

Article

Numerical Assessment of a 10 kW rSOC Exhaust Gas Afterburner with Preliminary Geometric Scaling Considerations

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Abstract

The integration of reversible solid oxide cell (rSOC) systems with industrial energy units can improve operational flexibility, but it also requires safe and efficient management of hydrogen-rich off-gas. This study presents the numerical design of an exhaust gas afterburner for a 10 kW rSOC stack, in which unreacted hydrogen mixed with steam is oxidized using the hot air stream employed for stack purging. A finite-volume CFD approach was applied using a non-premixed combustion model, a $k-\omega$ SST turbulence model, and GRI-Mech 3.0 chemistry, followed by a thermo-mechanical assessment of the chamber. For the reference case, the unreacted hydrogen stream was 1.16661×10^{-4} kg/s, corresponding to approximately 14 kW of chemical energy. The simulations predicted a localized reaction zone directly downstream of the burner outlet, accompanied by rapid hydrogen consumption and a fluid-temperature range of approximately 492–930 °C. The thermo-mechanical analysis predicted a maximum total deformation of 2.2189 mm and a maximum axial displacement of approximately 2.21 mm for the analyzed steady-state operating point. These results characterize the temperature, species, and deformation fields of the 10 kW reference configuration. The 100 kW and 1 MW variants should be treated only as preliminary geometric extrapolations, because they were not verified by separate CFD/CSD calculations.

Keywords: rSOC; hydrogen combustion; exhaust gas afterburner; CFD; thermal-FSI; non-premixed combustion; hydrogen-rich off-gas

1. Introduction

Reversible solid oxide cells (rSOCs) are regarded as promising devices for long-duration energy storage and sector coupling because they can operate alternately in solid oxide electrolysis (SOE) mode and solid oxide fuel cell (SOFC) mode [1,2]. In SOE operation, electrical energy and steam are converted into hydrogen, whereas in SOFC operation, hydrogen is converted back into electricity and heat. Owing to this bidirectional functionality, rSOC systems are attractive for industrial and power-generation applications that require improved flexibility, better integration of renewable electricity, and efficient use of high-temperature heat streams [1,2].

Despite these advantages, the practical deployment of rSOC-based systems depends not only on stack performance, but also on the safe and efficient design of hot balance-of-

Academic Editor: Jun Cong Ge

Received: 20 June 2026

Revised: 23 July 2026

Accepted: 28 July 2026

Published: 5 August 2026

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plant components. In particular, hydrogen-rich off-gases leaving high-temperature solid oxide systems may still contain a non-negligible amount of chemical energy, and their recovery by auxiliary burners or afterburners can improve overall heat integration and system efficiency [3,4]. Previous studies on SOFC systems have shown that the combustion of anode off-gases can support fuel utilization, thermal integration, and preheating duties, while dedicated CFD studies have also highlighted the importance of afterburner temperature distribution and thermal safety for reliable operation of the overall system [3–5].

From a combustion point of view, hydrogen-rich off-gases are challenging because their behavior differs from that of conventional hydrocarbon fuels. The combustible stream may be strongly diluted with steam, and water vapor is known to affect hydrogen oxidation kinetics, flame temperature, and pollutant formation [6]. Moreover, numerical studies of hydrogen combustion have shown that the predicted flame structure and thermal field may depend not only on the adopted turbulence–combustion interaction model, but also, in high-temperature cases, on the treatment of radiative heat transfer [7–10]. In practical devices, the burner configuration and operating mode are further constrained by the high temperatures of both the fuel-side and air-side streams, which influence ignition risk, flame stabilization, and heat transfer to the surrounding structure [3,5,6]. For this reason, numerical methods are particularly useful at the design stage, because they make it possible to assess the coupled flow, combustion, and thermal fields before prototype testing [3–5,7,8].

The system considered in this work is part of the HYDROGIN project, i.e., a modular rSOC installation intended for integration with industrial energy units in order to improve operational flexibility and increase the use of renewable energy. In the analyzed arrangement, the afterburner is one of the key hot-zone components cooperating with the rSOC stack and the FE1 heat exchanger. Its role is to oxidize the residual hydrogen leaving the cell together with steam, while the hot air stream used for stack purging is supplied separately as the oxidizer. According to the design assumptions for the 10 kW reference case, the unreacted hydrogen stream equals 0.000116661 kg/s, which corresponds to approximately 14 kW of chemical energy. The FE1 heat exchanger is placed downstream of the afterburner and is intended to recover heat for preheating the steam directed to the stack.

Against this background, the aim of the present study is to assess, by numerical means, the design of an exhaust gas afterburner dedicated to cooperation with a 10 kW rSOC stack and to formulate a practical scaling approach for higher-capacity variants. The work focuses on whether the proposed configuration enables stable oxidation of the hydrogen–steam off-gas under representative operating conditions and whether the chamber maintains acceptable thermo-mechanical behavior in steady operation. The results indicate that the reference 10 kW configuration provides a feasible and compact solution for hydrogen-rich off-gas utilization, while scaling to 100 kW and 1 MW can be approached by increasing the characteristic flow areas of the nozzle and outlet channel. At the same time, the larger variants should be treated as engineering extrapolations, because separate CFD/CSD verification was not reported for them.

The recent literature further confirms the relevance of this research direction. Muhammed and Jayanti showed that ReSOC-based systems can provide both power and storage functions in renewable-energy microgrids, but their practical operation depends on the appropriate integration of high-temperature components and operating strategy [11]. Wu et al. demonstrated that, in SOFC cogeneration systems, performance assessment should also include stack operating safety and exergy-efficiency improvement, not only electrical and thermal efficiency [12]. In parallel, recent experimental work on afterburner systems fueled with hydrogen–methane mixtures confirmed the growing practical interest in hydrogen-containing combustion systems and showed that burner configuration

and operating conditions strongly affect thermal behavior [13]. These recent studies indicate that the development of safe and efficient hydrogen-rich off-gas afterburners remains an important issue for integrated high-temperature electrochemical energy systems.

2. Materials and Methods

2.1. System Configuration

The analyzed afterburner was developed as part of the HYDROGIN concept [14], i.e., a modular reversible solid oxide cell (rSOC) installation intended for integration with industrial energy systems. In the hot section of the installation, the key components are the rSOC stack, the FE1 heat exchanger, the exhaust gas afterburner, and the high-temperature valve Z1. The afterburner is located upstream of the FE1 heat exchanger. Its role is to oxidize the residual hydrogen leaving the stack together with steam, while the air stream used for stack purging is introduced separately as the oxidizer. The FE1 heat exchanger is placed at the afterburner outlet and is used to preheat the steam supplied to the fuel electrode of the stack. The detailed numerical analysis presented in this work concerns the 10 kW reference configuration.

2.2. Reference Case and Process Inputs

According to the 0D process calculations, the unreacted hydrogen stream for the 10 kW installation equals 0.000116661 kg/s. Assuming a lower heating value of 120 MJ/kg, this corresponds to approximately 14 kW of chemical energy carried by the hydrogen-rich off-gas. These values were used as the basis for defining the reference operating case analyzed numerically in the present study.

2.3. Afterburner Geometry and Materials

In the construction of the burner and combustion chamber, the design was intentionally based on commercially available subcomponents. The burner head was a PERUN hand torch, acetylene–oxygen type S 371-5952, PG-216PZ, selected because its rated power reached up to 65 kW. The PE-RUN torch head was not used as a standard acetylene–oxygen burner operating in its original mode. In the present configuration, it was used as a commercially available burner-head geometry for introducing and distributing the hydrogen–steam stream. The oxidizer was not supplied through the burner together with the fuel, but separately as hot air entering the chamber. This arrangement was adopted to avoid premixing hydrogen and oxygen inside the burner at elevated temperatures. At this stage, the suitability of the component was therefore assessed mainly from the geometrical and flow-distribution points of view. The combustion chamber consisted of a ceramic tube enclosed in a steel shell terminated with a 160/80 reduction. The outer chamber structure was made of 316L stainless steel, whereas the inner liner was a ceramic tube with a purity of 99%. The fuel-side inlet supplied the hydrogen–steam mixture through the burner head, while the oxidizer entered the chamber separately.

2.4. Computational Domain and Mesh

Separate computational representations were prepared for the fluid domain and for the coupled solid domain of the chamber. This enabled analysis of both the reacting flow field and the thermal response of the surrounding structure. The flow domain was discretized using a polyhedral mesh with a near-wall layer. The reported mesh size was 4.6 million control volumes. Additional local refinement was introduced in the burner outlet region. According to the source documentation, a mesh-sensitivity check was performed and the adopted mesh density was considered sufficient to reproduce the temperature field and the distribution of reactions in the combustion chamber. Figures 1–3 show the

geometry of the combustion chamber, burner, and fluid domain used in the numerical analysis.

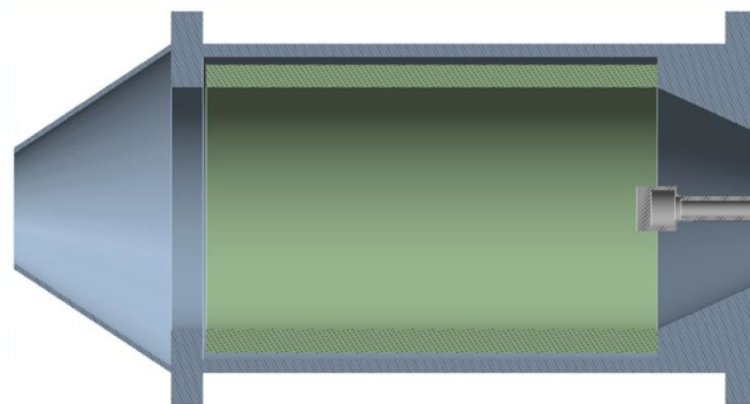


Figure 1. Cross-section of combustion chamber.

