil} = \text{constant} \implies R_{dil,2} = f(R_{dil,1}) \quad (4.9)$$

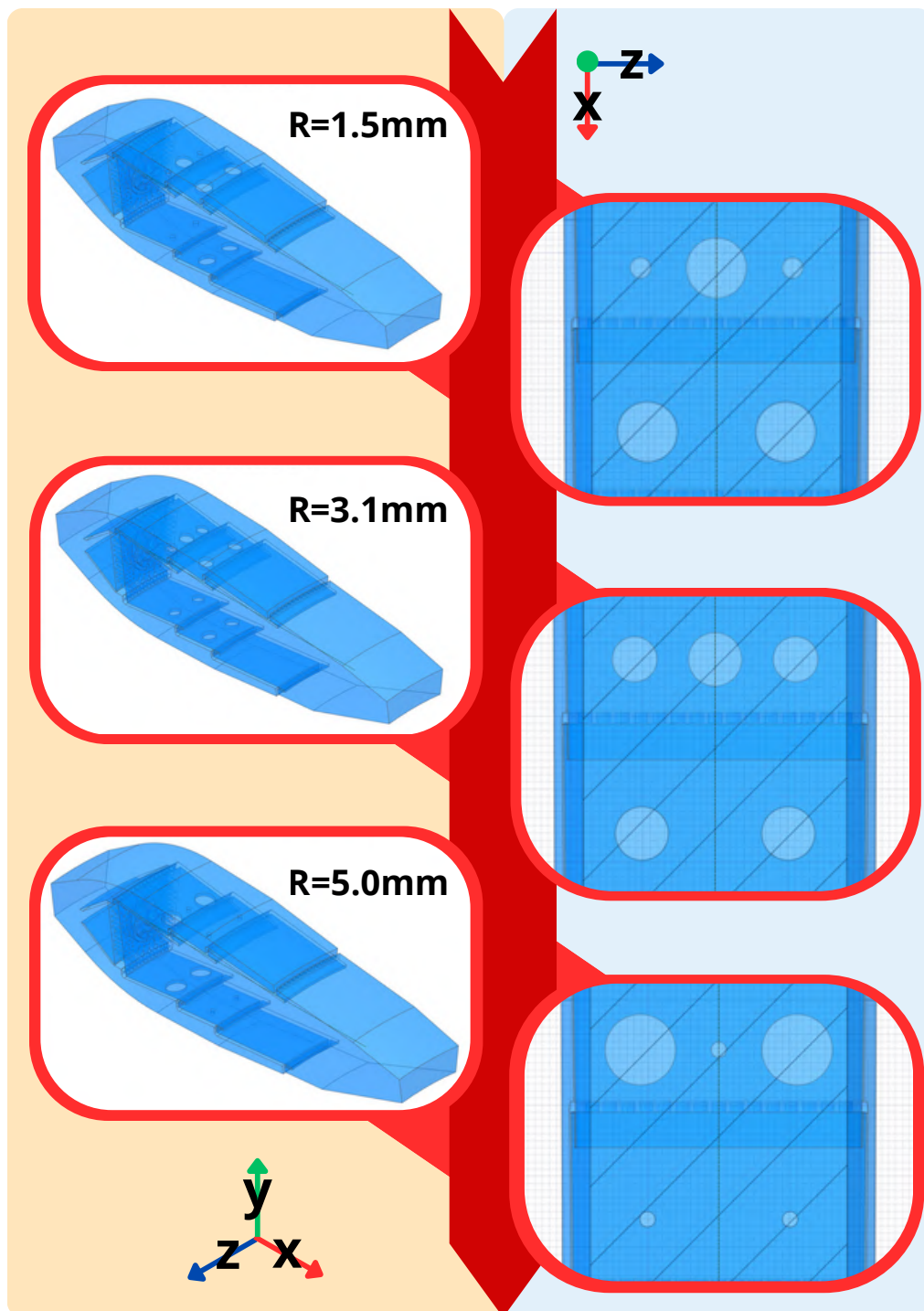


Figure 4.3: Variation of dilution hole geometry: comparison between three values of the parameter identifying the diameter of the main dilution holes in the primary zone. (In the figure case: $N_{slices} = 26$)

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Optimization Strategy via Adaptive Surrogate Models

Bayesian optimization methodology: from Gaussian Processes to the hybrid strategy with Matérn kernel for NO_x minimization.

ABSTRACT

This chapter describes the numerical optimization strategy implemented to minimize NO_x emissions, overcoming the high computational cost of CFD simulations through **Bayesian Optimization**. The methodology is distinguished by an adaptive approach: in response to instabilities encountered with the classic Gaussian kernel on non-smooth response surfaces, a transition was made to the **Matérn 3/2** covariance class, ensuring robustness even in the presence of discrete variables. Design space exploration was guided by the *Expected Improvement* criterion.

5.1 Introduction to the Methodology

Bayesian Optimization is a sequential strategy for finding the global optimum of expensive black-box functions. It uses a surrogate model (usually Gaussian Processes) to estimate the function's behavior and an acquisition function to balance exploration and exploitation, drastically reducing the number of evaluations needed to converge to the solution.

The design of a low-emission aeronautical combustor is configured as a constrained non-linear optimization problem, where the objective function (the NO_x emission index) cannot be expressed in closed form. The evaluation of this function depends on the numerical solution of Reynolds-Averaged Navier-Stokes (RANS) equations coupled with detailed chemical kinetics models for hydrogen. Given the “stiff” nature of the reactions and the complexity of turbulence, the computational cost of a single simulation makes the use of direct optimization algorithms (such as Genetic Algorithms or *Gradient-Based* methods), which would require hundreds or thousands of evaluations, prohibitive [29].

To overcome this complexity, this thesis work adopted an approach based on **Surrogate Models** and specifically on **Gaussian Process Regression (GPR)**. A distinctive element of the methodology presented here is its *flexibility*: the numerical strategy was evolved during the experimental campaign to adapt to encountered needs.

5.2 Mathematical Foundations of Gaussian Processes

A Gaussian Process (GP) is a statistical technique used to construct an approximation (metamodel) of the CFD simulator response, $y(\mathbf{x})$, where $\mathbf{x} \in \mathcal{D} \subset \mathbb{R}^d$ represents the vector of design parameters (d). The fundamental assumption is that the objective function can be modeled as a realization of a stochastic process $Y(\mathbf{x})$ defined by:

$$Y(\mathbf{x}) = \mu(\mathbf{x}) + Z(\mathbf{x}) \quad (5.1)$$

In which:

- $\mu(\mathbf{x})$ is the mean function, capturing the global trend of the data (in this work, $\mu(\mathbf{x}) = \mu$, an unknown constant to be estimated, configuring an *Ordinary Kriging*).
- $Z(\mathbf{x})$ is a zero-mean stochastic process with covariance defined by a kernel function $k(\mathbf{x}, \mathbf{x}')$:

$$Z(\mathbf{x}) \sim GP(0, k(\mathbf{x}, \mathbf{x}')) \quad (5.2)$$

Given a set of n observations $D_n = \{\mathbf{x}_i, y_i\}_{i=1}^n$, the posterior predictive distribution for a new point $\mathbf{x}^*$ is Gaussian, with mean $\hat{y}$ (the predicted value) and variance s^2 (the prediction uncertainty) given by [30]:

$$\hat{y}(\mathbf{x}^*) = \hat{\mu} + \mathbf{k}^{*T} \mathbf{K}^{-1} (\mathbf{y} - \mathbf{1}\hat{\mu}) \quad (5.3)$$

$$s^2(\mathbf{x}^*) = \sigma^2 \left(1 - \mathbf{k}^{*T} \mathbf{K}^{-1} \mathbf{k}^* + \frac{(1 - \mathbf{1}^T \mathbf{K}^{-1} \mathbf{k}^*)^2}{\mathbf{1}^T \mathbf{K}^{-1} \mathbf{1}} \right) \quad (5.4)$$

Where $\mathbf{K}$ is the $n \times n$ covariance matrix with elements $K_{ij} = k(\mathbf{x}_i, \mathbf{x}_j)$ and $\mathbf{k}^*$ is the vector of covariances between the new point and the observed ones.

5.3 The Role of the Kernel: Physical Meaning and Derivation

The kernel function $k(\mathbf{x}, \mathbf{x}')$ is not a simple algebraic construct for interpolation but constitutes the heart of Bayesian inference, effectively encapsulating *a priori information* about the system physics. The choice of kernel determines three fundamental properties of the surrogate model:

1. **Correlation:** Defines how relevant information obtained at a point $\mathbf{x}_i$ is for predicting the value at a point $\mathbf{x}_j$.
2. **Differentiability:** The kernel defines the function space in which the surrogate lives. In particular, the kernel's behavior near the origin determines whether generated functions will be smooth (C^∞) or rough (C^0, C^1).
3. **Power Spectrum:** By the Wiener-Khinchin theorem, the kernel is the Fourier transform of the process's Power Spectral Density (PSD) [30]. Choosing a kernel is equivalent to hypothesizing which spatial frequencies compose the physical phenomenon.

The two kernels used in this work and the theoretical reasons that led to preferring the Matérn class are analyzed below.

5.3.1 The Gaussian Kernel and its Limitations

In the initial phase of optimization, the *Squared Exponential* (or Gaussian) kernel was used, defined as:

$$k_{SE}(r) = \sigma^2 \exp\left(-\frac{r^2}{2l^2}\right) \quad (5.5)$$

Where $r = |\mathbf{x} - \mathbf{x}'|$ is the Euclidean distance. Expanding in a Taylor series around $r = 0$, it is noted that the kernel contains only even powers of r . This implies that the generated stochastic process is infinitely differentiable (C^∞) in mean square.

Although mathematically elegant, this property of "infinite derivability" was severely criticized by Stein [31] as an unrealistic assumption for modeling real physical phenomena. Confirming this, in the context of this work, such an assumption proved inadequate for two main reasons:

- **Discrete Nature of Parameters:** One of the fundamental parameters, the number of sectors N_{slices} , is an integer variable. Although the surrogate treats it as continuous (relaxation), the real physical response exists only for discrete values, introducing an intrinsic "roughness" in the response surface that a C^∞ model struggles to interpolate without oscillations.
- **Objective Function Sensitivity:** The combustor response (EINO_x) as a function of geometric parameters (N_{slices}, r_{dil}) is governed by strongly non-linear RANS equations. Small geometric variations can entail significant changes in mixing efficiency and temperature peaks.

The Wiener-Khinchin Theorem states that the kernel (covariance function) and the Power Spectral Density (PSD) are a Fourier transform pair. Defining the kernel means operating an a priori filtering: the choice of parameters determines which spatial frequencies (oscillations or length scales) the model can represent. A "smooth" kernel (like the Squared Exponential) excludes high frequencies, assuming a physical phenomenon devoid of abrupt variations.

This implies that the real response surface, despite being continuous, may present abrupt changes in slope ("kinks") or narrow valleys. The attempt to force an infinitely smooth surface onto data presenting these characteristics led to ill-conditioning problems of the covariance matrix, requiring an excessive regularization term (*nugget*) which caused optimization stagnation.

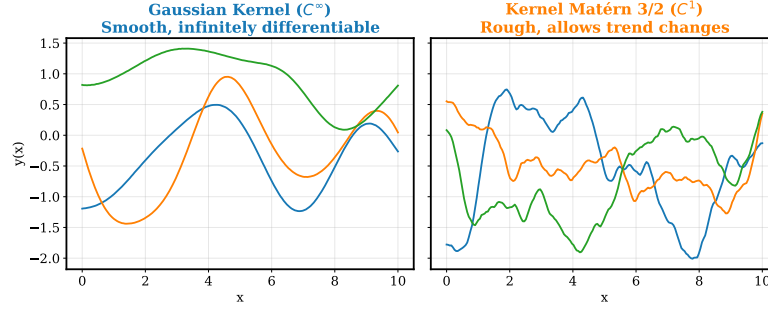


Figure 5.1: Comparison between stochastic process realizations generated by Gaussian Kernel (left) and Matérn 3/2 (right). It is noted how the Gaussian produces extremely smooth curves (C^∞), while the Matérn allows local slope variations (C^1), adapting better to physical phenomena with rapid changes.

5.3.2 The Matérn Kernel

To overcome the limitations exposed above, the **Matérn** class of covariance functions was adopted. The main reasons for this choice lie in the different differentiability properties of the adopted kernel, more in line with the expected function.

The Bessel functions of the second kind ($Y_n(x)$), also known as Weber or Neumann functions, are linearly independent solutions of Bessel's differential equation. Unlike functions of the first kind ($J_n(x)$), they present a singularity at the origin ($x = 0$), where they tend to infinity. They are essential for describing physical phenomena with cylindrical or spherical symmetry in domains not including the symmetry axis, such as wave propagation in radial waveguides or thermal distribution in cylindrical shells.

Physical Interpretation: Whittle's Equation

Whittle (1954) [32] demonstrated that a random field with Matérn covariance is the stationary solution of a specific **Stochastic Partial Differential Equation (SPDE)** driven by white noise:

$$\left(\frac{2\nu}{l^2} - \Delta\right)^{\frac{\nu}{2} + \frac{d}{4}} Z(\mathbf{x}) = \mathcal{W}(\mathbf{x}) \quad (5.6)$$

Where Δ is the Laplacian operator and $\mathcal{W}(\mathbf{x})$ is Gaussian white noise. In physical terms, using a Matérn kernel is equivalent to modeling the combustor response to geometric parameter variations as a stochastically damped spatial dynamic system.

The general analytical form of the kernel is given by [30]:

$$k_\nu(r) = \sigma^2 \frac{2^{1-\nu}}{\Gamma(\nu)} \left(\frac{\sqrt{2\nu}r}{l}\right)^\nu K_\nu\left(\frac{\sqrt{2\nu}r}{l}\right) \quad (5.7)$$

where K_ν is the modified Bessel function of the second kind and ν is the parameter controlling differentiability.

5.3.3 Matérn 3/2: The Optimal Choice

Specifically, the **Matérn 3/2** kernel was selected (setting $\nu = 1.5$). For this half-integer value, the Bessel function simplifies, leading to the formula implemented in the optimization code:

$$k_{3/2}(r) = \sigma^2 \left(1 + \frac{\sqrt{3}r}{l} \right) \exp \left(-\frac{\sqrt{3}r}{l} \right) \quad (5.8)$$

Why this choice? Unlike the Gaussian, the Matérn 3/2 generates processes of class C^1 (differentiable only once). This mathematical property is fundamental: it allows the surrogate to model functions that are continuous and have a continuous first derivative, but whose second derivative may be discontinuous. Physically, this means the model is capable of adapting to rapid trend changes in NO_x production (for example, when a geometric configuration approaches a very narrow local optimum) without suffering from numerical instabilities or having to excessively "smooth" the response. This guaranteed more robust convergence and a more faithful representation of combustor sensitivity to design parameters.

5.4 Infill Criterion: Expected Improvement (EI)

Once the surrogate model is built, it is necessary to decide which new point to simulate. The choice is guided by the maximization of **Expected Improvement (EI)**. As thoroughly discussed by Jones in his work on the taxonomy of global optimization methods [33], EI is the most effective criterion for balancing the two conflicting needs of optimization:

Mathematically, assuming the best value found so far is f_{min} , the improvement at a generic point $\mathbf{x}$ is defined as $I(\mathbf{x}) = \max(0, f_{min} - Y(\mathbf{x}))$. Since $Y(\mathbf{x})$ is a random variable with normal distribution $\mathcal{N}(\hat{y}, s^2)$, the expected value of such improvement is calculable in closed form [34]:

$$EI(\mathbf{x}) = (f_{min} - \hat{y})\Phi \left(\frac{f_{min} - \hat{y}}{s} \right) + s\phi \left(\frac{f_{min} - \hat{y}}{s} \right) \quad (5.9)$$

Where $\Phi(\cdot)$ is the cumulative distribution function of the standard normal and $\phi(\cdot)$ is the probability density function of the standard normal. The equation above elegantly highlights the balance:

- **First Term:** Dominant when $\hat{y}$ is much smaller than f_{min} (high probability of improving the record). This term guides local exploitation.
- **Second Term:** Proportional to s (standard error). Dominant when uncertainty is high, even if the predicted mean is not promising. This term guides global exploration, preventing the algorithm from getting trapped in local minima.

Using EI therefore allows sampling not only where we "think" the minimum is, but also where it "could" be, based on Kriging statistical uncertainty.

*Exploration vs
Exploitation:*

- **Local Search (Exploitation):**
Exploring zones where the model predicts low values of the objective function.
- **Global Search (Exploration):**
Exploring zones where model uncertainty is high (i.e., where we have not yet sampled).

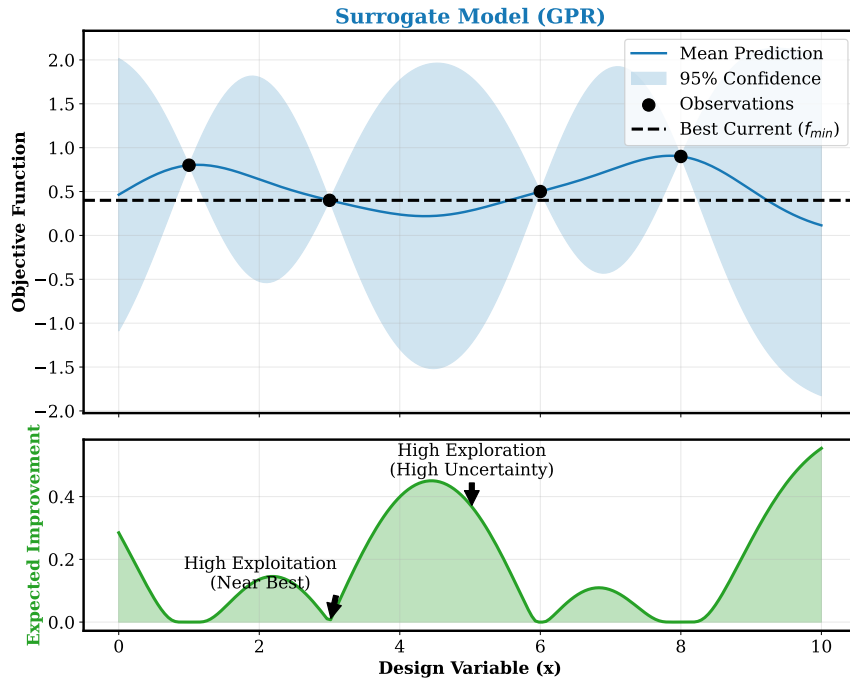


Figure 5.2: Representation of the EI criterion. Top: the surrogate function (blue mean) with uncertainty area (gray). Bottom: the EI acquisition function. It is noted how EI is high both where the mean is low (Exploitation) and where uncertainty is high (Exploration).