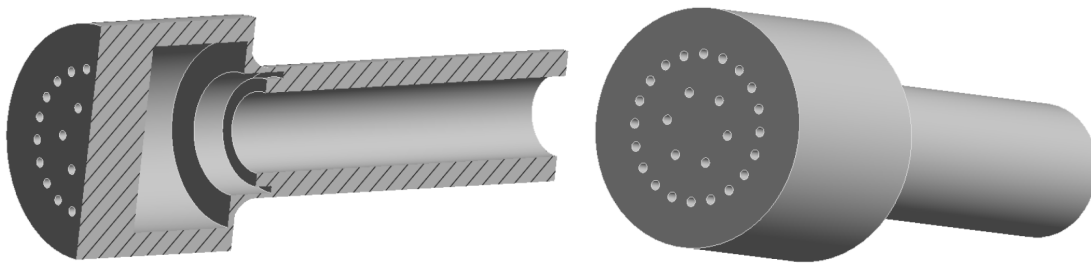


Figure 2. Cross-section of the burner.

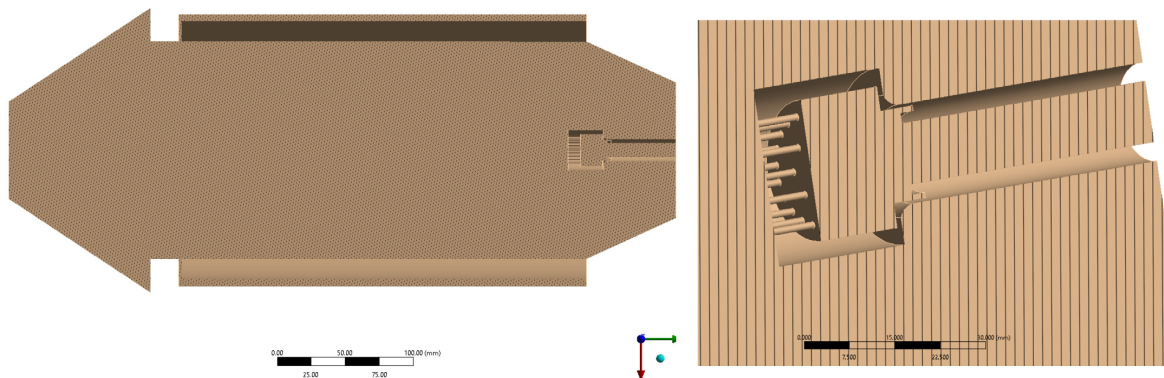


Figure 3. Cross-section of the fluid domain.

Mesh Independence Study

A mesh independence study was performed in order to assess the sensitivity of the numerical solution to the spatial discretization of the fluid domain. Five polyhedral meshes were tested, containing approximately 1.6, 2.4, 3.3, 4.6, and 6.0 million control volumes, respectively. In all cases, the mesh refinement was concentrated in the burner outlet region and near the fluid–solid interface, where the steepest gradients of temperature and species concentration were expected.

The convergence of the solution with increasing mesh density was evaluated using three monitored quantities directly relevant to the objectives of the study: the maximum fluid temperature in the reaction zone, the maximum temperature in the metallic chamber wall, and the area-averaged hydrogen mole fraction at the outlet. These quantities were

selected because they characterize, respectively, the thermal intensity of the combustion process, the thermal loading of the structure, and the completeness of hydrogen oxidation.

With increasing mesh density, all monitored quantities approached asymptotic values. The coarsest meshes showed noticeable deviations, particularly for the outlet hydrogen mole fraction, whereas the two finest meshes yielded only minor changes in all monitored parameters. Between the fourth and the fifth mesh, the relative change in maximum fluid temperature was 0.03%, the relative change in maximum metal temperature was 0.05%, and the relative change in the outlet hydrogen mole fraction was 0.87%. These results indicate that the solution became effectively mesh-independent at the level of approximately 4.60 million control volumes.

On this basis, the mesh containing approximately 4.6 million control volumes was selected for the remaining CFD calculations as a compromise between numerical accuracy and computational cost. Figure 4 presents a close-up view of the computational mesh generated for the analyzed geometry.



Figure 4. Close up of the generated mesh of the analyzed geometry.

Figure 5 presents the mesh-independence study for the reference afterburner, based on deviations from the results obtained with the finest mesh.

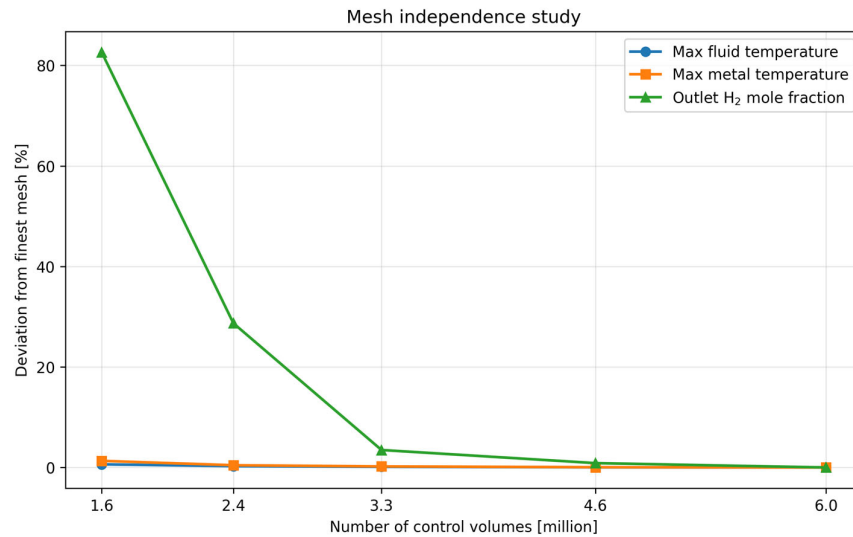


Figure 5. Mesh independence study for the reference afterburner. The deviations of the monitored quantities with respect to the finest mesh are shown as functions of the number of control volumes.

2.5. Numerical Model

This section describes the numerical approach adopted in the present study. In particular, it outlines the CFD, CSD, thermal-FSI, and combustion models used to analyze the behavior of the investigated afterburner configuration.

2.5.1. CFD Model

In the fluid domain, the starting point for the CFD computation is to define a universal set of mass, momentum, and energy balance equations for the fluid as follows [15]:

- Balance of mass— ρ

$$\frac{\partial}{\partial t}(\rho) + \text{div}(\rho \mathbf{v}) = 0, \quad (1)$$

- Balance of momentum— $\rho \mathbf{v}$

$$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \text{div}(\rho \mathbf{v} \otimes \mathbf{v}) + p \mathbf{I} = \text{div}(\mathbf{t}^c) + \rho \mathbf{b}, \quad (2)$$

- Balance of energy— e

$$\frac{\partial}{\partial t}(\rho e) + \text{div}(\rho e + p) \mathbf{v} = \text{div}(\mathbf{t}^c \mathbf{v} + \mathbf{q}_{fluid}^c) + \rho \mathbf{b} \cdot \mathbf{v}, \quad (3)$$

where $\rho = \rho(\mathbf{x}, t)$ —fluid density, which generally depends on the time t and the location $\mathbf{x}$, $\mathbf{v} = v_i \mathbf{e}_i$ —fluid velocity, p —thermodynamic pressure, $\mathbf{I} = \delta_{ij} \mathbf{e}_i \otimes \mathbf{e}_j$ —unity tensor, $\mathbf{t}^c = \mathbf{t} + \mathbf{R} + \mathbf{D}$ —the viscous, turbulent and diffusive flux of momentum, $\mathbf{b}$ —mass force of Earth's gravity, $e = u + \frac{v^2}{2}$ —which is the sum of the internal and kinetic energy, and $\mathbf{q}_{fluid}^c = \mathbf{q} + \mathbf{q}^+ + \mathbf{q}^{ph} + \dots$ —total heat flux in the fluid.

In order to take into account the influence of the turbulent transport of momentum and the turbulent transport of heat, the fluid should possess a set of additional equations governing the evolution of turbulent primary parameters, for instance, turbulent kinetic energy k and turbulent dissipation energy ω [16,17]:

$$\frac{\partial}{\partial t}(\rho k) + \text{div}(\rho k \mathbf{v}) = \text{div}(\mathbf{J}_k) + S_k \quad (4)$$

$$\frac{\partial}{\partial t}(\rho \omega) + \text{div}(\rho \omega \mathbf{v}) = \text{div}(\mathbf{J}_\omega) + S_\omega \quad (5)$$

where $\mathbf{J}_k$, $\mathbf{J}_\omega$ —diffusive flux of k and diffusive flux of ω with sources S_k, S_ω (various definitions from different authors exist in the literature). For each finite volume of the computational grid, seven equations were solved (one each for mass, energy, k and ω transport balance, and three momentum balance equations).

The adoption of the k – ω SST model was justified in the works of [18–22].

2.5.2. Radiation Model

Radiative heat transfer was included because previous studies on hydrogen combustion have shown that radiation may affect flame temperature, heat-release distribution, and thermal loading, especially at elevated temperatures [8,10,23–25].