5.5 Hybrid and Adaptive Optimization Strategy

In light of the theoretical considerations exposed, the optimization campaign was conducted adopting a mixed approach, characterized by an evolution of the surrogate model in response to system behavior. The strategy was articulated in two distinct phases:

Phase 1: Initial Exploration (Iterations 1-9)

The first 30 *infill* simulations (following the 21 initial DoE points) were guided using **Gaussian Kriging**. In this sparse sampling phase (*coarse*), the hypothesis of high spatial correlation allowed for a first global exploration. However, the method's effectiveness was initially limited by the presence of a regularization *nugget*: by effectively transforming the exact interpolator into an approximate regressor, the model tended to re-propose the same sampling points, causing search stagnation. To overcome this issue, after the seventh iteration (about 40 total simulations), the *nugget* was forced to zero. Although this momentarily restored interpolating capacity, after just two further iterations, the rigidity of the Gaussian kernel—incapable of adapting to response surface irregularities without relaxation—caused the numerical explosion of predicted values (*covariance matrix ill-conditioning*), rendering the model unusable for predicting subsequent points.

Phase 2: Refinement and Convergence (Iterations > 10)

Following the instabilities encountered with the Gaussian kernel, the surrogate was replaced with the **Matérn 3/2** model. This transition unlocked the optimization: the capacity of the C^1 class kernel to follow local gradients and curvature changes allowed reducing the *nugget* back to zero (or to infinitesimally small values managed adaptively), guaranteeing exact interpolation. This guided the algorithm towards high-performance geometric configurations that had been previously ignored by the too "rigid" Gaussian model. In both phases, the selection of new points was governed by the EI acquisition function, automatically balancing exploration and exploitation.

5.6 Design Space and Variables

Geometric parametrization was defined to act directly on the physical variables controlling the thermal NO_x formation mechanism (Zeldovich mechanism), namely peak temperature and residence time, in strict compliance with aeronautical sizing constraints [26, 27].

5.6.1 Optimization Variables

The design space $\mathcal{D}$ consists of two independent variables:

- **Number of Sectors N_{slices} :** Discrete variable. Modifies combustor periodicity and the physical volume of the primary zone, directly influencing recirculation vortex structure and flame stability.
- **Radius of the first row of holes $r_{dil,1}$:** Continuous variable. Regulates dilution air distribution within the sector. The radius of the second row, $r_{dil,2}$, is a dependent variable calculated analytically to satisfy the total area conservation constraint.

Variation of $r_{dil,1}$ modifies the momentum and penetration of transverse jets (*Jet-in-Crossflow*), fundamental parameters for ensuring rapid *quenching* of combustion products. Model initialization occurred via a 21-point **Latin Hypercube Sampling (LHS)**. Sample size was chosen to uniquely cover every possible integer value of N_{slices} in the range of interest [35].

5.7 Workflow Implementation

The optimization architecture follows a *Human-in-the-loop* approach, necessary to manage heterogeneity between the pre-processing environment (Windows/SpaceClaim) and the massive calculation environment (Linux/HPC).

The iterative cycle is articulated in the following phases:

1. **Learning (Python/Excel):** The `excel_kriging.py` script updates the surrogate model (Gaussian or Matérn depending on the operational phase) by integrating new available CFD data.

2. **Acquisition Optimization:** The *Expected Improvement* (EI) function is maximized on the surrogate space to identify optimal candidates.
3. **Manual Selection:** The operator selects 3 to 5 configurations for the next batch, typically balancing 2 *Best Improvement* points (exploration) and 1-3 *Minimum Prediction* point(s) (exploitation), while contextually applying a filter on simulations at points already analyzed; this expedient is necessary when the surrogate acts as a regressor (presence of nugget).
4. **Execution:** The process continues with automatic parametric CAD generation, meshing, and the launch of parallel CFD calculation on the HPC cluster.
5. **Loop Closure:** Numerical results (EINOx) are extracted and re-inserted into the database to start the next iteration.

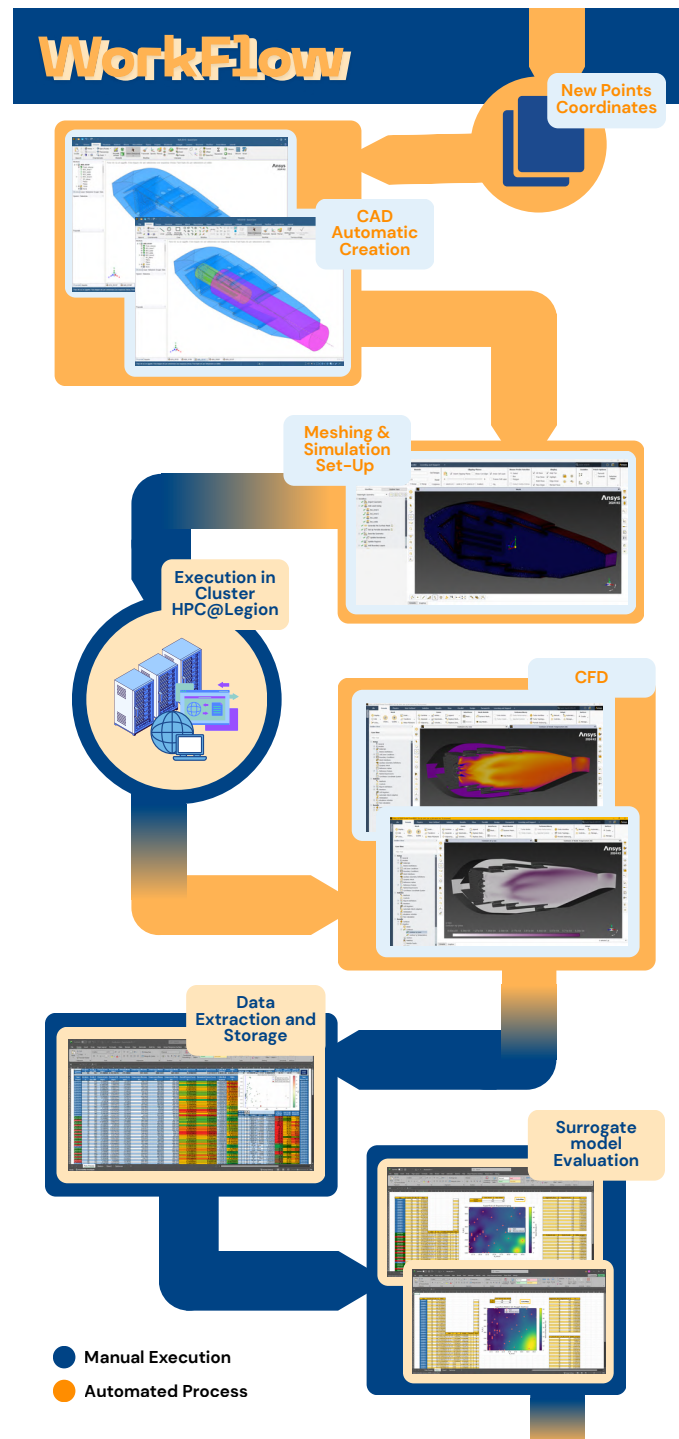


Figure 5.3: Overall flowchart of the optimization procedure: integration between adaptive surrogate model optimization, CAD modeling, and CFD simulation.

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From Optimization to Physics: Surrogate Analysis and Flame Structure Classification

Performance analysis, statistical validation, revised methodological framework and phenomenological classification of flame structures.

ABSTRACT

This chapter illustrates the results of the optimization campaign conducted on the hydrogen aeronautical combustor. Through a database of 74 CFD simulations, the process allowed identifying a global optimum capable of reducing NO_x emissions by 62.18 % compared to the initial average. The statistical validation of the surrogate model based on the Matérn 3/2 kernel and a detailed phenomenological analysis correlating geometry to the different flame topologies encountered are presented. The final quantitative analysis demonstrates how the "strained flame" regime is the key physical mechanism for the thermal abatement of pollutants in the optimal design.

For the combustor optimization process, a total of 74 CFD simulations were performed. The design space exploration strategy was distributed as follows:

- **21 simulations** constitute the initial database (DoE).
- **30 simulations** were guided via 9 iterations (of variable size) of a standard Kriging-based surrogate.
- **9 simulations** were guided via 3 iterations of a surrogate with Matérn 3/2 kernel, trained on the accumulated database of the previous 51 simulations.
- **3 simulations** added in visually poorly explored points of the domain.
- **11 simulations** guided by pattern search logic around the three local minima identified in the database.

The minimum marking the end of the optimization work corresponds to simulation number 68. This configuration records an improvement of **−62.18%** compared to the average EINO_x values calculated with the initial database simulations ($EINO_{x,mean} \approx 20.6 \text{ g/kg}$) and a **−4.31%** improvement compared to the minimum of the aforementioned database. The absolute minimum EINO_x value corresponds to 7.786 g/kg. The analysis of the behavior of the surrogate models that guided the process follows below.

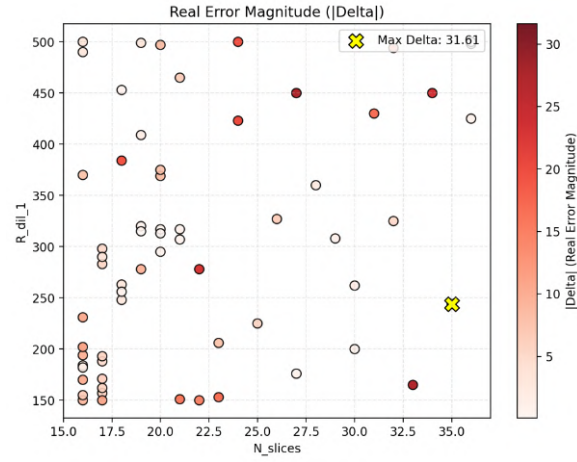
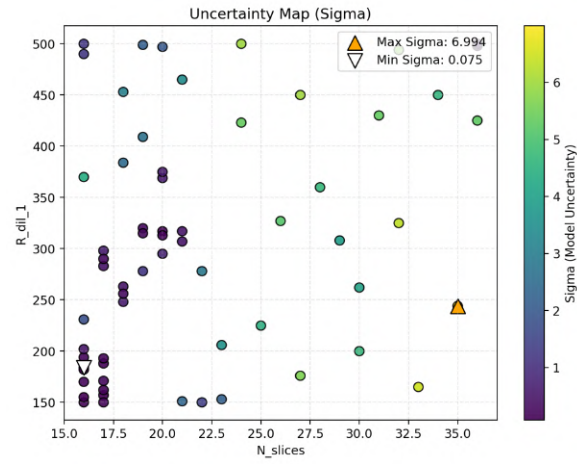
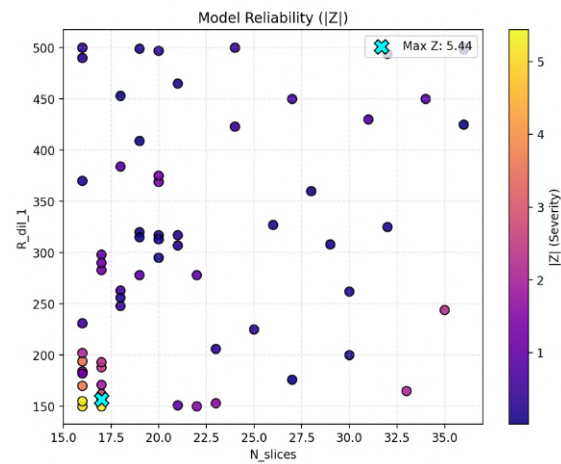
6.1 Surrogate Model Validation

The termination of the global exploration phase, which occurred after the evaluation of 63 design points, was decreed based on a diagnostic campaign. Using the Leave-One-Out Cross Validation (LOOCV) technique, fundamental graphical indicators were generated to discriminate between physiological surrogate uncertainty and potential systematic errors.

6.1.1 Correlation between Error and Uncertainty

The first level of verification concerned the local coherence of the model. Figure 6.1 reports the spatial scatter plots for the three key quantities: the actual absolute error (δ_{LOO}), the predicted uncertainty (σ_{LOO}), and the standardized residual ($|Z|$).

From the direct comparison between the maps, a strong topological correlation emerges: regions characterized by the largest deviations from CFD systematically coincide with areas where the model declares the highest estimation variance. This behavior is indicative of an "honest" model: the surrogate correctly recognizes zones of sparse information by widening confidence intervals. Consequently, by normalizing the error to obtain the residual $|Z|$, it is observed that peaks are attenuated and almost all points fall within the statistical reliability range $|Z| \leq 2$.

(a) Actual absolute error δ_{LOO} (b) Predicted uncertainty σ_{LOO} (c) Standardized residual $|Z|$ **Figure 6.1:** Spatial scatter plots for the three key quantities of the surrogate model.

6.1.2 Global Statistical Analysis (Z Residual Distribution)

To verify the validity of probabilistic assumptions, the frequency distribution of standardized residuals Z was analyzed. Theoretically, if the model were perfect, Z should follow a standard normal distribution $\mathcal{N}(0, 1)$. The obtained histogram (fig. 6.2) shows a bell curve well-centered on zero. Statistical parameters confirm the goodness of fit:

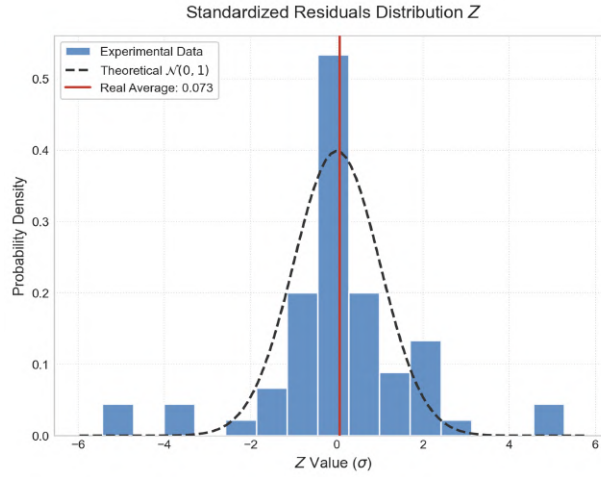


Figure 6.2: Frequency distribution of standardized residuals Z .

- **Mean ($\mu_Z \approx 0.07$):** The negligible value indicates the absence of global bias; the model tends neither to systematically overestimate nor underestimate emissions.
- **Symmetry:** The distribution tails are balanced, excluding significant drift phenomena in the data.

6.1.3 Spatial Independence Verification (Z Heatmap)

The final test concerned the search for residual spatial structures in the error. A response surface was generated by interpolating Z values (fig. 6.3). The map appears "flat" and devoid of coherent gradients. The absence of defined clusters leads to a fundamental operational conclusion: the used model does not introduce biases that privilege or penalize specific zones of the parameter space.

6.2 Reasons for Stopping Optimization with Surrogate

Having demonstrated the relative quality of the generated surrogate, it was decided to terminate global search operations, focusing on a local search (pattern search). Three considerations led to this decision:

- **Process Timing:** Despite using the HPC platform, the average timing per simulation stands at 24 hours. After 63 simulations, the process had reached 20 days of computation. Considering also the final refinement phase, it was determined that further resource usage was not worth the benefit of a potential marginal improvement of the current model.

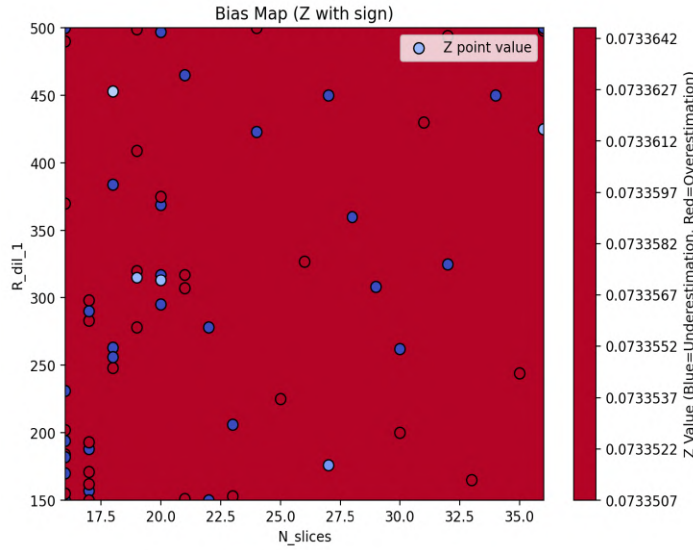


Figure 6.3: Map of standardized residuals Z for spatial independence verification.

- **Stagnation of Expected Improvement:** Although the Expected Improvement (E.I.) value is not the only metric to determine model saturation, decreasing values indicate a lower predicted probability of finding "global" improvements distant from the current minimum. Given the stagnant character of E.I. values in the last iterations, it was decided to terminate the global search.
- **Local Over-confidence (Scatter Z Analysis):** An in-depth analysis of the standardized residual scatter plot Z (fig. 6.4) highlighted a criticality in the zone of interest. Observing the bottom-left corner of the graph, corresponding to the area where the algorithm concentrated minimum points, an over-confidence behavior is noted: despite high sampling density lowering predicted uncertainty (σ), real residuals remain significant. This indicates that the continuous surrogate, at a local level, can no longer adequately model the roughness of the objective function, making the addition of further points based on model variance inefficient.

6.3 Modeling Criticalities in Discrete Spaces and Methodological Proposal

The considerations exposed in this section derive from a critical analysis conducted *a posteriori* on the entire optimization process. Operational experience allowed highlighting limitations and emergent behaviors that, although theoretically predictable, manifested their real extent to the operator only during simulation activities.

6.3.1 The Impact of Parameter Discrete Nature

The main criticality lies in the intrinsically discrete nature of the design space which, despite the adoption of advanced kernels like Matérn (more robust

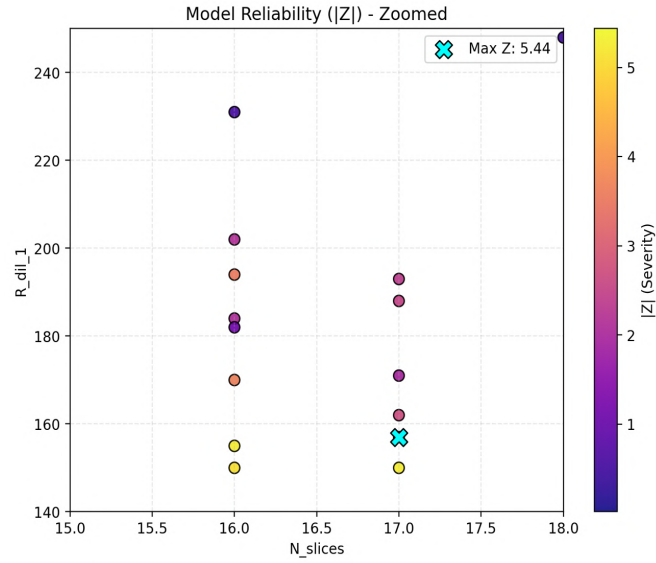


Figure 6.4: Analysis of the Z residual scatter plot highlighting local over-confidence phenomena.

than standard Kriging in handling irregularities), hinders the creation of a sufficiently regular and locally predictive response surface.

Exemplary is the impact of the parameter N_{slices} (number of combustor angular sectors): being an integer quantity, its variation induces discrete modifications not only on the computational mesh volume but also on mixer geometry and the total outflow area of dilution holes. This behavior was quantitatively confirmed during the pattern search phase: the transition from design point (16, 195) to (17, 195) — despite representing a unitary parametric variation — resulted in a sudden increase in EINOx from 7.81 g/kg to 9.32 g/kg. Jumps of such magnitude, also observed for parameter $r_{dil,1}$, confirm the presence of physical non-linearities and discontinuities that a continuous interpolator cannot capture without introducing artifacts or local estimation errors.

6.3.2 Optimization Workflow Revision

Analysis of encountered numerical instabilities falsified the intuitive assumption that "increasing point density monotonically improves the model". On the contrary, excessive local clustering in the presence of discontinuous responses degrades the global quality of the predictor. In light of this evidence, a methodological revision of the optimization workflow is proposed for future applications on analogous domains:

- **Pure Exploration Phase:** In early iterations, the surrogate should be guided exclusively by the global Expected Improvement criterion or space-filling logics, imposing minimum distance constraints between points to avoid premature clustering.
- **Decoupling Local Refinement:** Once promising areas are identified, local refinement (pattern search) should proceed independently of the global surrogate update. Points generated in this phase, being very

Numerical instabilities such as covariance matrix ill-conditioning problems required the adoption of an adaptive nugget in the Matérn kernel and precluded the use of the standard kernel.

close to each other, should not be re-inserted into the training database (to avoid numerical instabilities) but used as a validation set to verify local predictive capacity. Alternatively, replacing the original point in the database with the new refined point can be evaluated, provided this results in better representativeness of local behavior in the model, while avoiding the coexistence of quasi-coincident points.

- **Surrogate as "Qualitative Map":** The goal of the surrogate model must be limited to creating a "topological" map distinguishing macro-regions of interest (low emissions) from those to be discarded, renouncing the pretension of guiding fine convergence to the absolute minimum.
- **Physical Integration:** Final selection of optimum points must integrate physical criteria beyond numerical ones. It is necessary to exclude configurations that, while minimizing the mathematical objective function (EINO_x), present physically unstable or non-robust flame structures (e.g., risk of blow-off or flashback), thus avoiding wasted computational resources in refining technically inadmissible regions.

In conclusion, the hybrid approach outlined here aims to mitigate the "blindness" of the pure mathematical model, valuing the surrogate as a tool for qualitative exploration and delegating detailed optimization to punctual verification guided by the physics of the problem.

In subsequent paragraphs, a qualitative analysis of results will be performed, classifying the parameter space based on different observed flame structures, followed by a quantitative study of temperature distributions for the most representative configurations.

6.4 Phenomenological Analysis: Flame Structure Classification

To understand the physical reasons governing performance differences highlighted by the mathematical model, a qualitative analysis of flow and temperature fields was conducted. Starting from the response surface generated by the Matérn surrogate (fig. 6.5), the solution domain was subdivided into four macro-regions ("clusters") defined based on the NO_x production interval.

Within these zones, 16 representative simulated cases were selected and subjected to advanced post-processing via ANSYS CFD-Post. The analysis utilized two types of visualization:

- **3D Volumetric Rendering:** Generation of temperature isosurfaces ($T > 1550$ K) to identify the shape and extent of the flame core, together with 3D streamline visualization to trace fluid dynamic evolution inside the combustor.
- **Thermal Tomography:** Extraction of temperature profiles on 7 transverse planes perpendicular to the main outflow axis, positioned at strategic heights (from $z = 10$ mm to $z = 192$ mm, as per fig. 6.6), to evaluate mixture homogeneity and hot-spot persistence.

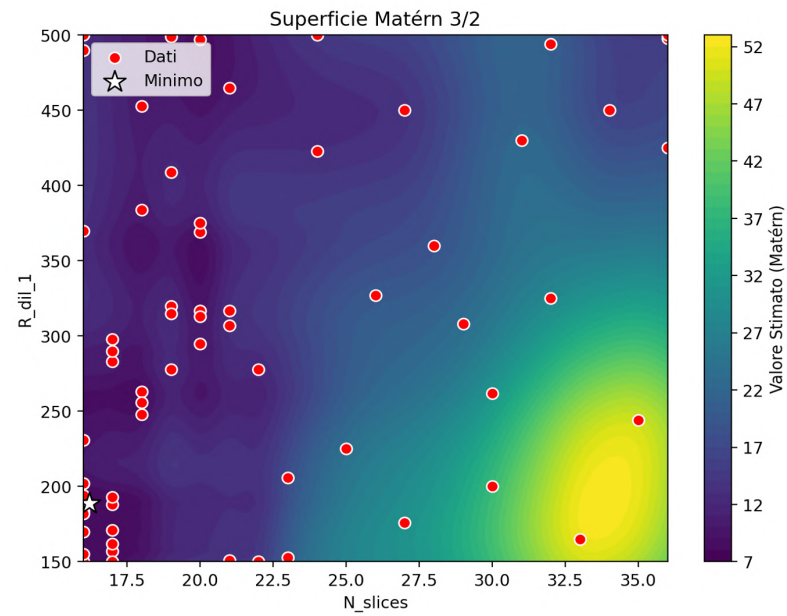


Figure 6.5: Response surface generated by the Matérn surrogate model.

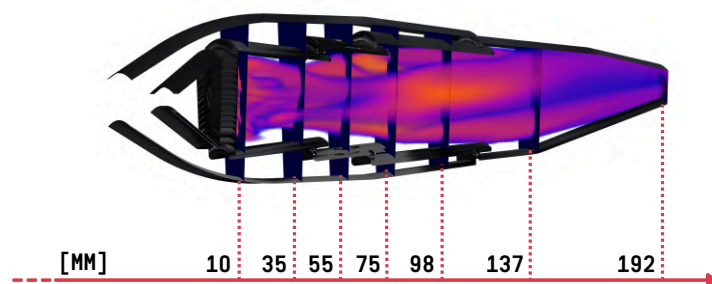


Figure 6.6: Positioning of transverse planes for thermal tomography analysis.

Based on observations, it was possible to reclassify the design space not only numerically but as a function of emergent flame topological structures. Figure 6.7 illustrates this classification, ordered from the highest performing configuration (A) to the critical one (D).

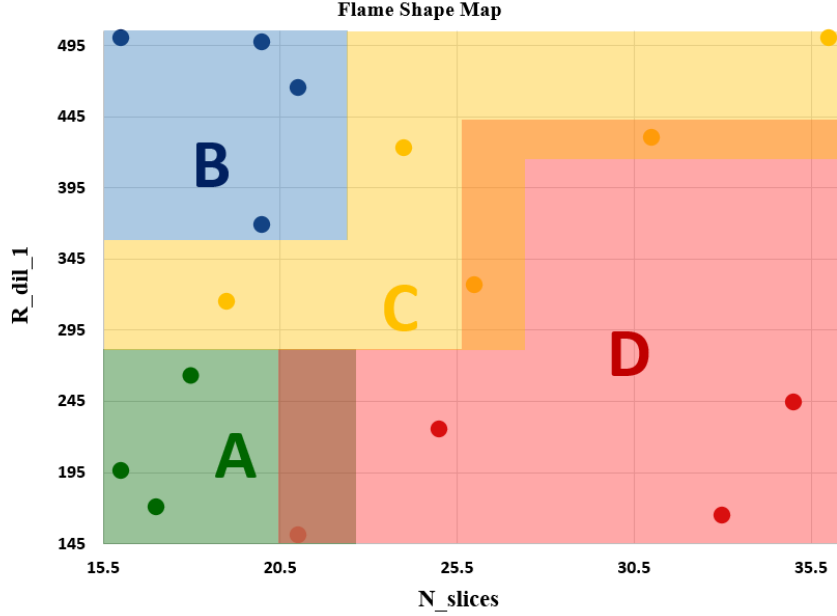


Figure 6.7: Map of flame structures classified by morphological typology.

The proposed classification is as follows:

- **Zone A (Green):** Low emissions ($EINO_x < 10$ g/kg). Sample mean: 8.15 g/kg.
- **Zone B (Light Blue):** Medium-low emissions ($10 \text{ g/kg} < EINO_x < 20$ g/kg). Sample mean: 10.32 g/kg.
- **Zone C (Yellow):** Medium-high emissions ($20 \text{ g/kg} < EINO_x < 30$ g/kg). Sample mean: 16.45 g/kg.
- **Zone D (Red):** High emissions ($EINO_x > 45$ g/kg). Sample mean: 41.55 g/kg.

Note: Intermediate case N21R151 showed hybrid characteristics, structurally positioning itself as a transition between topology A and topology D.

The four identified flame topologies are discussed in detail below.

6.4.1 Structure A – Distributed Flame ("Perforated Cross")

This configuration represents the design optimum. The interaction between mixer geometry and dilution jet penetration guarantees excellent mixing, allowing the reaction zone to distribute uniformly over much of the available volume ("perforated cross" topology). The absence of stagnant recirculations and effective dilution prevent the formation of concentrated high-temperature nuclei (hot-spots). Reaction occurs in a diffuse lean-premixed regime, minimizing thermal NO_x production.

6.4.2 Structure B – Bifurcated Flame ("Y-Shape")

Typical of configurations with high primary dilution radius values ($r_{dil,1}$), this structure is characterized by a concentration of hot flow in the central zone of the angular sector. Excessive inlet air flow ("primary air") tends to inhibit reaction at sector margins (local quenching effect or ultra-lean mixture), confining chemical activity to a central core assuming a "Y" shape. Although emissions remain contained, the lower spatial distribution of the flame favors the birth of minor hot-spots along the central axis.

6.4.3 Structure C – Tri-Columnar Flame ("III-Shape")

This topology emerges from the combination of low radial opening and strong primary air inflow. The evolution of the "Y" structure leads to the fragmentation of the flame front into three distinct vertical zones ("III-Shape"), distributed along the meridian direction. In this configuration, chemical kinetics appears significantly faster than local mixing: intense and localized temperature peaks are observed, especially in initial combustor sections, indicating combustion less controlled by dilution mechanisms.

6.4.4 Structure D – Edge Confined Flame ("- Shape")

This represents the worst-case in terms of emissions. Typically characterized by low values of $r_{dil,1}$ (and consequent strong air inflow in the secondary zone), this configuration pushes hot flow towards the azimuthal extremes of the angular sector (periodic walls). In these peripheral zones, mixing is poorly efficient and the fluid is less affected by the cooling effect of central dilution air. The result is a flame dominated by chemical kinetics ("fast chemistry") rather than mixing, with the formation of extreme hot-spots persisting to the outlet, generating massive quantities of nitrogen oxides.

In subsequent paragraphs, a more quantitative analysis of temperature distributions will be performed to corroborate the visual observations discussed here. To complete the morphological investigation, Appendix B contains the complete atlas of temperature sections for all analyzed cases, organized according to the proposed classification, to allow an overview of recurring structures.

6.5 Quantitative and Statistical Analysis of Flame Structures

To corroborate the morphological observations previously exposed, a quantitative statistical analysis was conducted on flow and temperature fields for the four representative cases (A, B, C, D). The investigation is based on the extraction of fluid dynamic data on twelve cut planes perpendicular to the main outflow axis (x). For each configuration, three fundamental indicators are presented:

- **Axial Temperature Statistics:** Trend of mean temperature and standard deviation ($\pm 1\sigma$) along the longitudinal combustor axis.

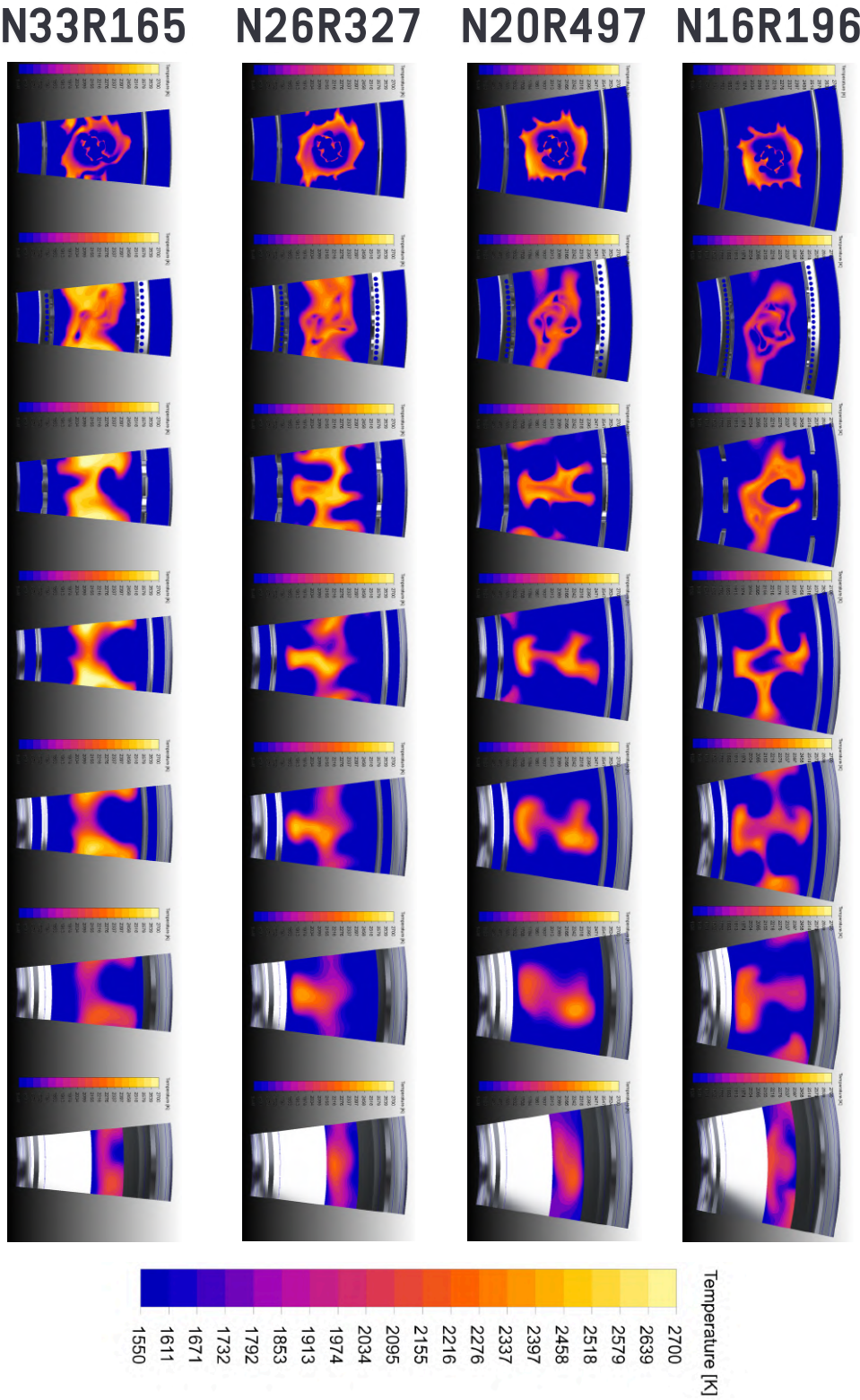


Figure 6.8: Visualization of flame evolution in the four highlighted structure typologies.

- **Cumulative Histograms (Stacked Plots):** Percentage distribution of fluid mass into temperature bands, to quantify the volume occupied by hot zones ($T > 2200$ K).
- **Scatter Plots (T vs Z):** Pointwise correlation between temperature and Mixture Fraction (Z).

The mixture fraction Z , used to trace the mixing progress state, was defined in this work as the total elemental mass fraction of hydrogen. Since the fuel is composed of pure hydrogen ($Y_{H,fuel} = 1$) and the oxidant is devoid of it ($Y_{H,ox} = 0$), this quantity acts as a normalized passive scalar ($0 \leq Z \leq 1$). Its calculation was performed by summing the weighted contributions of hydrogen-containing species according to the formula:

$$Z = Y_{H_2} + \frac{2.016}{18.015}Y_{H_2O} + \frac{1.008}{17.007}Y_{OH} + Y_H \quad (6.1)$$

Where Y_i represents the mass fraction of the i -th species (molecular hydrogen, water, hydroxyl radical, and atomic hydrogen) and numerical coefficients represent ratios between atomic/molecular masses to extract elemental H content.