The momentum flux is defined in terms of the radiative energy flux as follows:

$$\tau^{rad} = \left(\delta_{ij} \frac{\varphi_1}{3} + \varphi_2 \Lambda_i \Lambda_j \right) \vec{e}_i \otimes \vec{e}_j \quad (6)$$

where

$$\varphi_1 = -1 + \sqrt{4 - 3\lambda} \quad (7)$$

$$\varphi_2 = \frac{2 - \sqrt{4 - 3\lambda}}{\lambda} \quad (8)$$

$$\Lambda_i = \frac{q_i^{rad}}{\sqrt{\lambda}}, \quad \lambda = \vec{q}^{rad} \cdot \vec{q}^{rad} \quad (9)$$

The radiative heat flux is defined in the implicit form of an integro-differential equation:

$$\text{div} \vec{q}^{rad} = \alpha [4e_b - g] \quad (10)$$

where

α —absorption coefficient, m^{-1} ;

e_b —blackbody emissive power, W/m^2 ;

g —incident radiation energy defined by relation (11).

$$g = \int_{4\pi} i' d\hat{\omega}' \quad (11)$$

where

i —radiation intensity, W/m^2 ;

$\hat{\omega}'$ —solid angle.

The radiation intensity is not known a priori, and its determination requires solving the integro-differential closure equation (Equation (12)):

$$\frac{\partial}{\partial t} i + \nabla(\vec{\Omega} i) = -\kappa i + \alpha i_b + \frac{\sigma}{4\pi} \int_{4\pi} i' d\hat{\omega}' \quad (12)$$

where

i —radiation intensity, W/m^2 ;

$\vec{\Omega}$ —propagation direction, $|\vec{\Omega}| = 1$;

i_b —blackbody radiation intensity, W/m^2 ;

σ —scattering coefficient, m^{-1} .

The above model describes the interaction of radiation passing through the mixture by means of absorption, scattering, and transmission. This means that absorption and scattering change the intensity of the heat flux in certain directions within the considered control volume, while the volume itself emits new radiation. Radiation transport is additionally subject to the assumptions that the surface and the medium are “gray,” the medium

is in a local state of thermodynamic equilibrium, the refractive index is equal to one, and the hemispherical and total emissivities are equal.

In the CFD calculation, radiative heat transfer was included using the standard P1 radiation model available in ANSYS Fluent 2023 R2. The P1 model is an approximation of the radiative transfer equation in which radiation transport is represented by a diffusion-type equation for the incident radiation. This approach is less computationally demanding than full angular radiation models and is commonly used in engineering simulations of high-temperature reacting flows when radiation must be included but is not the main focus of the analysis.

The use of the P1 model was justified by the presence of a high-temperature reaction zone and water vapor in the combustion products. In the analyzed hydrogen–steam case, H₂O was the main participating radiating species, while H₂, O₂, and N₂ were treated as non-dominant radiating components. The wall surfaces were treated as gray diffuse surfaces, and gas-phase scattering was neglected. Radiation was included in the final CFD calculations, and the resulting temperature field was used in the subsequent thermo-mechanical assessment.

The gas absorption coefficient, including the contribution of water vapor, was calculated using the domain-based weighted-sum-of-gray-gases model (WSGGM) available in ANSYS Fluent.

2.5.3. Combustion Model

The reacting flow was analyzed using a finite-volume CFD approach. A non-premixed combustion model was adopted because both the fuel and oxidizer streams entered the system at elevated temperatures. Under such conditions, the documentation states that only the fuel mixture could be fed through the burner head, because direct introduction of oxygen into the burner would result in immediate ignition inside the burner. The documented CFD setup included a $k-\omega$ turbulence model and the GRI-Mech 3.0 reaction mechanism comprising 53 species and 325 reactions. The non-premixed combustion model was selected because the hydrogen–steam stream and the oxidizer stream are supplied to the afterburner separately. In this configuration, combustion is controlled mainly by mixing between the fuel-side and air-side streams, rather than by a premixed flame introduced at the inlet. A premixed model would therefore not represent the actual feeding arrangement of the device. GRI-Mech 3.0 was used because it provides detailed H/O reaction chemistry and includes the main intermediate species involved in hydrogen oxidation, such as H, O, OH, HO₂, and H₂O₂. This was important because the study not only assesses the temperature field, but also the local distribution of selected species in the reaction zone. The kinetic parameters were taken from the literature sources listed in the project materials. The influence of steam on hydrogen oxidation kinetics was considered in accordance with the literature data reported for steam-diluted hydrogen combustion, while the numerical treatment of hydrogen combustion was aligned with previously published CFD studies [6,7].

Figure 6 compares detailed chemical kinetic mechanisms in terms of the number of species and reactions, showing the increase in mechanism size with fuel complexity.

Based on a comparison of mechanism size and complexity, GRI-Mech 3.0 was selected for the present study as a compromise between chemical detail and computational cost.

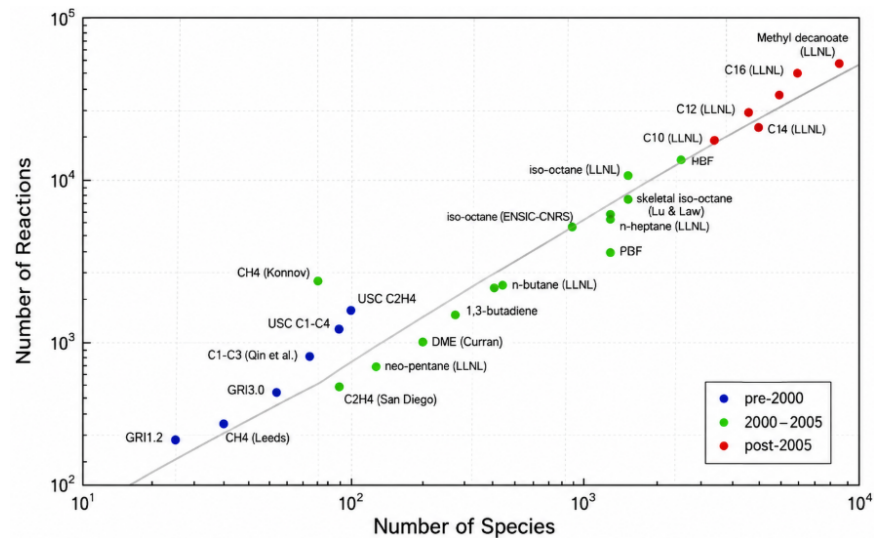


Figure 6. Comparison of detailed chemical kinetic mechanisms in terms of the number of species and reactions. Blue, green, and red markers denote mechanisms developed before 2000, during 2000–2005, and after 2005, respectively. The figure illustrates the general increase in mechanism size with increasing fuel complexity [26].

Table 1 presents selected representative Arrhenius parameters for elementary reactions relevant to steam-diluted hydrogen oxidation. These reactions are shown only to illustrate the main H/O/HO₂/H₂O₂ pathways. They do not constitute a separate reduced mechanism used in the CFD calculation. The CFD model used the complete GRI-Mech 3.0 mechanism, containing 53 species and 325 reactions. The rate constant is expressed as $k = A T^n \exp(-E/RT)$; the units of A depend on reaction order and follow the conventional kinetic format of the source mechanism, while E is given in cal/mol. Table 2 presents selected Arrhenius parameters for representative hydrogen oxidation reactions affected by water vapor.

Table 1. Main burner and outlet dimensions used in the CFD model for the 10 kW reference case.

Parameter	Unit	Value
Number of nozzle holes	—	26
Diameter of a single nozzle hole	m	0.0012
Radius of a single nozzle hole	m	0.0006
Total nozzle cross-sectional area	m ²	2.94053×10^{-5}
Chamber outlet diameter	m	0.072
Chamber outlet radius	m	0.036
Nozzle channel length	m	0.01

Table 2. Selected Arrhenius parameters for representative elementary reactions of hydrogen oxidation influenced by water vapor, based on literature data from [6].

No.	Reaction	A	n	E
5	$O + H_2 = OH + H$	1.30×10^{04}	2.8	5922.0
6	$H + O_2 = OH + O$	1.90×10^{14}	0.0	16,812.0
7	$H + O_2 + M = HO_2 + M$	8.00×10^{17}	−0.8	0.0
10	$H_2O + O = OH + OH$	1.50×10^{10}	1.1	17,260.0
12	$HO_2 + O = OH + O_2$	2.44×10^{13}	0.0	−446.0
14	$H + HO_2 = OH + OH$	8.40×10^{13}	0.0	874.0
16	$HO_2 + HO_2 = H_2O_2 + O_2$	4.20×10^{14}	0.0	11,982.0

17	$\text{HO}_2 + \text{HO}_2 = \text{H}_2\text{O}_2 + \text{O}_2$	1.30×10^{11}	0.0	−1630.0
18	$\text{OH} + \text{OH} (+\text{M}) = \text{H}_2\text{O}_2 (+\text{M})$	7.40×10^{13}	−0.4	0.0
k_0	—	0.23×10^{19}	−0.90	−1700.0

The non-premixed combustion model was used because the hydrogen–steam stream and the oxidizer stream were introduced separately into the afterburner. The fuel-side stream passed through the burner head, whereas the hot air stream was supplied separately to the chamber. Therefore, the reaction zone was governed mainly by mixing between the two streams, not by a premixed flame imposed at the inlet.