6.5.1 Case A: N16R196 – The Global Optimum

Analysis of the optimal case quantitatively confirms the dominance of mixing mechanisms over chemical kinetics. Observing the axial statistical trend (fig. 6.10), an extremely gradual and quasi-linear increase in mean temperature relative to the axial coordinate is noted. Heat release is completed, marking the end of the primary reaction, only beyond half of the dilution zone ($z > 0.15$ m). Standard deviation (σ) remains contained, with punctual temperature peaks rarely exceeding 2500 K.

The mass distribution by temperature bands (fig. 6.11) highlights the absence of vast overheated regions: the fraction of fluid at very high temperature ($T > 2200$ K) remains marginal, never exceeding 10 % of the total mass passing through critical sections.

Of crucial importance is the analysis of the $T - Z$ scatter diagram (fig. 6.12). The point cloud (scatter) is positioned significantly below the adiabatic equilibrium curve, even near the stoichiometric mixture. This deviation is the physical signature of a high aerodynamic strain rate. Intense turbulence and strong velocity gradients induced by geometry generate a high scalar dissipation rate, which removes heat from the flame front faster than the chemical reaction can produce it to reach equilibrium. It is precisely this "strained flame" mechanism that limits thermal peaks and, consequently, thermal NO_x production.

6.5.2 Case B: N20R497 – The Competitor

Configuration B shows remarkable similarity to the optimum, confirming itself as a high-quality sub-optimal solution. Comparison of axial distributions (fig. 6.9) highlights minimal deviations: kinetics appear slightly faster in initial phases ($z < 0.05$ m), while maintaining comparable flame length. However, slightly higher local temperature peaks and greater standard deviation at the

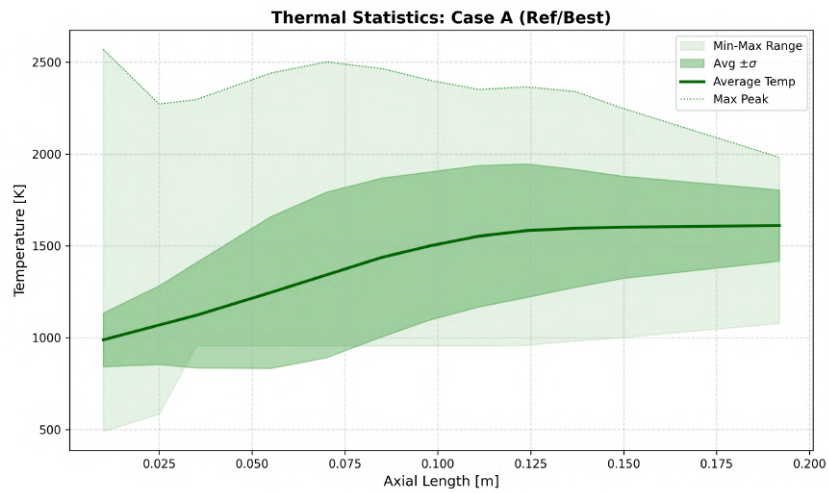


Figure 6.10: Axial trend of mean temperature and standard deviation for Case A.

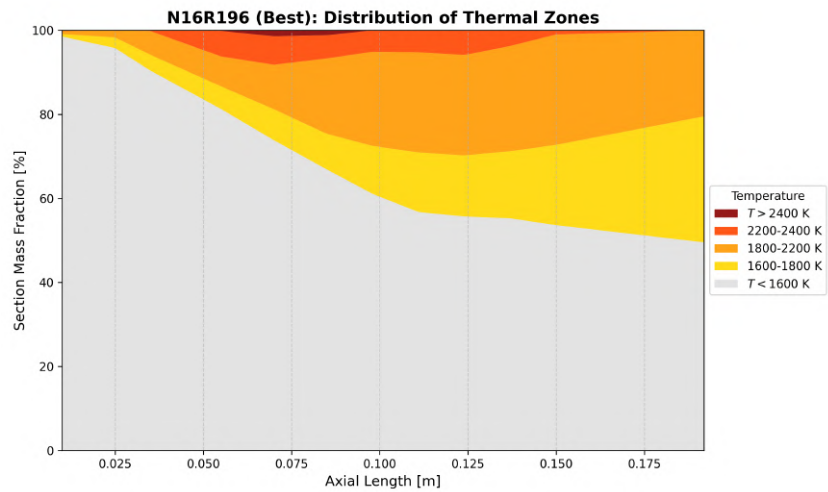


Figure 6.11: Cumulative histogram of mass distribution by temperature bands (Case A).

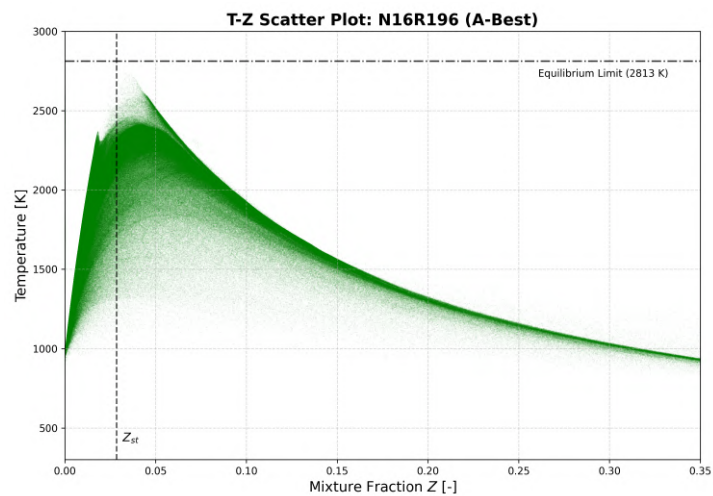


Figure 6.12: T-Z scatter plot for Case A highlighting deviation from adiabatic equilibrium.

combustor outlet are recorded, a symptom of lower outlet profile homogeneity (worse pattern factor).

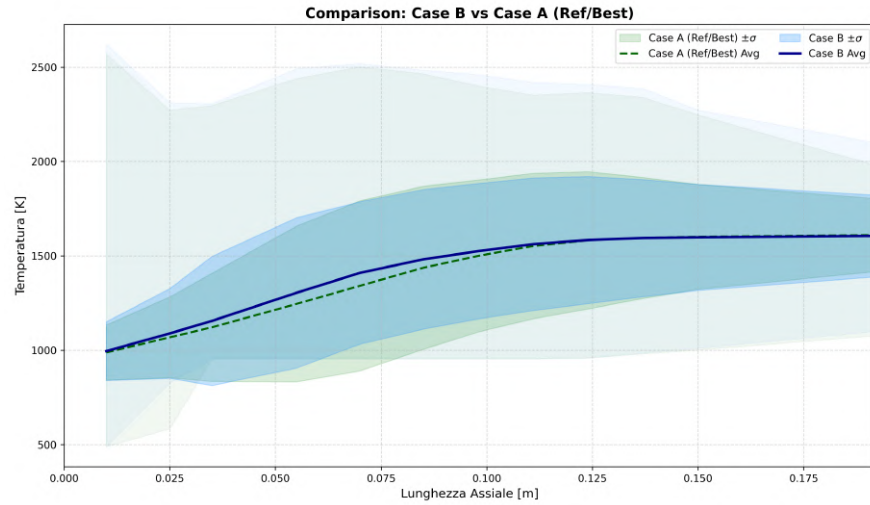


Figure 6.9: Comparison of axial thermal trends between Case A and Case B.

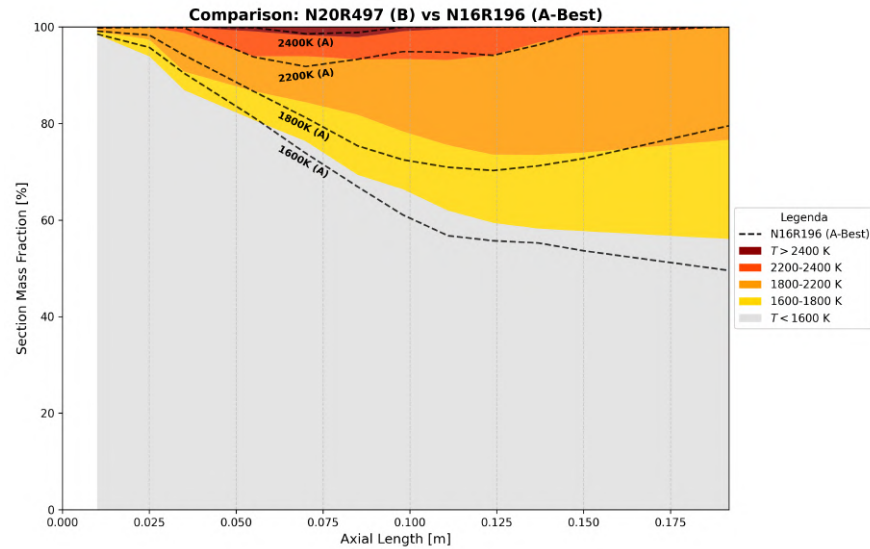


Figure 6.13: Cumulative histogram of mass distribution by temperature bands (Case B compared to Case A).

The scatter plot (fig. 6.14) also shows behavior analogous to case A, although the density of points near equilibrium temperature is slightly higher. These differences, albeit subtle, are sufficient to justify the recorded emissions increase ($EINO_x \approx 8.66$ vs 7.78 g/kg).

6.5.3 Case C: N26R327 – Transition to "Fast Chemistry" Regime

With case C, a radical change in combustion regime is observed. Heat release occurs abruptly (fig. 6.15): axial thermal gradients are steep and standard

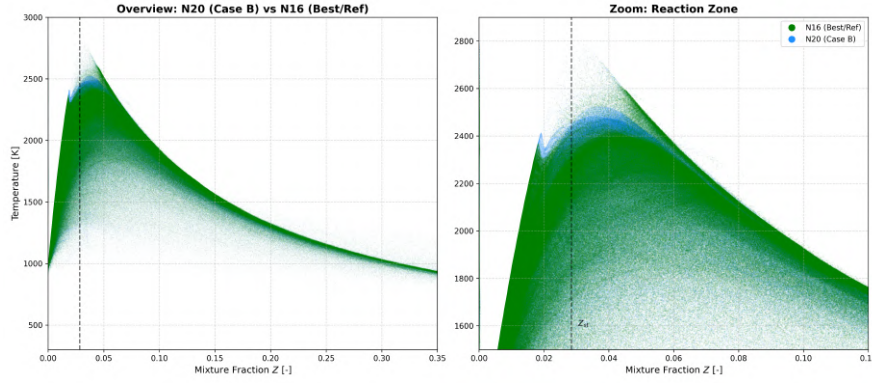


Figure 6.14: Comparison of T-Z scatter plots between Case A and Case B.

deviation in the primary zone ($x < 0.065$ m) is significantly wider compared to the optimal case.

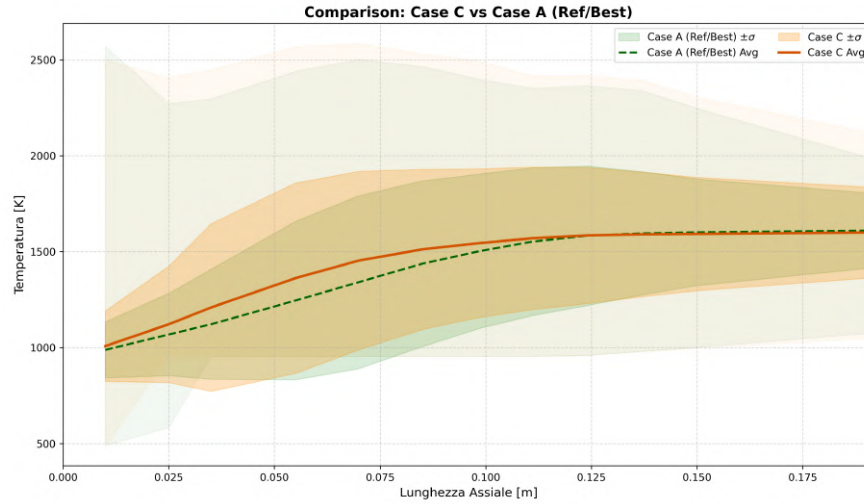


Figure 6.15: Comparison of axial thermal trends between Case A and Case C.

The mass histogram (fig. 6.16) quantifies this criticality: in the secondary zone, over 15 % of fluid mass is found at temperatures exceeding 2200 K. From the $T - Z$ graph (fig. 6.17), the lower impact of aerodynamic strain clearly emerges. Points in phase space frequently reach temperatures close to 2500 K around stoichiometric, indicating that mixing is not sufficiently rapid to prevent the attainment of local equilibrium conditions.

6.5.4 Case D: N33R165 – The Worst Case

Case D represents the extreme of phenomena observed in case C, outlining a structure dominated by fast chemistry limit. Heat release is exhausted almost instantaneously at the inlet of the dilution zone (fig. 6.18), with temperature peaks recording a marked increase, widely exceeding 2500 K.

The mass fraction analysis (fig. 6.19) is unmerciful: the extent of very high temperature zones ($T > 2200$ K) in this case exceeds that of medium temperature zones ($T > 1800$ K) of the optimal case.

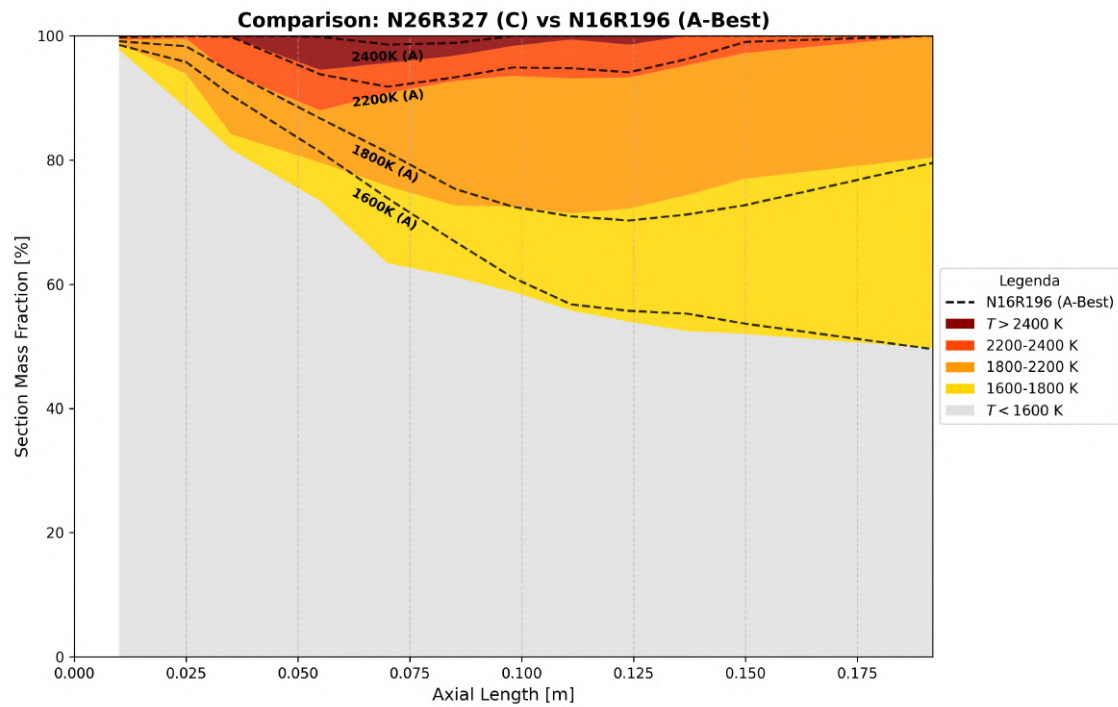


Figure 6.16: Cumulative histogram of mass distribution by temperature bands (Case C compared to Case A).

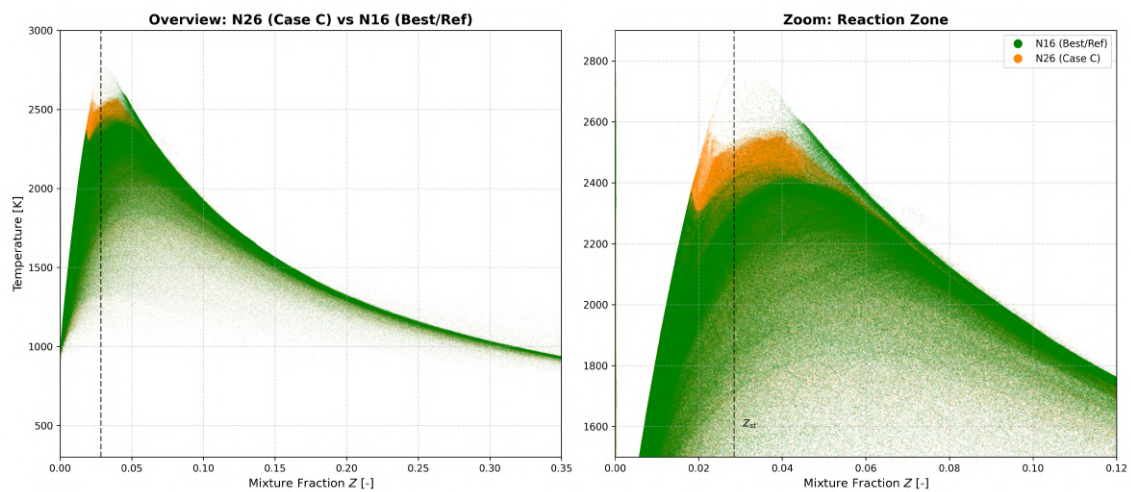


Figure 6.17: Comparison of T-Z scatter plots between Case C and Case A.

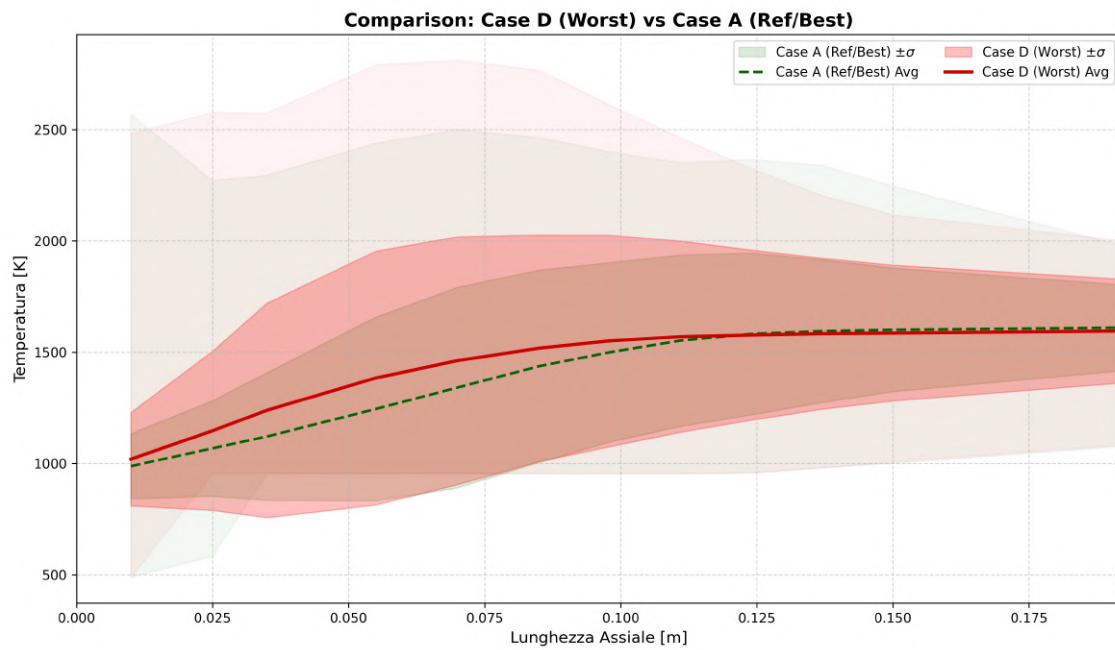


Figure 6.18: Comparison of axial thermal trends between Case A and Case D..

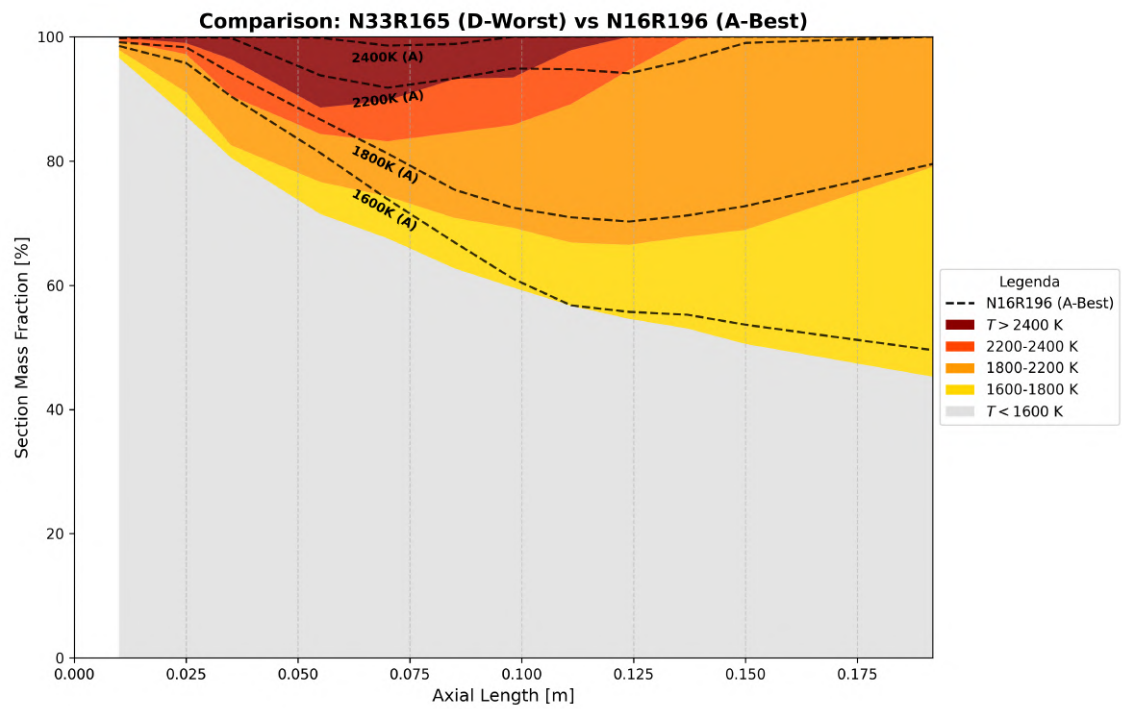


Figure 6.19: Cumulative histogram of mass distribution by temperature bands (Case D compared to Case A).

The final scatter plot (fig. 6.20) provides definitive proof: around stoichiometric mixture, point distribution touches the theoretical adiabatic limit ($T_{max} \approx 2813$ K). In these regions, the scalar dissipation rate is negligible; the flame is free to anchor and burn at the maximum possible temperature, maximizing NO_x production according to the Zeldovich mechanism.

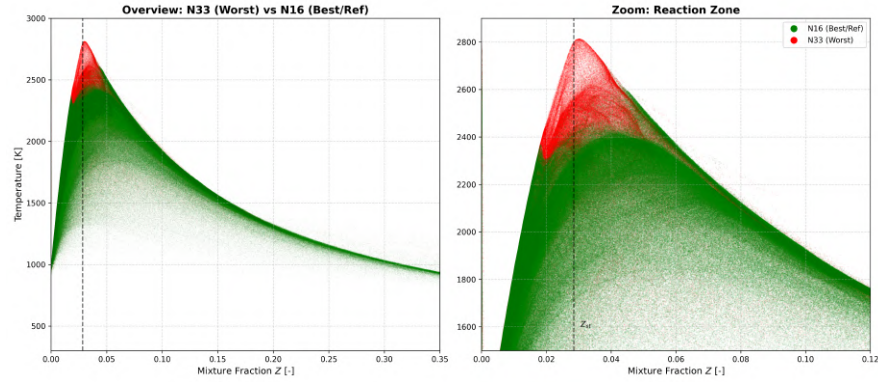


Figure 6.20: Comparison of T-Z scatter plots between Case A and Case D.

6.6 Overview and Performance Map

Ultimately, an attempt was made to synthesize nitrogen oxide formation mechanisms by correlating the two physical quantities governing their kinetics: temperature and residence time. Figure 6.21 maps the four configurations correlating high-temperature mass fraction with local mean axial velocity (assumed as an inverse proxy of residence time).

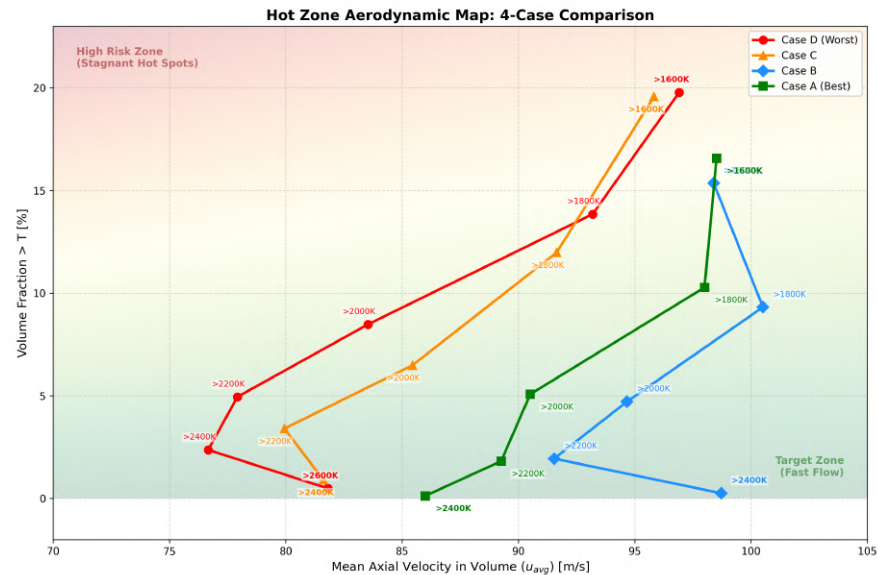


Figure 6.21: Performance map: correlation between high-temperature masses and mean axial velocity.

Theoretically, ideal configurations should locate in the bottom-right quadrant (minimal hot masses transported at high speed, thus low residence

time). Although this trend is verified for extreme cases (A vs D), an apparent anomaly is noted in the A-B comparison, where case B would seem to show more favorable mean velocities. This discrepancy highlights the limits of the one-dimensional assumption: mean axial velocity does not capture complex recirculation structures (toroidal vortices) essential for flame stabilization. It is probable that in case B, despite having high axial velocities, fluid remains trapped in high-temperature recirculation zones longer than suggested by the mean, or that the recirculation zone topology itself is less efficient in dissipating heat compared to the "distributed" design of case A.

Thesis Conclusions

The optimization work presented in this chapter allowed exploring and understanding the complex interaction between geometry and combustion physics in a hydrogen burner. Through a hybrid approach, combining the exploratory efficiency of surrogate models (Kriging/Matérn) with the local precision of pattern search, it was possible to identify a geometric configuration capable of reducing NO_x emissions by 62.18 % compared to the initial mean reference.

Post-hoc analyses revealed that such improvement is not the result of a simple parametric adjustment, but of a transition towards a different combustion regime. The optimal design (N16R196) favors a "distributed" flame structure, where interaction between jets and the central vortex maximizes aerodynamic strain rate. This prevents the mixture from staying in adiabatic equilibrium conditions, keeping peak temperatures systematically below the critical threshold for thermal Zeldovich mechanism activation.

Conversely, inefficient configurations (like case D) suffer from excessive geometric confinement inhibiting transverse mixing, leading to flames dominated by fast chemistry and the formation of vast thermal hot-spots. Although this study is limited by the use of steady RANS approximation — which does not allow investigating thermoacoustic instabilities or transient flashback phenomena — and by the discrete nature of geometric parameters, obtained results provide robust guidelines for preliminary design of fuel-flexible or hydrogen-based combustors, highlighting how maximizing macroscopic mixing remains the keystone for sustainable decarbonization of aeronautical propulsion.

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Appendices

Appendix A

Simulation Database

Analysis of operating parameters and optimization results

ABSTRACT

This database collects the CFD simulation results for the different combustor configurations. The nomenclature of symbols, the analytical formulations used for calculating performance indices, and the detailed results for each analyzed design point are reported below.

Database Reading Guide

1. Operating and Geometric Parameters

- N_{sl} : Number of angular sectors (slices) into which the domain is divided / number of injectors.
- R_{dil} : Radial position of primary dilution holes ($R \cdot 100$ [mm]).
- $\dot{m}_{air}, \dot{m}_{H_2}$: Inlet mass flow rates of air and hydrogen [kg/s].

2. Flow Field Results

- $\bar{U}_{out}$: Mean velocity of burnt gases at the outlet section [m/s].
- $T_{max}, T_{min}, T_{avg}$: Maximum, minimum, and mass-weighted average temperatures on the outlet surface [K].

3. Quality and Emission Indices

OPF (Overall Pattern Factor): Outlet temperature profile non-uniformity index. Low values indicate better mixing.

$$OPF = \frac{T_{max} - T_{avg}}{T_{avg}} \quad (A.1)$$

NPF (Normalized Pattern Factor): Outlet temperature profile non-uniformity index. Low values indicate better mixing.

$$NPF = \frac{T_{max} - T_{min}}{T_{avg}} \quad (A.2)$$

EINOx (Emission Index of NOx): Grams of nitrogen oxides produced per kilogram of fuel burned.

$$EINOx = \frac{Y_{NOx} \dot{m}_{air}}{\dot{m}_{fuel}} \times 1000 \quad \left[\frac{g_{NOx}}{kg_{fuel}} \right] \quad (A.3)$$

4. Optimization Metrics

Parameters related to the optimization algorithm (Kriging / Pattern Search):

- **Type:** Point generation strategy (e.g., initial *Database*, local *Pattern Search*, *Exploitation*).
- **EI (Expected Improvement):** Expected Improvement value of the objective function.
- **Kernel / Nugget:** Statistical hyperparameters of the surrogate model (Gaussian Process).
- **Δ Values [%]:** Percentage deviation from the expected value (E_{NOx}), the average value (DB_{avg}), or the minimum value (DB_{min}) of the reference database.

Title: N(N_{sl}) R(R_{dil})

N_{sl} [–]	R_{dil} [100 · mm]	$\dot{m}_{air}$ [m/s]	$\dot{m}_{H2}$ [m/s]	$\bar{U}_{out}$ [m/s]	T_{max} [K]	T_{min} [K]	T_{avg} [K]
OPF		NPF		Y_{NOx}		$EINOx$ [g/kg]	

N(36) R(425)

36	425	27.5	0.199	271.126	1890.734	1048.486	1597.137
0.184		0.527		1.35e-04		18.633	

N(35) R(244)

35	244	27.5	0.199	270.199	2038.834	1081.641	1593.756
0.279		0.601		3.58e-04		49.408	

N(34) R(450)

34	450	27.497	0.199	271.595	1820.537	1077.13	1599.501
0.138		0.465		1.19e-04		16.44	

N(33) R(165)

33	165	27.501	0.199	270.823	2002.294	1083.068	1596.271
0.254		0.576		3.73e-04		51.552	

N(32) R(494)

32	494	27.5	0.2	270.88	2045.359	1041.759	1596.79
0.281		0.629		1.50e-04		20.72	

N(31) R(430)

31	430	27.499	0.2	271.188	2071.454	1057.19	1597.882
0.296		0.635		1.62e-04		22.357	

N(30) R(262)

30	262	27.503	0.2	271.804	1936.978	1060.541	1600.587
0.21		0.548		2.24e-04		30.853	

N(29) R(308)

29	308	27.5	0.2	271.948	1915.864	1082.005	1601.159
0.197		0.521		1.70e-04		23.373	

N(28) R(360)

28	360	27.498	0.2	272.006	1943.138	1087.836	1602.019
0.213		0.534		1.36e-04		18.733	

N(27) R(176)

27	176	27.506	0.2	271.605	2032.943	1047	1600.212
0.27		0.616		2.20e-04		30.128	

N(26) R(327)

26	327	27.5	0.2	271.343	2115.672	1050.619	1599.858
0.322		0.666		1.43e-04		19.591	

Title: $N(N_{sl})$ $R(R_{dil})$

N_{sl} [–]	R_{dil} [100 · mm]	$\dot{m}_{air}$ [m/s]	$\dot{m}_{H2}$ [m/s]	$\bar{U}_{out}$ [m/s]	T_{max} [K]	T_{min} [K]	T_{avg} [K]
OPF		NPF		Y_{NOx}		$EINOx$ [g/kg]	

N(25) R(225)

25	225	27.501	0.201	273.342	1819.67	1078.545	1607.825
0.132		0.461		1.73e-04		23.678	

N(24) R(423)

24	423	27.5	0.201	271.282	2041.163	1024.635	1600.166
0.276		0.635		9.55e-05		13.051	

N(23) R(206)

23	206	27.5	0.201	271.707	2010.111	1041.655	1601.516
0.255		0.605		1.29e-04		17.674	

N(22) R(278)

22	278	27.499	0.202	272.895	2087.581	1087.802	1606.276
0.3		0.622		9.09e-05		12.387	

N(21) R(465)

21	465	27.5	0.201	271.49	2130.066	1038.714	1601.199
0.33		0.682		7.39e-05		10.091	

N(20) R(295)

20	295	27.5	0.202	273.531	2020.359	1118.591	1608.418
0.256		0.561		7.40e-05		10.08	

N(19) R(409)

19	409	27.499	0.203	270.696	2415.32	1038.066	1597.843
0.512		0.862		8.98e-05		12.196	

N(18) R(384)

18	384	27.5	0.202	272.137	2338.263	1110.534	1604.842
0.457		0.765		7.69e-05		10.45	

N(17) R(188)

17	188	27.499	0.202	273.163	2017.722	1033.668	1608.108
0.255		0.612		5.99e-05		8.137	

N(16) R(370)

16	370	27.498	0.203	270.97	2416.46	1033.336	1601.052
0.509		0.864		9.48e-05		12.856	

Title: N(N_{sl}) R(R_{dil})

N_{sl} []	R_{dil} [100 · mm]	$\dot{m}_{air}$ [m/s]	$\dot{m}_{H2}$ [m/s]	$\bar{U}_{out}$ [m/s]	T_{max} [K]	T_{min} [K]	T_{avg} [K]
<i>OPF</i>		<i>NPF</i>		Y_{NOx}		E_{INOx} [g/kg]	
<i>Iter</i>		#Data		<i>Label</i>		<i>Type</i>	
<i>EI</i>	E_{NOx}	ΔE_{NOx} [%]	ΔDB_{avg} [%]	ΔDB_{min} [%]		Kernel	Nugget

N(18) R(248)

18	248	27.5	0.202	274.108	1992.238	1129.912	1611.06
0.237		0.535		6.81e-05		9.25	
1		22		20EI/14E.min		Exploration	
1.72	6.433	43.79	-55.08	13.68		STD	1e-8

N(18) R(263)

18	263	27.5	0.202	274.309	1939.472	1125.682	1611.816
0.203		0.505		6.29e-05		8.548	
1		23		12EI/13E.min		Exploration	
1.725	6.429	32.97	-58.48	5.06		STD	1e-8

N(18) R(256)

18	256	27.495	0.202	274.234	1940.783	1131.452	1611.796
0.204		0.502		6.33e-05		8.605	
1		24		1EI/1E.min		Exploitation	
1.738	6.414	34.14	-58.21	5.75		STD	1e-8

N(36) R(498)

36	498	27.5	0.199	271.49	1873.979	1041.089	1598.329
0.172		0.521		1.09e-04		15.103	
2		25		3EI/3E.min		Exploration	
6.544	1.603	842.31	-26.65	85.61		STD	1e-8

N(16) R(231)

16	231	27.499	0.203	273.032	2083.214	1054.376	1608.224
0.295		0.64		7.10e-05		9.632	
2		26		10EI/9E.min		Exploration	
6.311	1.826	427.54	-53.22	18.38		STD	1e-8

N(36) R(500)

36	500	27.5	0.199	271.574	1865.504	1047.56	1598.674
0.167		0.512		1.08e-04		14.933	
2		27		1EI/1E.min		Exploitation	
7.003	1.141	1208.43	-27.48	83.52		STD	1e-8