In ANSYS Fluent, the non-premixed model was coupled with GRI-Mech 3.0 through the chemistry table used by the combustion model. The fuel and oxidizer compositions were defined according to the inlet data, and the GRI-Mech 3.0 mechanism was used as the chemical kinetic mechanism for hydrogen oxidation. The model then used the tabulated chemistry to determine the local temperature and species composition as a function of the mixture state. This allowed the calculation to include the main H/O reaction pathways and intermediate species, including H, O, OH, HO₂, and H₂O₂, while keeping the computational cost lower than the direct finite-rate integration of all reactions in every control volume.

2.5.4. CFD Solver Settings

For clarity, the main CFD solver settings used in the reference calculation are summarized in Table 3. The table lists the adopted solver type, discretization schemes, turbulence and combustion models, radiation model, and convergence criteria used.

Table 3. Main CFD solver settings used in the reference calculation.

Setting	Adopted option
Solver type	pressure-based
Time treatment	Steady-state
Pressure–velocity coupling	coupled
Momentum discretization	Second-order upwind
Energy discretization	Second-order upwind
Turbulence model	k– ω SST
Turbulence discretization	Second-order upwind
Species transport/combustion	Non-premixed combustion model
Chemical mechanism	GRI-Mech 3.0, 53 species and 325 reactions
Turbulence–chemistry coupling	Mixture-fraction/PDF approach with chemistry table generated from GRI-Mech 3.0
Radiation model	P1 radiation model
Convergence criteria	Residuals below 10^{-5} for continuity, momentum, turbulence and species; residual below 10^{-6} for energy
Wall treatment	Default correlation-based y^+ -insensitive near-wall treatment for the SST k– ω model.
Gas absorption coefficient treatment	Domain-based WSGGM, with H ₂ O as the principal participating radiating species

2.5.5. CSD Model

In analogy to the CFD set of governing equations, the appropriate set of CSD governing equations is determined as follows [27,28]:

- Balance of mass— ρ

$$\frac{\partial}{\partial t}(\rho) + \text{div}(\rho \mathbf{v}) = 0 \quad (13)$$

- Balance of momentum— $\rho \mathbf{v}$.

$$\frac{\partial}{\partial t}(\rho \mathbf{v}) + \text{div}(\rho \mathbf{v} \otimes \mathbf{v}) = \text{div}(\boldsymbol{\sigma}) + \rho \mathbf{b} \quad (14)$$

- Balance of energy—

$$\frac{\partial}{\partial t}(\rho e) + \text{div}(\rho e + p) \mathbf{v} = \text{div}(\boldsymbol{\sigma} \mathbf{v} + \mathbf{q}_{\text{solid}}^c) + S_e \quad (15)$$

where $\boldsymbol{\sigma}$ —elastic stress tensor, $\mathbf{q}_{\text{solid}}^c$ —total heat flux in the solid, and S_e —source. To the set of CSD governing equations, additional evolution equations describing the behavior of the solid material can be added, e.g., the evolution of plastic strain, evolution of kinematic hardening, and evolution of isotropic hardening, etc. Here, CSD is a direct analogy for CFD. Both methods use the same balance equations (mass, momentum and energy).

2.5.6. Thermal-FSI Assessment

In addition to the CFD analysis, the chamber was subjected to thermo-mechanical assessment. The purpose of this part of the study was to verify whether the thermal loads generated in the reacting-flow calculation could be accommodated by the chamber structure. From the energy-conversion perspective, coupled fluid–solid analysis is important because the interaction between thermal flow processes and the structural response may influence both operational safety and the overall performance of the device [29,30]. The source materials indicate that both the fluid and solid domains were included in the computational workflow and that the structural response was evaluated in terms of deformation and directional displacement. Because the available documentation focuses mainly on the engineering outcomes, only the documented thermo-mechanical scope is reported here.

Thermal-FSI is based on coupling through the energy equation, i.e., one- and two-way heat energy exchanges between the fluid and the solid. Two-way thermal-FSI is frequently encountered in problems involving turbomachinery, heat exchangers, etc. An example of thermal-FSI is shown in Figure 7.

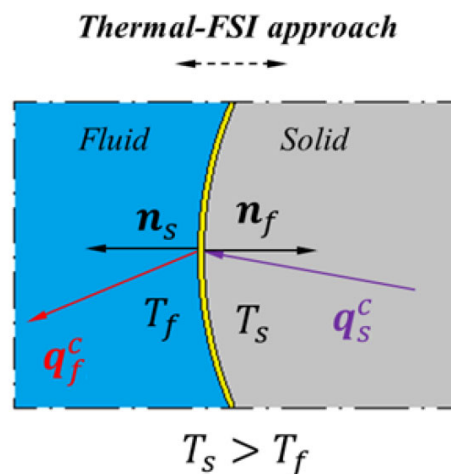


Figure 7. Conceptual diagram of one-way thermal-FSI coupling [31]; where $\mathbf{q}_s^c$ —total diffusive heat flux in the solid body; $\mathbf{q}_f^c$ —total diffusive heat flux in the fluid domain; T_s —solid temperature; T_f —fluid temperature; $\mathbf{n}$ —normal vector.

In the literature, two types of thermal-FSI analysis can be found [32–34]: one-way FSI and two-way FSI. In one-way FSI, after performing CFD calculations, the pressure and temperature field solutions are exported to the CSD solver, which then determines stresses and displacements based on these inputs. In one-way thermal-FSI, the heating or

cooling of the fluid by the solid body is implemented using Neumann-type boundary conditions.

The thermo-mechanical calculation was performed as a one-way thermal-FSI analysis. The temperature field obtained from the final CFD solution was transferred to the solid-domain model and used as the thermal load in the structural calculation. No feedback from the structural deformation to the flow field was included. The interfaces between the solid components were treated as bonded contacts in the structural model. Local contact separation, frictional sliding, weld geometry, and weld-detail stresses were not included. The material models were linear elastic, with temperature-dependent thermal and mechanical properties, as listed in Tables 3–5.

The thermal-FSI method has been developed for many years, and some of its applications are described, among others, in works [26,35–37].

Table 4. Inlet parameters.

	Molar Mass Given by 0D Calculations [kg/kmol]	Mole Fraction Given by 0D Calculations [-]	Molar Flux Given by 0D Calculations [kmol/h]	Mass Flow [kg/h]	Mass Flow [kg/s]
N ₂	28.013	0.842	6.062	169.801	4.7167×10^{-2}
O ₂	31.999	0.158	1.137	36.396	1.0110×10^{-2}
H ₂	2.016	0.070	0.208	0.420	0.117×10^{-3}
H ₂ O	18.015	0.930	2.767	49.860	13.850×10^{-3}

Table 5. Brass properties [38].

Temperature [°C]	Density [kg/m ³]	Re [MPa]	Rm [MPa]	Poisson Ratio [-]	Young Modulus [GPa]	Specific Heat [J/kgK]	CTE [1/°C]
20	8500	150	350	0.34	100	380	19×10^{-6}
100	8470	120	300	0.34	95	390	19.5×10^{-6}
200	8420	90	240	0.34	88	405	20×10^{-6}
300	8370	65	180	0.35	80	420	20.5×10^{-6}
400	8320	40	120	0.35	70	440	21×10^{-6}
500	8270	20	70	0.35	60	460	22×10^{-6}

2.6. Boundary Conditions

The boundary conditions for the CFD analysis were derived from the 0D calculations of the reference case. The fuel inlet was defined as a mass-flow inlet at 675 °C and consisted of a mixture with molar fractions of 0.07 H₂ and 0.93 H₂O. The oxidizer inlet was defined as a mass-flow inlet at 492 °C and consisted of air represented by molar fractions of 0.158 O₂ and 0.842 N₂. The outlet boundary condition was specified as a pressure outlet.

The corresponding component mass flow rates used in the calculations were 0.010110 kg/s for O₂ and 0.047167 kg/s for N₂.

The boundary conditions for CFD calculations were set as follows:

- Inlet—Mass flow inlet: 675 °C, 0.07 mol H₂, and 0.93 mol H₂O;
- Air inlet—Mass flow inlet: 492 °C, 0.158 mol O₂, and 0.842 mol N₂;
- Outlet—Pressure outlet.

For CSD calculations, the boundary conditions are shown in Figure 8.

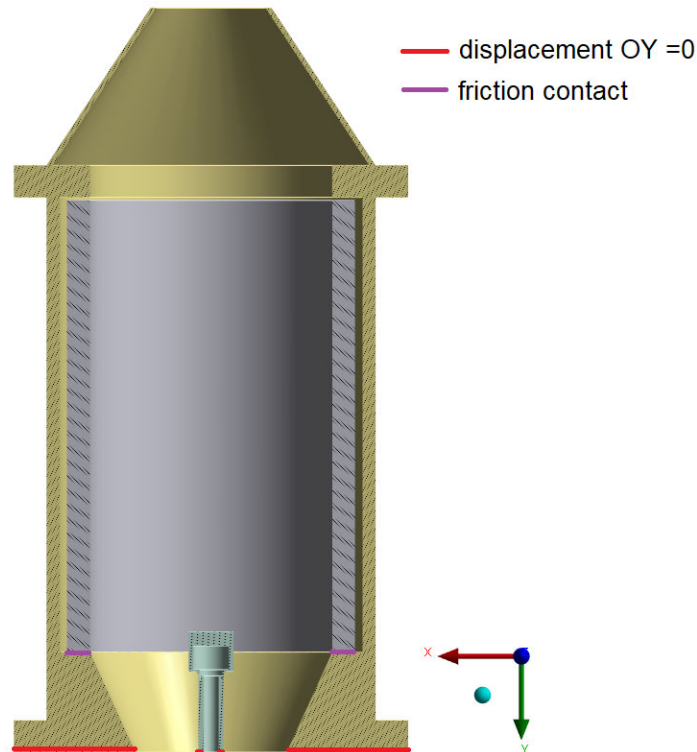


Figure 8. Structural boundary conditions used in the CSD calculation. The lower supporting surfaces were constrained by imposing $U_Y = 0$, and a frictional contact was defined between the ceramic liner and the surrounding steel structure.