N(17) R(283)

17	283	27.499	0.202	272.559	2178.157	1039.299	1605.576
0.357		0.709		7.60e-05		10.332	
3		28		14EI/14E.min		Exploration	
2.438	5.699	81.3	-49.82	26.98		STD	1e-8

Title: N(N_{sl}) R(R_{dil})

N_{sl} []	R_{dil} [100 · mm]	$\dot{m}_{air}$ [m/s]	$\dot{m}_{H2}$ [m/s]	$\bar{U}_{out}$ [m/s]	T_{max} [K]	T_{min} [K]	T_{avg} [K]
<i>OPF</i>		<i>NPF</i>		Y_{NOx}		E_{INOx} [g/kg]	
<i>Iter</i>		#Data		<i>Label</i>		<i>Type</i>	
<i>EI</i>	E_{NOx}	ΔE_{NOx} [%]	ΔDB_{avg} [%]	ΔDB_{min} [%]		Kernel	Nugget

N(17) R(298)

17	298	27.499	0.202	272.198	2246.503	1032.459	1604.305
0.4		0.757		8.11e-05		11.025	
3		29		15EI/15E.min		Exploration	
2.433	5.703	93.31	-46.45	35.5		STD	1e-8

N(17) R(290)

17	290	27.499	0.202	272.603	2208.848	1033.487	1605.784
0.376		0.732		7.63e-05		10.363	
3		30		1EI/1E.min		Exploitation	
2.456	5.681	82.43	-49.67	27.36		STD	1e-8

N(16) R(490)

16	490	27.498	0.203	270.576	2416.596	1051.276	1598.207
0.512		0.854		9.82e-05		13.314	
4		31		9EI/9E.min		Exploration	
75.547	-67.395	119.76	-35.34	63.63		STD	1e-8

N(16) R(500)

16	500	27.498	0.203	270.335	2416.452	1048.138	1596.874
0.513		0.857		9.65e-05		13.086	
4		32		1EI/1E.min		Exploitation	
85.713	-77.544	116.88	-36.45	60.83		STD	1e-8

N(24) R(500)

24	500	27.5	0.201	271.545	2134.276	1007.862	1601.207
0.333		0.703		1.05e-04		14.393	
5		33		19EI/19E.min		Exploration	
18.289	-10.119	242.24	-30.1	76.89		STD	1e-8

N(16) R(150)

16	150	27.498	0.203	273.293	2056.766	1073.881	1609.156
0.278		0.611		6.07e-05		8.239	
5		34		1EI/1E.min		Exploitation	
33.393	-25.257	132.62	-59.98	1.26		STD	1e-8

N(23) R(153)

23	153	27.499	0.201	271.685	2019.684	1022	1601.389
0.261		0.623		1.47e-04		20.117	
6		35		19EI/19E.min		Exploration	
14.729	-6.077	431.05	-2.3	147.24		STD	1e-8

Title: N(N_{sl}) R(R_{dil})

N_{sl} []	R_{dil} [100 · mm]	$\dot{m}_{air}$ [m/s]	$\dot{m}_{H2}$ [m/s]	$\bar{U}_{out}$ [m/s]	T_{max} [K]	T_{min} [K]	T_{avg} [K]
<i>OPF</i>		<i>NPF</i>		Y_{NOx}		E_{INOx} [g/kg]	
<i>Iter</i>		#Data		<i>Label</i>		<i>Type</i>	
<i>EI</i>	E_{NOx}	ΔE_{NOx} [%]	ΔDB_{avg} [%]	ΔDB_{min} [%]		Kernel	Nugget

N(21) R(151)

21	151	27.5	0.201	272.818	1925.533	1068.512	1605.697
0.199		0.534		1.04e-04		14.153	
6		36		4EI/4E.min		Exploration	
18.672	-10.137	239.61	-31.26	73.94		STD	1e-8

N(22) R(150)

22	150	27.499	0.202	273.286	1964.731	1063.15	1607.331
0.222		0.561		1.08e-04		14.769	
6		37		1EI/1E.min		Exploitation	
19.628	-11.1	233.06	-28.27	81.51		STD	1e-8

N(19) R(278)

19	278	27.499	0.203	272.787	2172.31	1014.672	1606.355
0.352		0.721		9.02e-05		12.248	
7		38		20EI		Exploration	
1.556	9.783	25.19	-40.52	50.52		STD	1e-8

N(16) R(155)

16	155	27.498	0.203	273.569	1981.871	1069.584	1610.179
0.231		0.567		6.25e-05		8.48	
7		39		6E.min		Exploitation	
none	8.232	3.01	-58.81	4.22		STD	1e-8

N(16) R(170)

16	170	27.499	0.203	273.449	2024.901	1068.946	1609.575
0.258		0.594		5.99e-05		8.121	
///		40		///		Database	
///	8.384	-3.13	-60.56	-0.2		STD	1e-8

N(21) R(307)

21	307	27.5	0.201	271.999	2139.153	1021.316	1602.624
0.335		0.698		9.61e-05		13.13	
8		41		none		Exploration	
none	11.337	15.82	-36.23	61.37		STD	0

N(21) R(317)

21	317	27.5	0.201	271.932	2167.895	1020.83	1602.304
0.353		0.716		9.51e-05		12.985	
8		42		none		Exploration	
none	11.245	15.47	-36.94	59.58		STD	0

Title: $N(N_{sl})$ $R(R_{dil})$

N_{sl} []	R_{dil} [100 · mm]	$\dot{m}_{air}$ [m/s]	$\dot{m}_{H2}$ [m/s]	$\bar{U}_{out}$ [m/s]	T_{max} [K]	T_{min} [K]	T_{avg} [K]
<i>OPF</i>		<i>NPF</i>		Y_{NOx}		E_{INOx} [g/kg]	
<i>Iter</i>		#Data		<i>Label</i>		<i>Type</i>	
<i>EI</i>	E_{NOx}	ΔE_{NOx} [%]	ΔDB_{avg} [%]	ΔDB_{min} [%]		Kernel	Nugget

N(16) R(194)

16	194	27.499	0.203	273.491	1997.893	1068.532	1609.697
0.241		0.577		5.90e-05		8.006	
8		43		17EI/17E.min		Exploration	
2.721	5.401	48.25	-61.11	-1.6		STD	0

N(16) R(202)

16	202	27.499	0.203	273.394	2010.835	1067.579	1609.481
0.249		0.586		6.73e-05		9.125	
8		44		2EI/2E.min		Exploitation	
3.111	5.015	81.96	-55.68	12.15		STD	0

N(19) R(320)

19	320	27.501	0.203	272.529	2262.782	1014.99	1605.134
0.41		0.777		8.96e-05		12.163	
9		45		10EI		Exploration	
1.788	10.361	17.4	-40.93	49.49		STD	0

N(16) R(184)

16	184	27.499	0.203	273.448	2016.387	1067.703	1609.627
0.253		0.589		6.19e-05		8.401	
9		46		1E.min		Exploitation	
none	7.38	13.85	-59.2	3.25		STD	0

N(19) R(315)

19	315	27.501	0.203	272.543	2268.75	1013.105	1605.276
0.413		0.782		9.07e-05		12.323	
9		47		1EI		Exploration	
1.85	9.926	24.15	-40.15	51.45		STD	0

N(20) R(317)

20	317	27.5	0.202	273.595	2044.786	1112.495	1608.54
0.271		0.58		7.13e-05		9.714	
9		48		15E.min		Exploitation	
none	7.563	28.43	-52.82	19.38		STD	0

N(20) R(313)

20	313	27.5	0.202	273.462	2055.705	1102.296	1608.2
0.278		0.593		7.24e-05		9.864	
9		49		///		Exploitation	
///	7.611	29.6	-52.09	21.23		STD	0

Title: N(N_{sl}) R(R_{dil})

N_{sl} []	R_{dil} [100 · mm]	$\dot{m}_{air}$ [m/s]	$\dot{m}_{H2}$ [m/s]	$\bar{U}_{out}$ [m/s]	T_{max} [K]	T_{min} [K]	T_{avg} [K]
<i>OPF</i>		<i>NPF</i>		Y_{NOx}		$EINOx$ [g/kg]	
<i>Iter</i>		#Data		<i>Label</i>		<i>Type</i>	
<i>EI</i>	E_{NOx}	ΔE_{NOx} [%]	ΔDB_{avg} [%]	ΔDB_{min} [%]		Kernel	Nugget

N(17) R(157)

17	157	27.499	0.202	273.11	2039.524	1049.764	1607.855
0.268		0.616		6.06e-05		8.232	
///		50		none		Database	
none	9.455	-12.94	-60.02	1.17		STD	0

N(16) R(182)

16	182	27.499	0.203	273.262	2037.107	1064.613	1609.001
0.266		0.604		6.19e-05		8.401	
9		51		4E.min		Exploitation	
none	7.398	13.55	-59.2	3.24		STD	0

N(20) R(369)

20	369	27.5	0.202	272.713	2110.686	1124.485	1606.639
0.314		0.614		6.92e-05		9.428	
10		52		5EI		Exploration	
0.713	8.363	12.73	-54.21	15.87		Matèrn 3/2	variable

N(20) R(375)

20	375	27.5	0.202	272.348	2188	1129.908	1605.344
0.363		0.659		7.58e-05		10.328	
10		53		6EI		Exploration	
0.707	8.39	23.09	-49.84	26.93		Matèrn 3/2	variable

N(17) R(150)

17	150	27.499	0.202	273.008	2063.957	1043.848	1607.417
0.284		0.635		6.39e-05		8.686	
10		54		1E.min		Exploitation	
none	7.944	9.34	-57.82	6.75		Matèrn 3/2	variable

N(17) R(171)

17	171	27.499	0.202	273.069	2033.476	1044.432	1607.697
0.265		0.615		5.97e-05		8.111	
10		55		4E.min		Exploitation	
none	7.954	1.97	-60.61	-0.32		Matèrn 3/2	variable

N(20) R(497)

20	497	27.5	0.202	272.375	2099.819	1100.065	1605.287
0.308		0.623		6.36e-05		8.661	
11		56		10EI		Exploration	
0.767	10.418	-16.87	-57.93	6.45		Matèrn 3/2	variable

Title: N(N_{sl}) R(R_{dil})

N_{sl} []	R_{dil} [100 · mm]	$\dot{m}_{air}$ [m/s]	$\dot{m}_{H2}$ [m/s]	$\bar{U}_{out}$ [m/s]	T_{max} [K]	T_{min} [K]	T_{avg} [K]
<i>OPF</i>		<i>NPF</i>		Y_{NOx}		E_{INOx} [g/kg]	
<i>Iter</i>		#Data		<i>Label</i>		<i>Type</i>	
<i>EI</i>	E_{NOx}	ΔE_{NOx} [%]	ΔDB_{avg} [%]	ΔDB_{min} [%]		Kernel	Nugget

N(19) R(499)

19	499	27.499	0.203	271.556	2156.829	1075.234	1602.673
0.346		0.675		7.03e-05		9.545	
11		57		2EI		Exploration	
0.8	11.036	-13.51	-53.64	17.31		Matèrn 3/2	variable

N(17) R(162)

17	162	27.499	0.202	273.08	2041.439	1040.402	1607.734
0.27		0.623		6.14e-05		8.343	
11		58		4E.min		Exploitation	
none	7.892	5.71	-59.48	2.54		Matèrn 3/2	variable

N(18) R(453)

18	453	27.5	0.202	271.769	2357.912	1105.852	1603.589
0.47		0.781		7.72e-05		10.49	
12		59		1EI		Exploration	
0.344	11.143	-5.86	-49.05	28.92		Matèrn 3/2	variable

N(17) R(193)

17	193	27.499	0.202	273.066	2051.864	1037.467	1607.653
0.276		0.631		6.15e-05		8.358	
12		60		1E.min		Exploitation	
none	7.919	5.55	-59.41	2.72		Matèrn 3/2	variable

N(27) R(450)

27	450	27.506	0.201	272.025	2054.075	1044.869	1601.77
0.282		0.63		9.99e-05		13.71	
///		61		none		Database	
none	17.338	-20.93	-33.41	68.49		Matèrn 3/2	variable

N(30) R(200)

30	200	27.503	0.2	272.005	1933.483	1086.754	1601.317
0.207		0.529		2.75e-04		37.855	
///		62		none		Database	
none	38.267	-1.08	83.85	365.24		Matèrn 3/2	variable

N(32) R(325)

32	325	27.5	0.2	269.842	2029.023	1045.308	1592.96
0.274		0.618		2.07e-04		28.51	
///		63		none		Database	
none	26.253	8.6	38.46	250.38		Matèrn 3/2	variable

Title: $N(N_{sl})$ $R(R_{dil})$

N_{sl} []	R_{dil} [100 · mm]	$\dot{m}_{air}$ [m/s]	$\dot{m}_{H2}$ [m/s]	$\bar{U}_{out}$ [m/s]	T_{max} [K]	T_{min} [K]	T_{avg} [K]
OPF		NPF		Y_{NOx}		$EINOx$ [g/kg]	
$Iter$		#Data		ΔDB_{avg} [%]		ΔDB_{min} [%]	

N(17) R(194)

17	194	27.499	0.202	273.121	2048.667	1042.019	1607.889
0.274		0.626		6.30e-05		8.56	
Pattern Search		64		-58.43		5.2	

N(16) R(193)

16	193	27.499	0.203	273.178	2059.235	1068.317	1608.616
0.28		0.616		6.42e-05		8.714	
Pattern Search		65		-57.68		7.1	

N(16) R(195)

16	195	27.499	0.203	273.573	1990.19	1056.447	1610.018
0.236		0.58		5.76e-05		7.812	
Pattern Search		66		-62.06		-3.98	

N(17) R(195)

17	195	27.499	0.202	272.978	2079.979	1036.517	1607.406
0.294		0.649		6.86e-05		9.319	
Pattern Search		67		-54.74		14.53	

N(16) R(196)

16	196	27.499	0.203	273.583	1981.67	1076.919	1609.966
0.231		0.562		5.74e-05		7.786	
Pattern Search		68		-62.18		-4.31	

N(17) R(196)

17	196	27.499	0.202	272.985	2078.194	1039.877	1607.493
0.293		0.646		6.57e-05		8.926	
Pattern Search		69		-56.65		9.7	

N(16) R(197)

16	197	27.499	0.203	273.359	2036.396	1058.66	1609.286
0.265		0.608		6.04e-05		8.198	
Pattern Search		70		-60.19		0.75	

N(16) R(171)

16	171	27.499	0.203	273.144	2087.285	1075.567	1608.557
0.298		0.629		6.76e-05		9.164	
Pattern Search		71		-55.49		12.63	

Title: $N(N_{sl})$ $R(R_{dil})$

N_{sl} []	R_{dil} [100 · mm]	$\dot{m}_{air}$ [m/s]	$\dot{m}_{H2}$ [m/s]	$\bar{U}_{out}$ [m/s]	T_{max} [K]	T_{min} [K]	T_{avg} [K]
<i>OPF</i>		<i>NPF</i>		Y_{NOx}		$EINOx$ [g/kg]	
<i>Iter</i>		#Data		ΔDB_{avg} [%]		ΔDB_{min} [%]	

N(16) R(198)

16	198	27.499	0.203	273.36	2032.568	1066.387	1609.373
0.263		0.6		6.12e-05		8.304	
Pattern Search		72		-59.67		2.06	

N(17) R(170)

17	170	27.499	0.202	273.067	2045.966	1039.642	1607.698
0.273		0.626		6.20e-05		8.426	
Pattern Search		73		-59.08		3.56	

N(17) R(172)

17	172	27.499	0.202	272.976	2058.098	1045.477	1607.438
0.28		0.63		6.43e-05		8.736	
Pattern Search		74		-57.57		7.37	

Appendix B

Flame Structure Atlas

Topological classification and visual analysis of CFD results

ABSTRACT

This appendix collects detailed visualizations of the thermal fields for the 16 selected representative cases. Each sheet reports the geometric configuration, performance indices, and a tomographic section of the temperature field, classified according to the morphological taxonomy (A-B-C-D) defined in Chapter 6.

Classification Legend

The sheets are color-coded based on the identified flame structure typology:

- | | |
|----------|---|
| A | Case A (Green) - Ref/Best: Distributed structure. Low emissions. |
| B | Case B (Blue): Bifurcated structure. Medium-low emissions. |
| C | Case C (Orange): Tri-columnar structure. Medium-high emissions. |
| D | Case D (Red) - Worst: Confined structure. High emissions. |

1. Operating and Geometric Parameters

- N_{sl} : Number of angular sectors (slices) into which the domain is divided / number of injectors.
- R_{dil} : Radial position of primary dilution holes ($R \cdot 100$ [mm]).
- $\dot{m}_{air}, \dot{m}_{H2}$: Inlet mass flow rates of air and hydrogen [kg/s].

2. Flow Field Results

- T_{max} : Maximum temperature at combustor outlet [K].

3. Quality and Emission Indices

OPF (Overall Pattern Factor): Outlet temperature profile non-uniformity index. Low values indicate better mixing.

$$OPF = \frac{T_{max} - T_{avg}}{T_{avg}} \quad (\text{B.1})$$

NPF (Normalized Pattern Factor): Outlet temperature profile non-uniformity index. Low values indicate better mixing.

$$NPF = \frac{T_{max} - T_{min}}{T_{avg}} \quad (B.2)$$

EINO_x (Emission Index of NO_x): Grams of nitrogen oxides produced per kilogram of fuel burned.

$$EINO_x = \frac{Y_{NO_x} \dot{m}_{air}}{\dot{m}_{fuel}} \times 1000 \left[\frac{g_{NO_x}}{kg_{fuel}} \right] \quad (B.3)$$

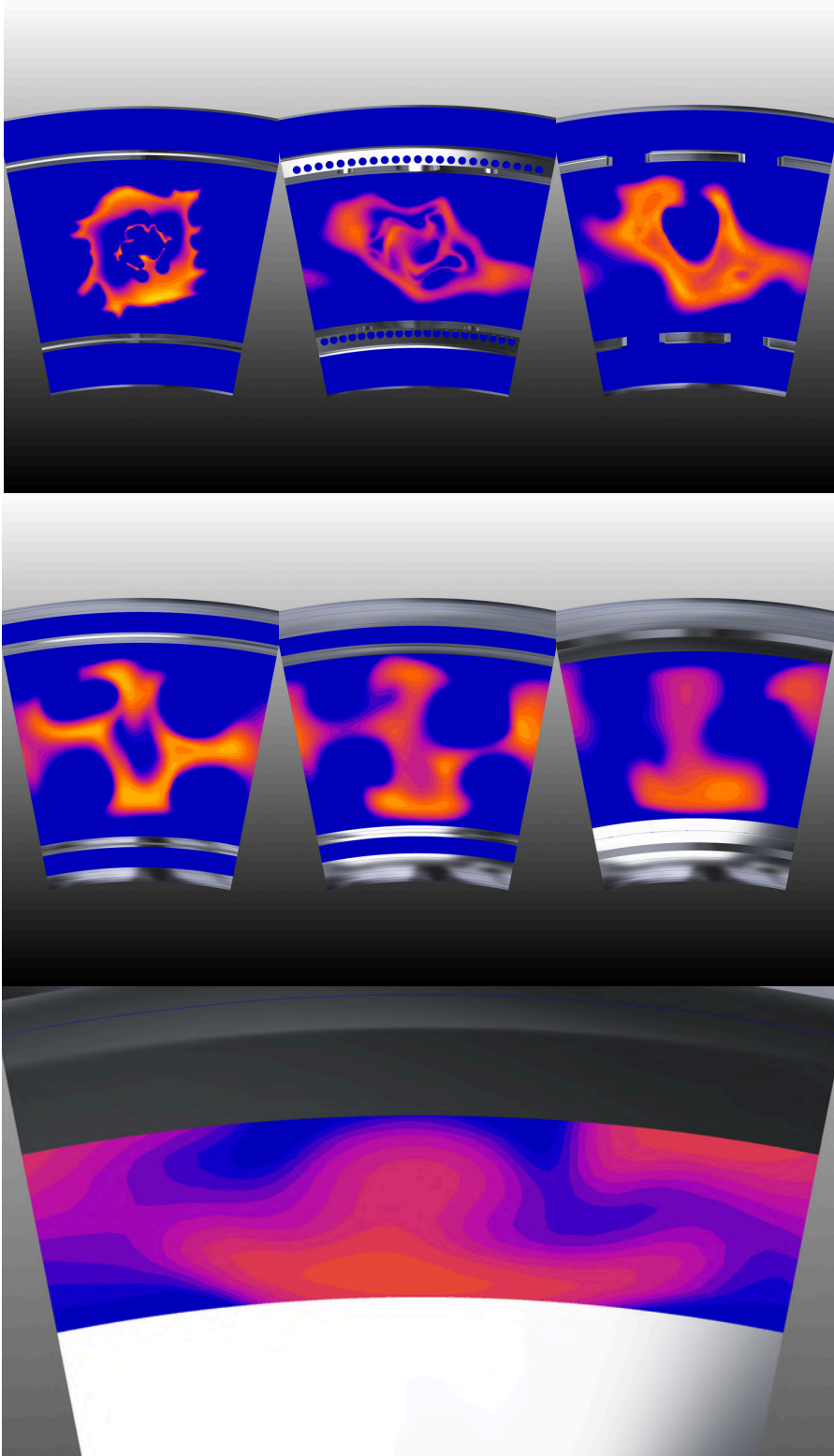
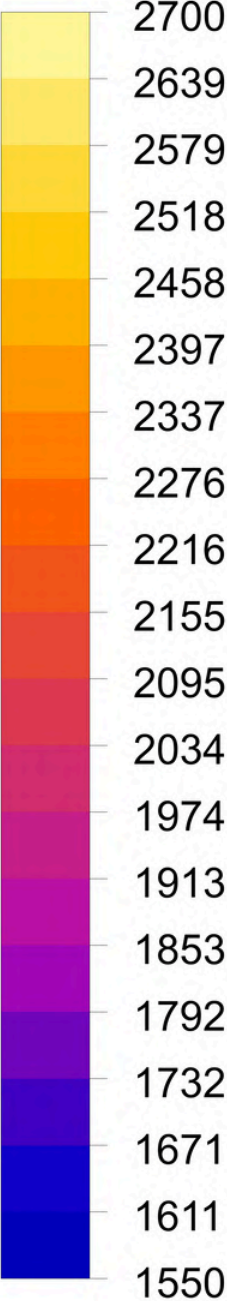
Simulation ID – Class (ID Color)			
Geometric and Operating Parameters (Input)			
N_{sl} (Sectors)	R_{dil} (Radius)	$\dot{m}_{air}$ (Air)	$\dot{m}_{H2}$ (Fuel)
COLORBAR X55 X35 X10 X137 X98 X75 X192			
Performance and Emission Indices (Output)			
OPF (Pattern)	NPF (Pattern)	T_{max} (Peak)	$EINO_x$ (Emissions)

Simulation N16 R196 – Shape A

Geometric and Operating Parameters

N_{sl} : 16	R_{dil} : 1.96 mm	$\dot{m}_{air}$: 27.5 kg/s	$\dot{m}_{H_2}$: 0.203 kg/s
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Temperature [K]



Performance and Emission Indices

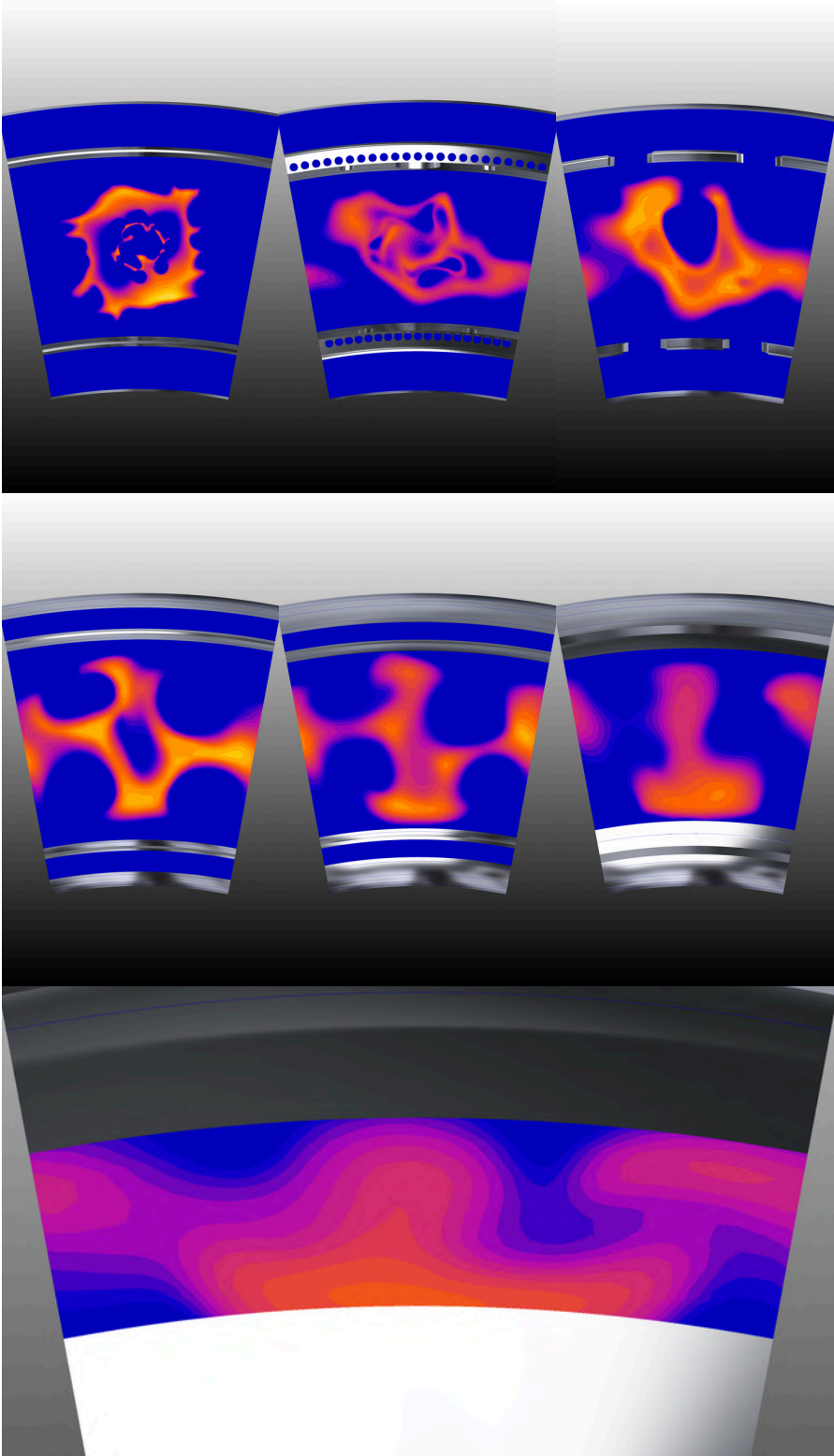
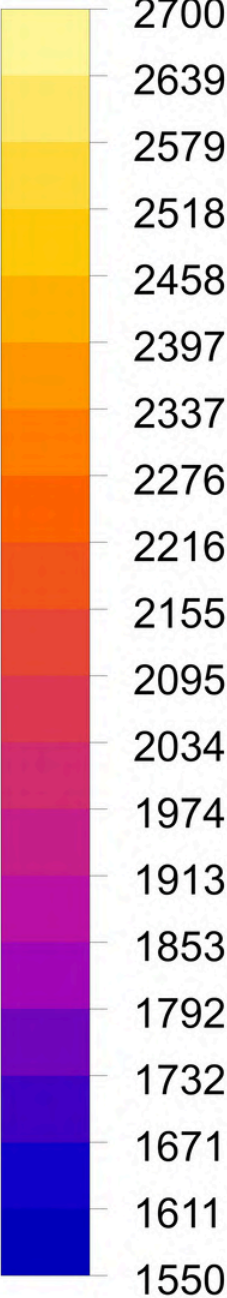
OPF : 0.23	NPF : 0.56	T_{max} : 1982 K	$EINO_x$: 7.78 g/kg
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Simulation N17 R171 – Shape A

Geometric and Operating Parameters

N_{sl} : 17	R_{dil} : 1.71 mm	$\dot{m}_{air}$: 27.5 kg/s	$\dot{m}_{H_2}$: 0.203 kg/s
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Temperature [K]



Performance and Emission Indices

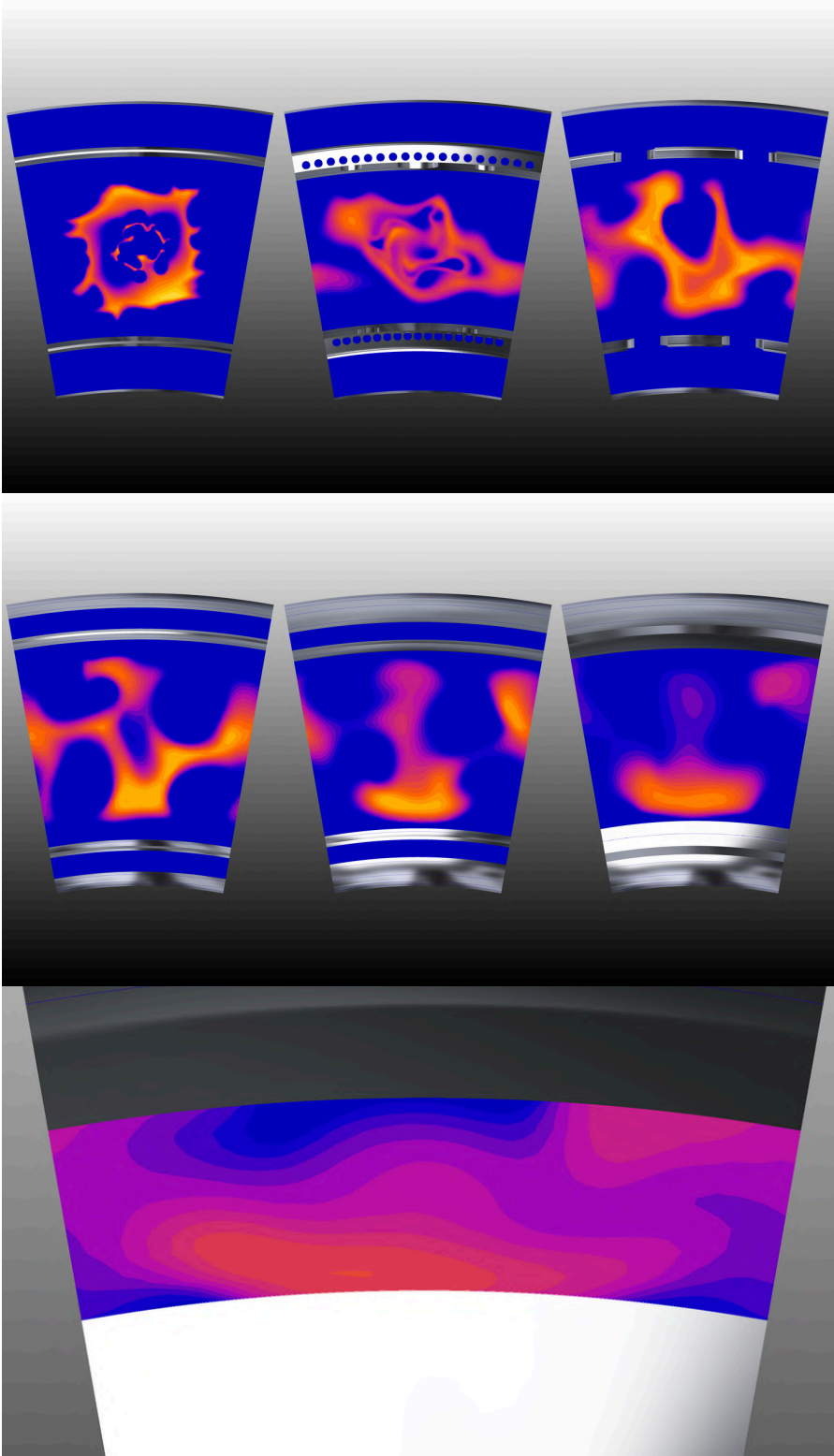
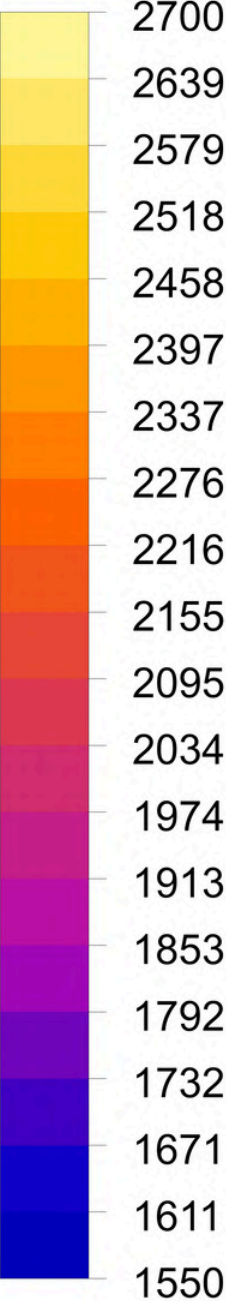
OPF : 0.26	NPF : 0.62	T_{max} : 2033 K	$EINO_x$: 8.11 g/kg
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Simulation N18 R263 – Shape A