The inlet data listed in Table 2 were taken from the 0D process calculations prepared for the 10 kW reference case of the HYDROGIN system. These calculations provided the composition and flow rates of the hydrogen–steam stream leaving the rSOC stack and of the air stream supplied to the afterburner. Therefore, the inlet mass flow rates, molar fractions, and stream temperatures used in the CFD model follow directly from the process balance of the reference operating point. The outlet was defined as a pressure outlet to represent the flow path from the afterburner toward the downstream FE1 heat exchanger.

Tables 4–7 contain material data used in the structural and thermo-mechanical parts of the analysis. They correspond to the materials assumed in the afterburner design: brass for the burner component, 316L stainless steel for the outer chamber, and WHIPOX ceramic material for the internal liner. These properties were introduced to calculate the thermal expansion and deformation of the chamber under the temperature field obtained from the CFD simulation.

Table 6. Properties of 316L stainless steel [39].

Temperature [°C]	Density [kg/m ³]	Re [Mpa]	Rm [Mpa]	Poisson's Ratio [-]	Young Modulus [Gpa]	Specific Heat [J/kgK]	Coefficient of Thermal Expansion [1/C]
25	8000	205	515	0.29	193	500	16×10^{-6}
900	7850	50	120	0.25	90	660	19.3×10^{-6}

Table 7. Ceramic pipe properties (WHIPOX) [40].

E11	E22, E33	G12	G13, G23	v12	v13, v23	Density	Coef. of Thermal Expansion 600 °C	Thermal Cond. 20 °C	Thermal Cond. 1000 °C	Specific Heat 20 °C	Specific Heat 600 °C	Specific Heat 1400 °C
GPa	GPa	GPa	GPa	–	–	kg/m ³	10 ^{−6} /K	W/mK	W/mK	J/gK	J/gK	J/gK
125	101.72	43.9	42.92	0.144	0.193	2800	7.5	3.1	1.55	1.02	1.22	1.31

Table 7 contains the following variables:

- E11—stiffness in direction 1;
- E22—stiffness in direction 2;
- E33—stiffness in direction 3;
- G12—shear stiffness in the 1–2 plane;
- G13—shear stiffness in the 1–3 plane;
- G23—shear stiffness in the 2–3 plane;
- v12—transverse strain in direction 2 caused by tensile loading in direction 1;
- v13—transverse strain in direction 3 caused by tensile loading in direction 1;
- v23—transverse strain in direction 3 caused by tensile loading in direction 2.

2.7. Preliminary Geometric Scaling Methodology

The detailed CFD/CSD analysis was performed only for the 10 kW reference afterburner. For larger nominal capacities, a preliminary geometric scaling rule was used to define the indicative dimensions of the nozzle channels and outlet passage. The scaling was based on increasing the characteristic flow cross-sectional areas while preserving the number of nozzle channels. For the 10 kW, 100 kW, and 1 MW variants, the radius of the single nozzle channel was specified as 0.0006 m, 0.001897 m, and 0.006 m, respectively, while the total nozzle cross-sectional area increased from $2.94053 \times 10^{-5} \text{ m}^2$ to $2.94 \times 10^{-4} \text{ m}^2$ and $2.941 \times 10^{-3} \text{ m}^2$. The outlet radius was scaled from 0.036 m to 0.113842 m and 0.36 m.

This procedure should be understood as a first-step geometric sizing method, not as a universal scaling law. Increasing the nominal capacity changes the flow rate, velocity field, turbulence level, residence time, fuel–air mixing, flame stabilization, and heat transfer to the chamber walls. For this reason, the 100 kW and 1 MW variants cannot be treated as verified designs on the basis of geometry alone.

The proposed scaling rule is applicable only as an initial design estimate for afterburners operating under conditions close to the reference case, i.e., steam-diluted hydrogen-rich off-gas, hot air as the oxidizer, comparable pressure level, and a similar burner/chamber arrangement. The final assessment of larger variants requires separate reacting-flow and thermomechanical calculations.

These larger-capacity variants were not subjected to separate CFD or thermo-mechanical calculations in the present study. Therefore, they should be regarded as preliminary engineering extrapolations of the numerically analyzed 10 kW design rather than fully verified afterburner configurations.

3. Results

This section presents the CFD and CSD results obtained for the 10 kW reference afterburner. The CFD part focuses on the temperature field and the spatial distributions of the main and intermediate species in the fluid domain, whereas the CSD part summarizes the thermo-mechanical response of the chamber under the thermal loading derived from the flow calculations. The results are shown in representative longitudinal and transverse sections through the burner outlet region and the combustion chamber.

3.1. CFD Results

Figure 9 presents the temperature field in the fluid domain on representative longitudinal and transverse sections through the burner outlet region. The temperature contours show the formation of a hot reaction core emerging from the burner outlet and extending downstream into the combustion chamber. In the longitudinal sections, the highest temperatures are concentrated in the central part of the reacting jet, whereas lower temperatures are observed in the peripheral regions of the chamber. The transverse section confirms that the hottest zone remains localized around the burner outlet and the central jet region.

Figure 10 presents the temperature distribution on a transverse plane located 2 mm downstream of the burner outlet. The results show a strongly non-uniform thermal field, with the highest temperatures concentrated in the central region corresponding to the reacting core. Elevated temperatures are also visible around the individual outlet channels, indicating intense local mixing and heat release immediately after the burner exit. In contrast, the surrounding chamber region remains significantly cooler, confirming that the hottest zone is confined to the near-axis region and does not spread over the entire cross-section. This distribution is consistent with the formation of a compact combustion zone directly downstream of the burner outlet.

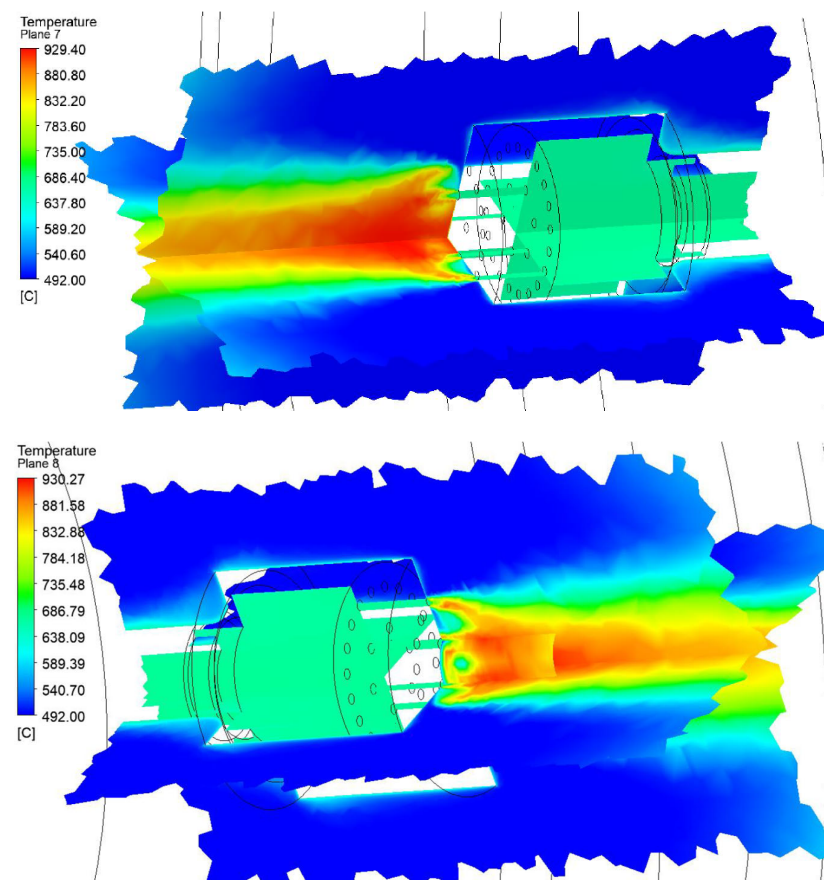


Figure 9. Temperature field in the cross-section of the burner.