Geometric and Operating Parameters

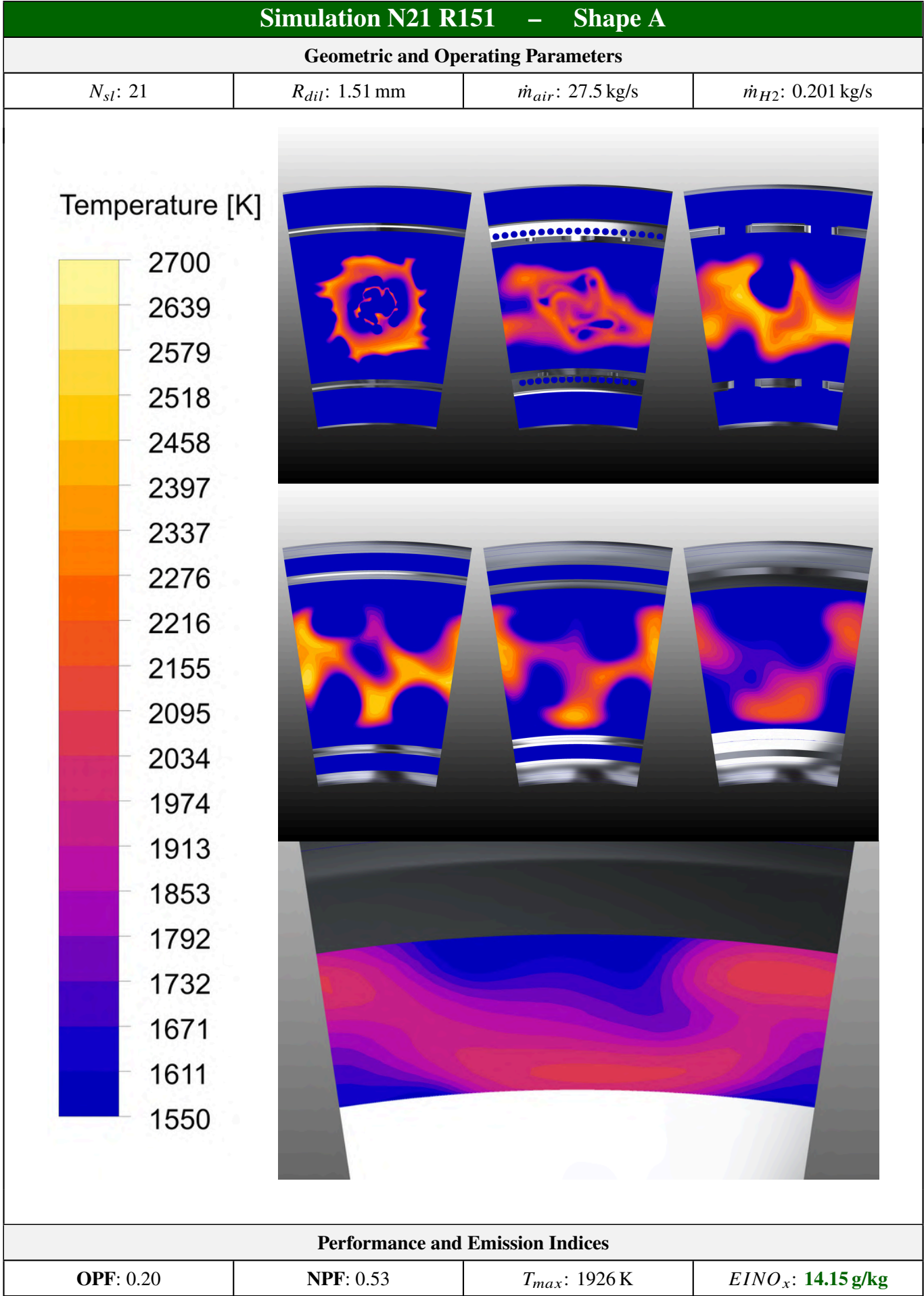
N_{sl} : 18	R_{dil} : 2.63 mm	$\dot{m}_{air}$: 27.5 kg/s	$\dot{m}_{H_2}$: 0.202 kg/s
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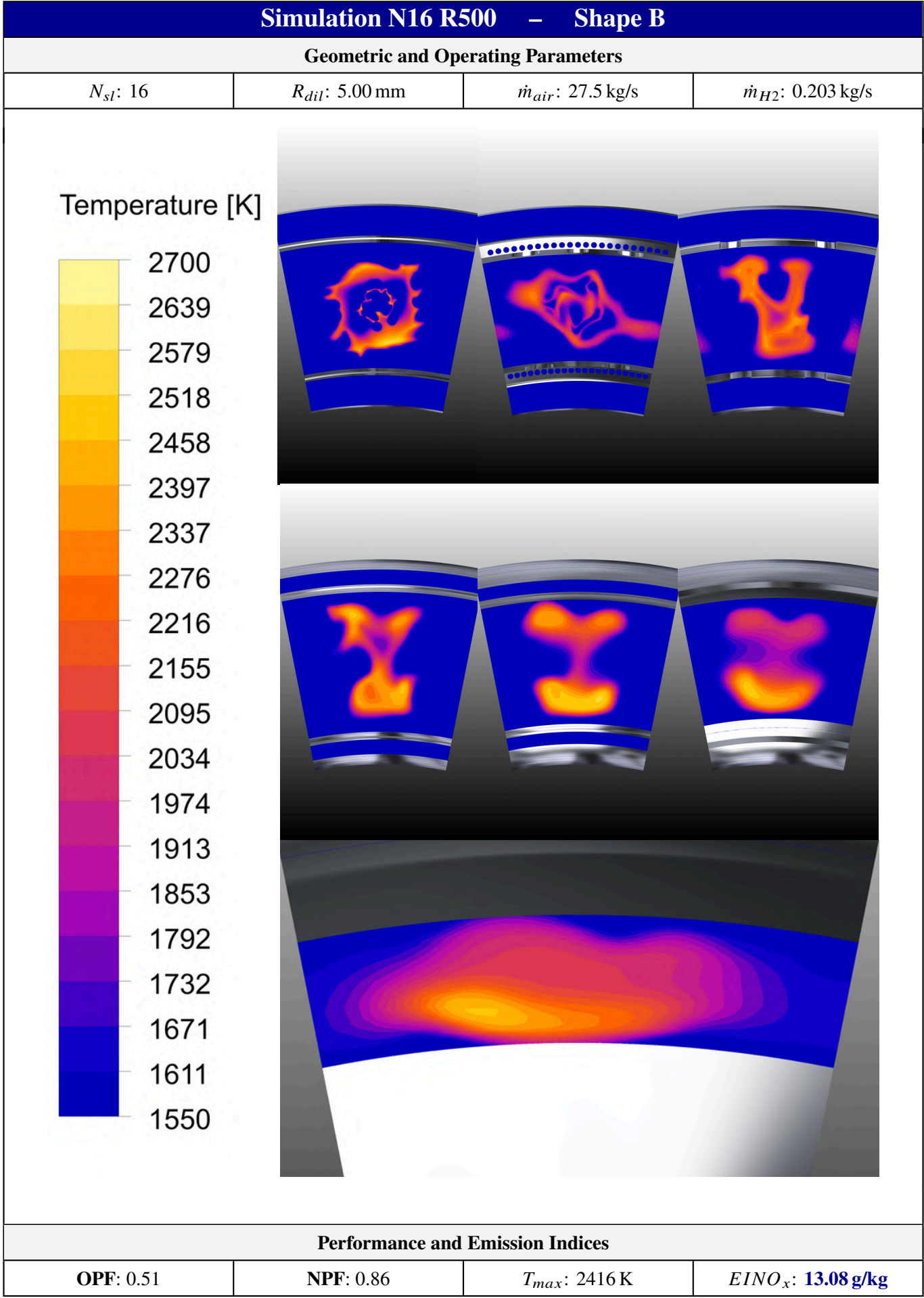
Temperature [K]

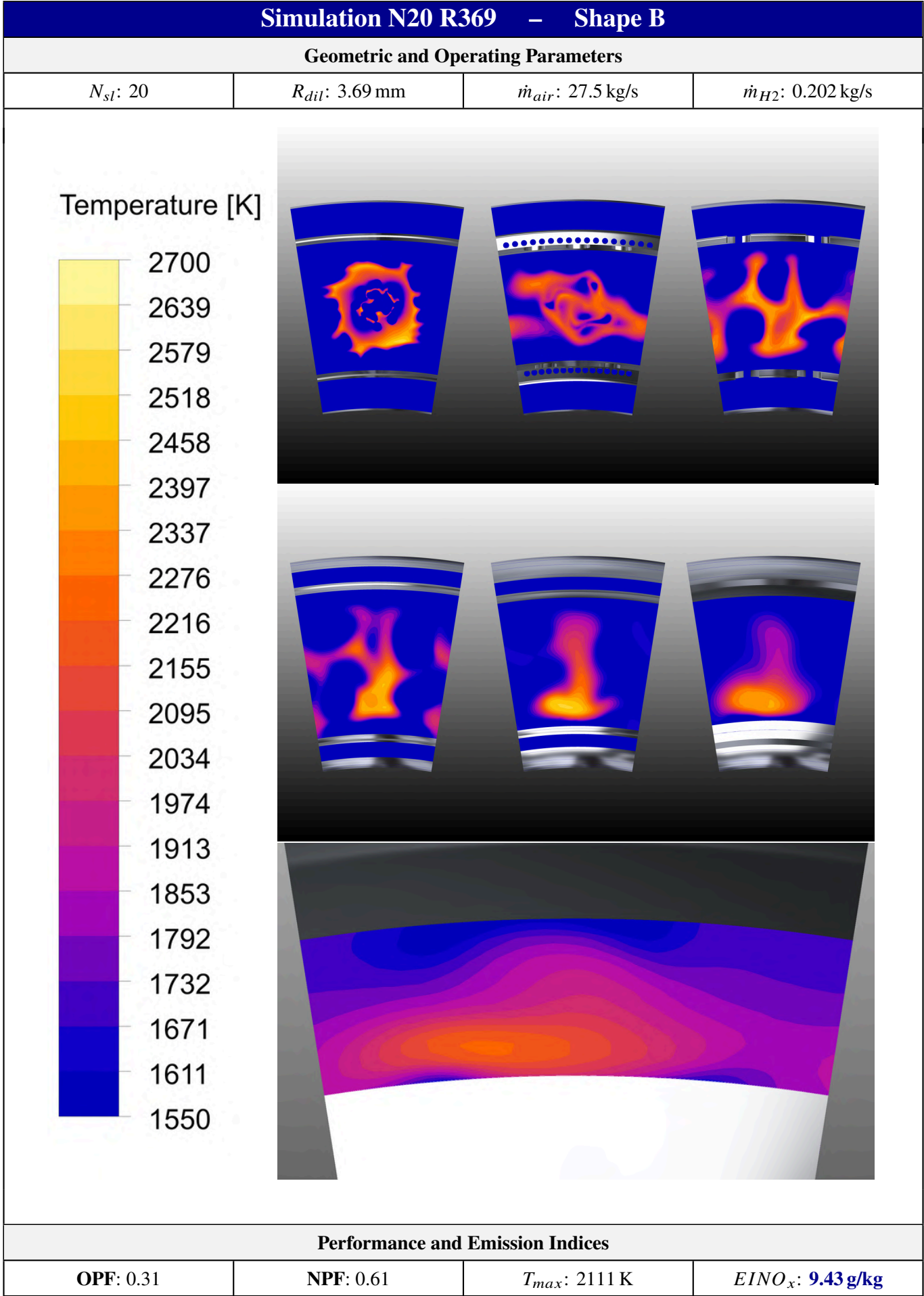


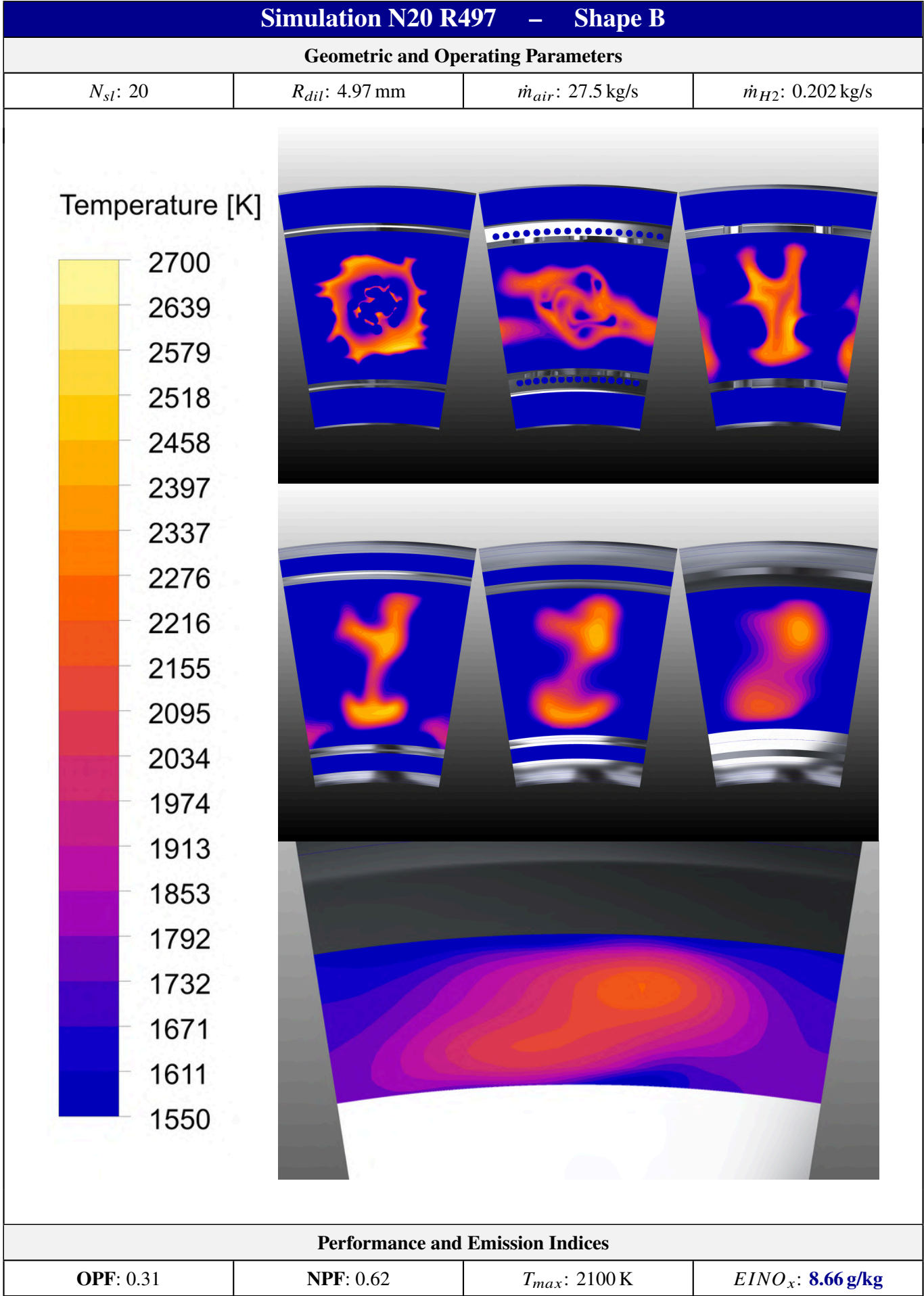
Performance and Emission Indices

OPF : 0.20	NPF : 0.50	T_{max} : 1939 K	$EINO_x$: 8.55 g/kg
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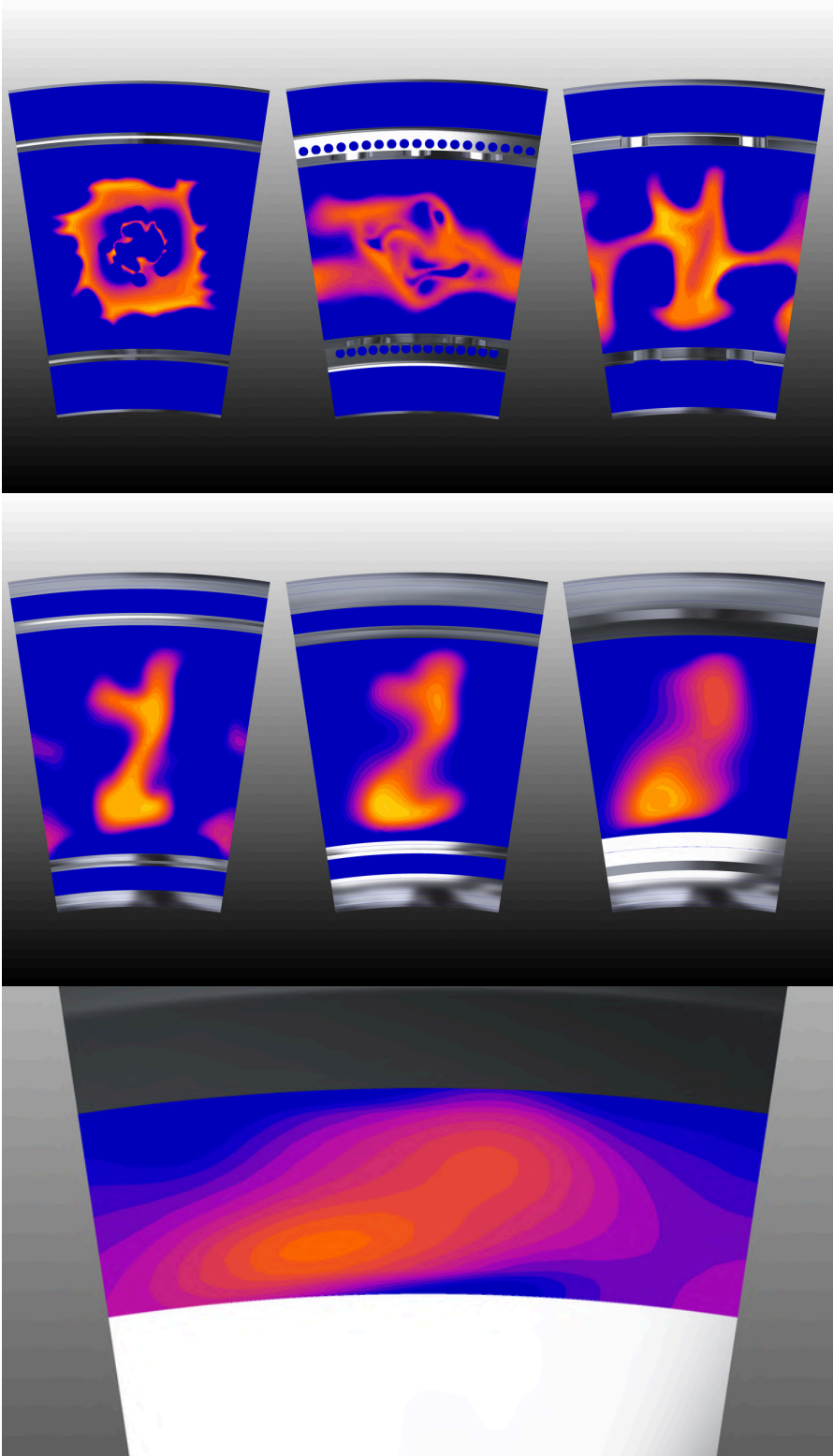
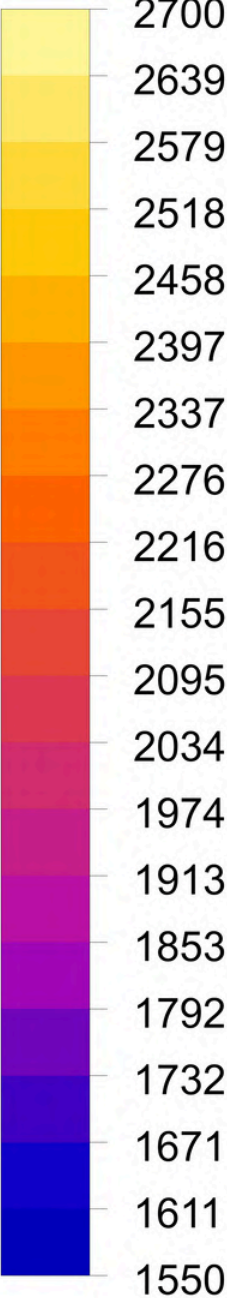


Simulation N21 R465 – Shape B

Geometric and Operating Parameters

N_{sl} : 21	R_{dil} : 4.65 mm	$\dot{m}_{air}$: 27.5 kg/s	$\dot{m}_{H_2}$: 0.201 kg/s
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Temperature [K]



Performance and Emission Indices

OPF : 0.33	NPF : 0.68	T_{max} : 2130 K	$EINO_x$: 10.09 g/kg
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