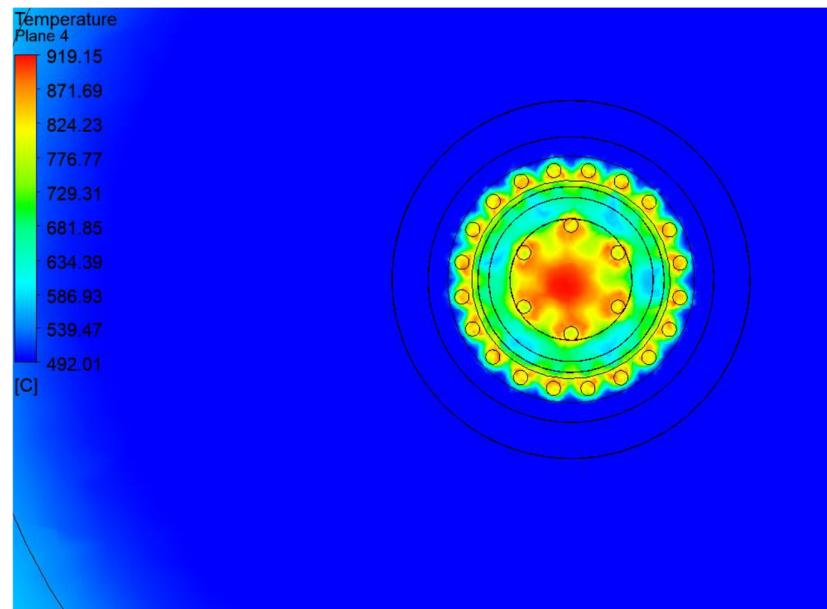


Figure 10. Temperature field on a transverse plane located 2 mm downstream of the burner outlet.

The species fields shown in the following figures provide further insight into the combustion process and the spatial structure of the reacting flow. Taken together, they illustrate the consumption of hydrogen, the distribution of the oxidizer stream, the formation of water vapor, and the presence of intermediate species within the reaction zone.

Figures 11–15 show the mole-fraction distributions of O_2 , N_2 , H_2 , H_2O , and HO_2 in the fluid domain. These fields were used to describe the development of the combustion process rather than only to identify individual species. The oxygen distribution shows depletion in the central reaction zone below the burner outlet, while nitrogen follows the main oxidizer stream and remains dominant outside the reaction core. Hydrogen is confined to a narrow region near the burner outlet and rapidly disappears downstream, which confirms fuel consumption close to the burner exit. Water vapor is present both as an inlet component and as a combustion product, with increased values in the central jet and downstream region. The HO_2 radical appears only in trace amounts and remains localized close to the reaction zone. Together, these distributions confirm that hydrogen oxidation is concentrated directly downstream of the burner outlet.

Overall, the CFD results indicate that combustion is concentrated in the region immediately downstream of the burner outlet. The temperature and species distributions are mutually consistent and confirm that hydrogen is rapidly consumed in the core of the reacting jet, while the surrounding chamber volume is dominated by the oxidizer stream and combustion products.

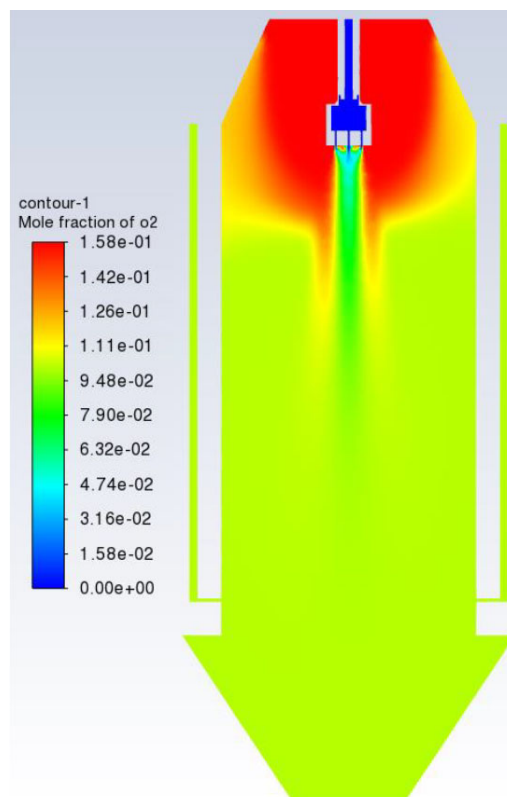


Figure 11. Longitudinal section through the fluid domain, showing the mole-fraction distribution of oxygen.

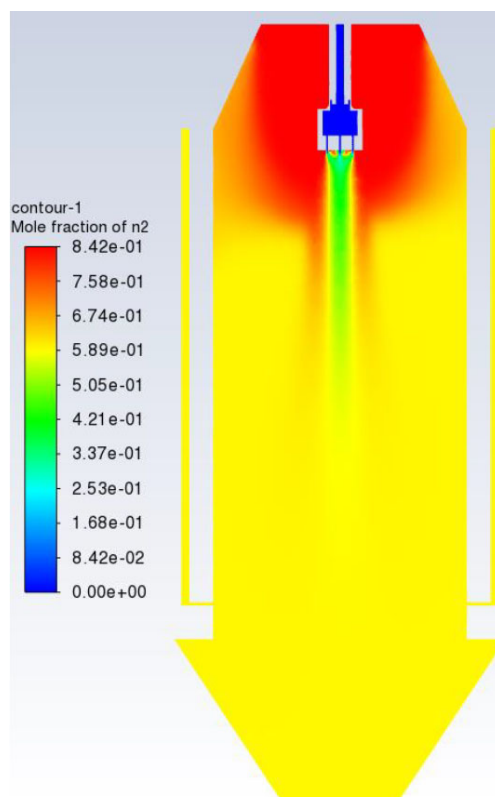


Figure 12. Longitudinal section through the fluid domain, showing the mole-fraction distribution of nitrogen.

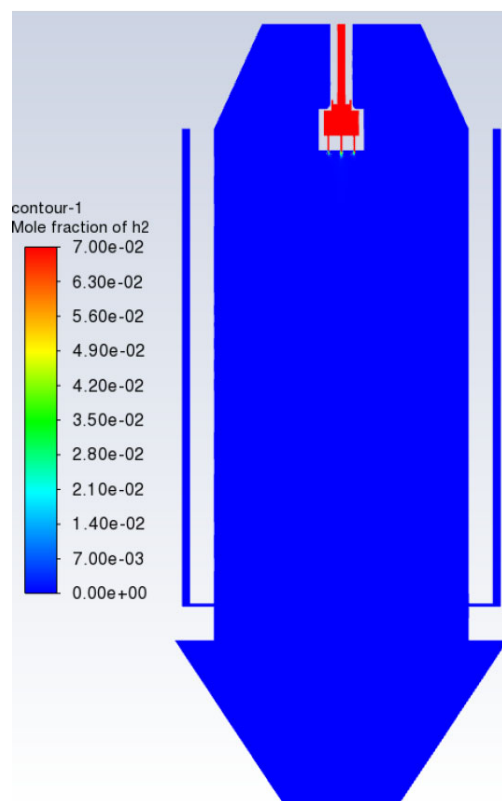


Figure 13. Longitudinal section through the fluid domain, showing the mole-fraction distribution of hydrogen.

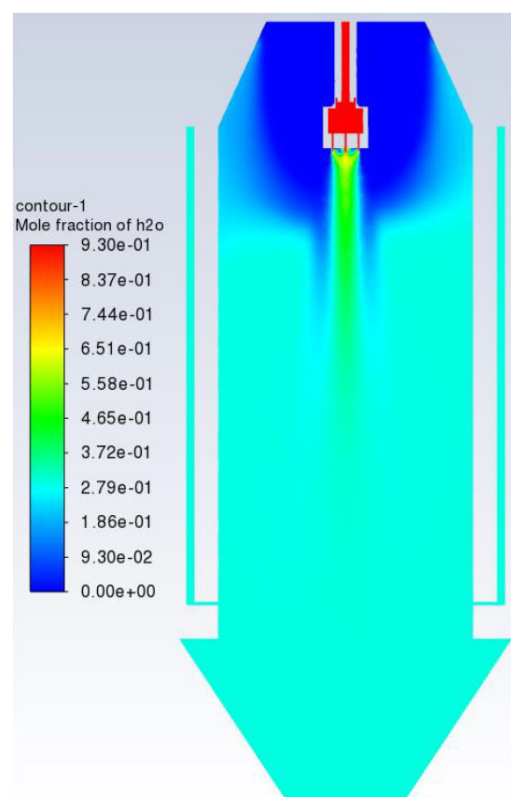


Figure 14. Longitudinal section through the fluid domain, showing the mole-fraction distribution of water vapor.

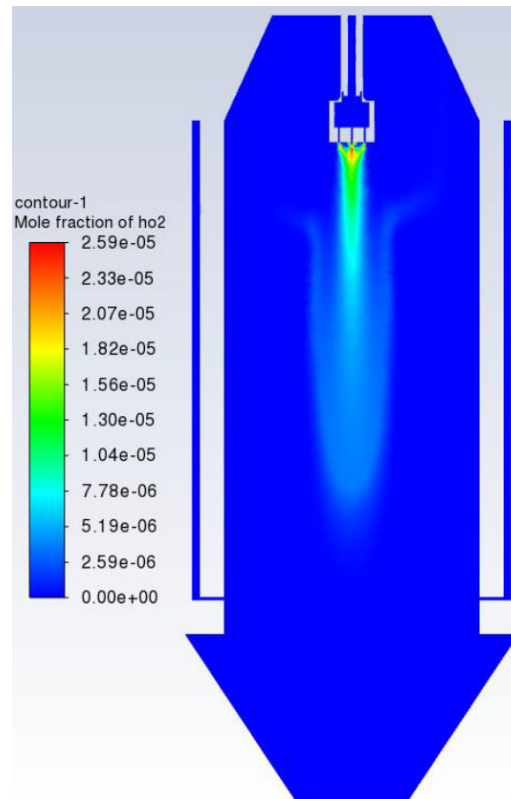


Figure 15. Longitudinal section through the fluid domain showing the mole-fraction distribution of the hydroperoxyl radical.

3.2. CSD Results

This section presents the thermo-mechanical response of the afterburner structure under the thermal loading generated by the reacting flow. The results obtained were used to assess the deformation level of the chamber and to verify whether the structural response remained acceptable under steady operating conditions.

Figure 16 shows the total deformation of the afterburner structure. The deformation increases along the chamber length toward the outlet section, where the highest values are observed. This result indicates that the thermally loaded chamber undergoes its largest structural response in the downstream region, which is exposed to the combined effect of elevated temperature and geometric transition.

Figure 17 presents the directional deformation along the Y-axis. The deformation pattern varies smoothly along the structure and indicates the dominant axial displacement of the chamber caused by thermal loading. This result is consistent with the thermo-mechanical assessment reported in the Abstract, according to which the maximum axial displacement remained limited to about 2.21 mm.

The CSD results confirm that the structural response of the analyzed afterburner remains limited under the considered steady operating conditions. For the analyzed steady-state operating point, the predicted maximum total deformation was 2.2189 mm, while the maximum axial displacement was approximately 2.21 mm.

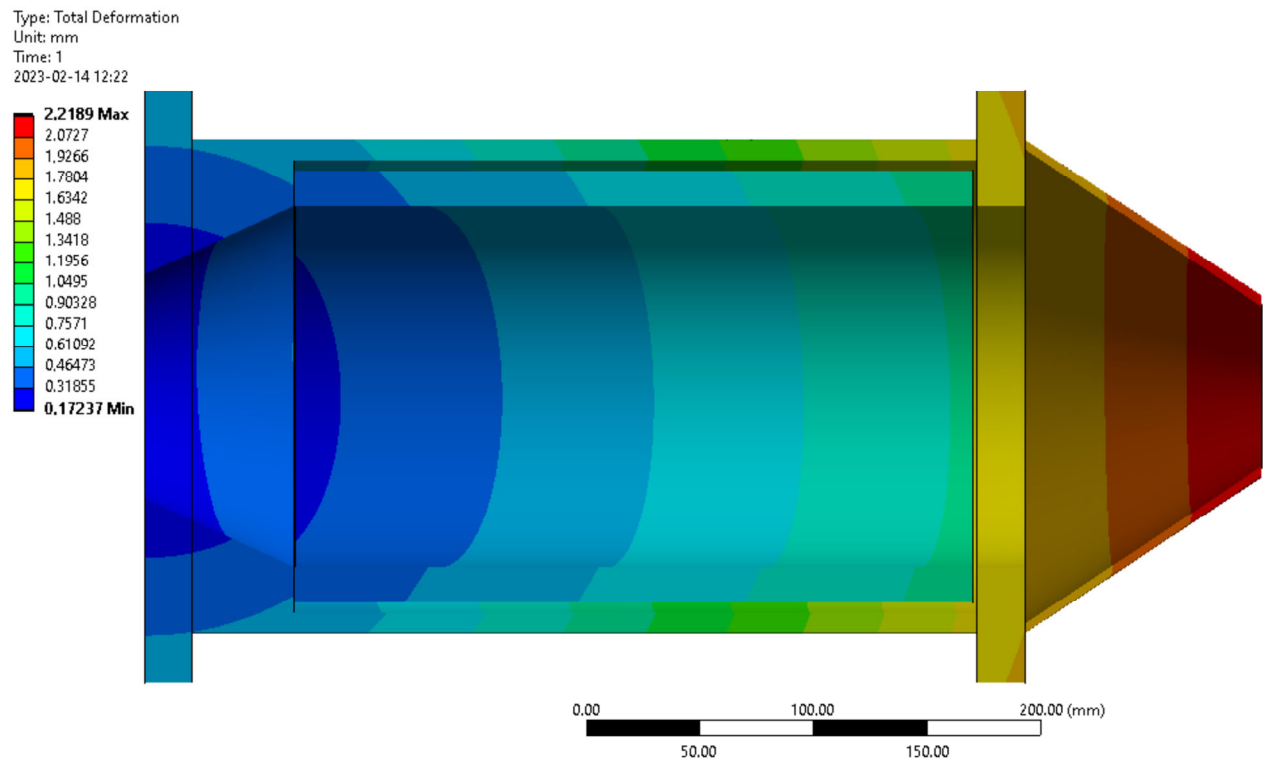


Figure 16. Total deformation of the afterburner structure predicted by the thermo-mechanical analysis.

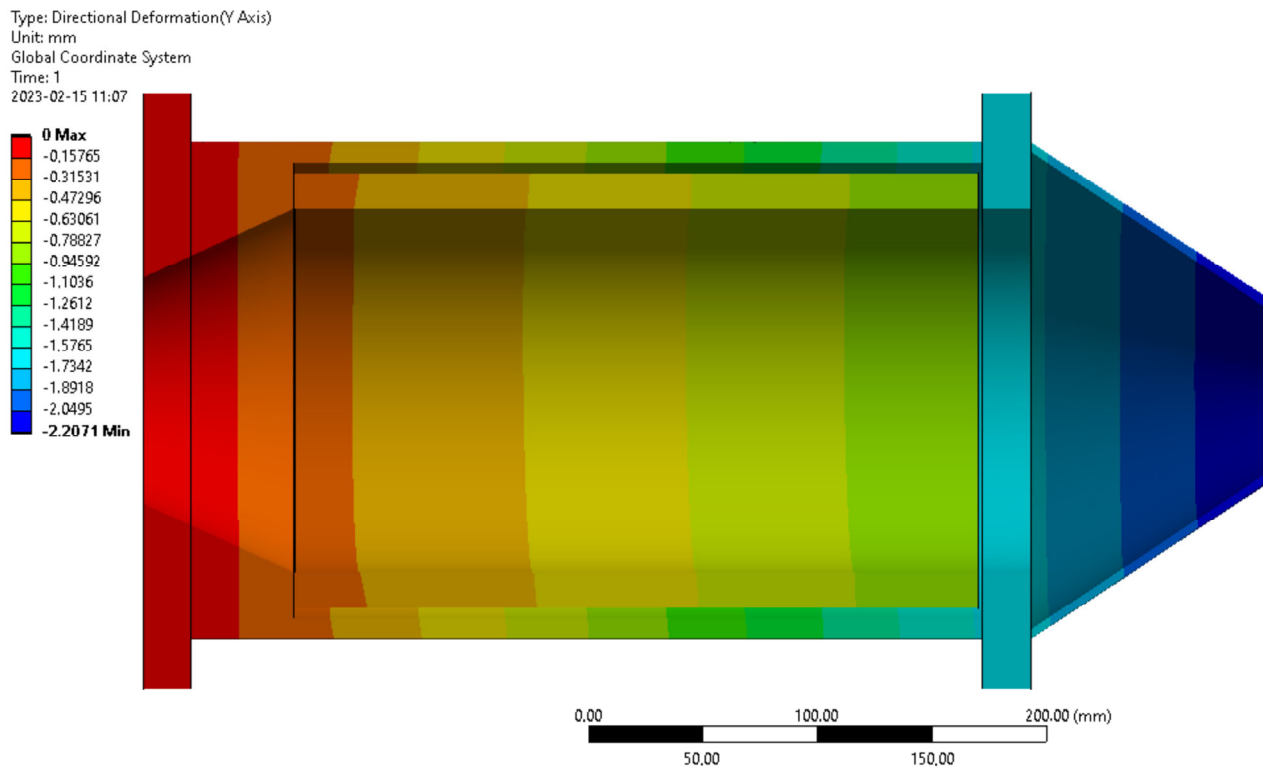


Figure 17. Directional deformation of the afterburner structure along the Y-axis predicted by the thermo-mechanical analysis.

4. Discussion

The main quantitative CFD and CSD results for the 10 kW reference afterburner are summarized in Tables 8 and 9. The CFD table presents the key thermal and species-related quantities of the reacting flow, whereas the CSD/thermal-FSI table summarizes the principal deformation measures of the chamber under thermal loading.

Table 8. Key quantitative CFD results for the 10 kW reference afterburner.

Parameter	Symbol	Unit	Value
Unreacted hydrogen mass flow rate	$\dot{m}_{H_2}$	kg/s	1.16661×10^{-4}
Chemical energy of unreacted hydrogen	$\dot{Q}_{chem}$	kW	14.0
Maximum temperature in the fluid domain	T_{max}	°C	930.27
Minimum temperature in the fluid domain	T_{min}	°C	492.00
Maximum oxygen mole fraction	x_{O_2max}	–	1.58×10^{-1}
Maximum nitrogen mole fraction	x_{N_2max}	–	8.42×10^{-1}
Maximum hydrogen mole fraction	x_{H_2max}	–	7.00×10^{-2}
Maximum water vapor mole fraction	x_{H_2Omax}	–	9.30×10^{-1}
Maximum HO ₂ mole fraction	x_{HO_2max}	–	2.59×10^{-5}

Table 9. Key quantitative CSD/Thermal-FSI results for the 10 kW reference afterburner.

Parameter	Symbol	Unit	Value
Maximum total deformation	$u_{tot,max}$	mm	2.2189
Minimum total deformation	$u_{tot,min}$	mm	0.1724
Minimum directional deformation (Y-axis)	$u_{y,min}$	mm	−2.2071
Maximum axial displacement	$u_{ax,max}$	mm	2.2100

The summarized results indicate that the analyzed afterburner operates within a temperature range of approximately 492–930 °C, while the maximum species levels remain consistent with the imposed inlet composition and the expected reaction products. From a structural point of view, the thermo-mechanical response is limited, with the maximum total deformation equal to 2.2189 mm and a maximum axial displacement of about 2.21 mm.

The results obtained for the 10 kW reference case support the working hypothesis that a compact afterburner can provide effective and thermally manageable oxidation of hydrogen-rich off-gas from an rSOC stack. The CFD fields show that the main reaction zone is formed immediately downstream of the burner outlet, where the highest temperatures are reached and hydrogen is rapidly consumed. At the same time, the species distributions indicate a physically consistent combustion pattern: oxygen is depleted in the reaction core, hydrogen disappears within a short downstream distance, water vapor dominates the product-rich region, and HO₂ remains confined to trace levels near the flame zone. Taken together, these results indicate that the proposed configuration provides stable oxidation of the hydrogen–steam mixture under the analyzed operating conditions.

From the combustion perspective, these findings are consistent with previous studies on SOFC and hydrogen-rich off-gas utilization, which emphasized that burner performance is governed by the coupling between mixing, flame localization, and thermal safety [3–5]. In the present case, the temperature field remains strongly localized around the central reacting jet, which is advantageous from the point of view of controlled combustion and heat recovery. This feature is particularly important in the considered HYDROGIN arrangement, because the afterburner operates upstream of the heat exchanger and therefore directly affects the thermal conditions available for steam preheating. The obtained temperature range, extending from approximately 492 °C to 930 °C, confirms that the

device is capable of recovering a significant fraction of the residual chemical energy carried by the unreacted hydrogen stream.

The results also confirm the importance of steam dilution in shaping the combustion behavior of the considered off-gas. In contrast to conventional hydrocarbon-fueled systems, the present mixture contains hydrogen that is strongly diluted with water vapor, which affects both flame structure and intermediate-species formation. This interpretation is in line with the literature showing that water vapor influences hydrogen oxidation kinetics, flame temperature, and radical pathways [6]. The very low HO_2 levels predicted in the present calculations suggest that the intermediate chemistry remains confined to a narrow region near the burner outlet and does not extend significantly into the downstream chamber volume. From a design perspective, this is favorable because it indicates that the combustion process remains spatially compact and does not spread uncontrollably through the whole chamber.

An important contribution of the present work, relative to many CFD-oriented afterburner studies, is the inclusion of the thermo-mechanical response of the chamber. The CSD/thermal-FSI results indicate that the largest structural response occurs in the downstream part of the chamber, where elevated temperature is combined with a geometric transition. Nevertheless, the maximum total deformation remains limited to 2.2189 mm, and the maximum axial displacement is approximately 2.21 mm. These values support the conclusion that the proposed chamber design is mechanically feasible under the analyzed steady conditions. This aspect is particularly relevant for practical implementation, because the safe integration of an afterburner in an rSOC hot section requires not only stable combustion but also predictable thermal expansion of the surrounding structure.

At the system level, the results indicate that the analyzed afterburner can be treated as a viable balance-of-plant component for hydrogen management and heat integration in rSOC-based energy systems. Its function is not limited to safe disposal of residual fuel; rather, it converts the residual chemical energy into a usable high-temperature stream that can support downstream heat recovery. In this sense, the proposed concept is aligned with the broader objective of improving the flexibility and thermal efficiency of integrated rSOC installations. The compactness of the reaction zone and the limited structural response both strengthen the practical relevance of the design at the reference 10 kW scale.

At the same time, the conclusions of the present study should be interpreted within the actual scope of the analysis. The detailed CFD/CSD analysis was carried out only for the 10 kW reference afterburner. Although a scaling rule was proposed for the 100 kW and 1 MW variants, these larger designs were not subjected to separate CFD or thermo-mechanical verification and should therefore be treated as engineering extrapolations rather than verified designs. This limitation is important, because the localization of the flame, heat-transfer intensity, and structural response may all change with scale even when geometric similarity is preserved.

Further work should therefore focus on three main directions. First, the numerical results should be complemented by experimental validation of temperature distribution and outlet composition for the reference design. Second, the larger-capacity variants should be verified using dedicated CFD/CSD calculations rather than by geometric scaling alone. Third, the analysis should be extended beyond the present steady-state framework to include transient operating scenarios relevant to rSOC integration, such as start-up, shut-down, and load-following conditions. Additional assessment of pollutant formation and radiative heat transfer would also improve the completeness of the design methodology for practical industrial deployment.

From an engineering perspective, the proposed afterburner concept offers three main advantages. First, the CFD results indicate that combustion remains spatially localized immediately downstream of the burner outlet, which supports controlled heat release and

efficient oxidation of the hydrogen-rich off-gas. Second, the predicted temperature range of approximately 492–930 °C confirms that the residual chemical energy of the unreacted hydrogen can be converted into a high-temperature stream suitable for downstream heat recovery. Third, the thermo-mechanical response of the chamber remains limited, with a maximum total deformation of 2.2189 mm and a maximum axial displacement of about 2.21 mm, which quantify the predicted structural response of the reference 10 kW configuration under the analyzed steady-state conditions.

At the same time, the present study has several important limitations that should be stated explicitly. The detailed CFD/CSD analysis was performed only for the 10 kW reference case, whereas the 100 kW and 1 MW variants were introduced on the basis of a scaling rule and should therefore be treated as engineering extrapolations rather than fully validated designs. In addition, the conclusions are based exclusively on numerical results, because no dedicated experimental validation of the temperature field, species distributions, or structural deformation is reported in the current manuscript. The analysis is also restricted to steady operating conditions and does not yet address transient states that are relevant for practical rSOC operation, such as start-up, shut-down, or rapid load changes.

The calculations were performed for one reference operating point obtained from the 0D process model of the 10 kW rSOC system. In practical operation, the gas composition, hydrogen content, steam dilution, air flow rate, and inlet temperatures may change with stack load and operating mode. These parameters can affect the reaction-zone location, peak temperature, hydrogen conversion, and heat transfer to the chamber walls. A higher hydrogen fraction may increase local heat release, while stronger steam dilution may reduce the flame temperature and slow down oxidation. Changes in the inlet temperature may also shift the reaction zone relative to the burner outlet. Therefore, the present results refer to the analyzed reference case. A separate sensitivity analysis is required to assess the behavior of the afterburner over a wider operating range.

The model was not validated against experimental measurements, because such data were not available for the analyzed afterburner. Therefore, the results should be treated as a numerical design assessment of the 10 kW reference case. The calculation was checked through a mesh independence study and by verifying the physical consistency of the predicted fields. The obtained distributions showed the expected combustion behavior: hydrogen was consumed near the burner outlet, oxygen was depleted in the reaction zone, water vapor was formed downstream, and the highest temperatures were localized close to the burner exit. The main modeling uncertainties are related to the turbulence–combustion interaction, radiation treatment, steady-state boundary conditions, material property data, and the lack of direct temperature and gas-composition measurements. Experimental validation should be carried out in the next stage of work.

Radiation was included in the CFD model because of the high temperatures expected in the reaction zone. However, no separate calculation without radiation was performed. Therefore, the present study does not quantify the isolated effect of radiation on gas temperature, wall temperature, or heat transfer to the chamber walls. This should be treated as a limitation of the analysis. A comparison of calculations with and without radiation is required in further work to determine the actual contribution of radiative heat transfer to the thermal loading of the afterburner.

The present thermo-mechanical analysis was limited to deformation under steady thermal loading. It does not include a full assessment of long-term structural integrity. In practical operation, the chamber may be exposed to repeated start-up and shut-down cycles, thermal stresses, cyclic loading, and local effects near welded joints. These factors may influence the fatigue life and durability of the afterburner. Therefore, the present CSD results should be treated as an initial structural assessment. Separate stress, fatigue, and welded-joint analyses are required before final qualification of the design.

The present work does not include a detailed operational analysis of the afterburner. The ignition procedure, flame stability during start-up and load changes, maintenance requirements, safety procedures, and manufacturing tolerances were not analyzed in the numerical model. These aspects are important for practical use of the device, but they require prototype testing and operation-oriented studies. Therefore, the present results should be treated as a numerical assessment of the reference design under the assumed operating conditions, not as a complete operational qualification of the afterburner.

These observations define the main directions for further work. The most important next step is experimental verification of the reference afterburner, including temperature measurements and outlet-gas characterization. This should be followed by separate CFD/CSD analyses of larger-capacity variants in order to verify whether the assumed scaling rule preserves both combustion stability and structural integrity. Further developments should also include transient simulations representative of flexible rSOC operation and, if possible, an extended assessment of emissions and additional heat-transfer effects.

5. Conclusions

The steady-state CFD calculation for the 10 kW reference afterburner predicted a localized reaction zone directly downstream of the burner outlet. In this region, the hydrogen mole fraction decreased rapidly, oxygen was depleted, and increased water vapor concentration was observed. The calculated fluid-temperature range was approximately 492–930 °C.

The thermo-mechanical calculation predicted a maximum total deformation of 2.2189 mm and a maximum axial displacement of approximately 2.21 mm under the transferred steady-state temperature field. These results describe the predicted thermal, species, and deformation fields for the analyzed reference operating point.

The conclusions are limited to the numerically analyzed 10 kW configuration. No conclusions regarding combustion stability, operational safety, or structural integrity under transient and off-design conditions can be drawn without additional numerical and experimental verification. The 100 kW and 1 MW variants should be treated as preliminary engineering extrapolations because they were not verified by separate CFD/CSD calculations.

Experimental validation is required before the predictive accuracy of the proposed CFD/CSD methodology can be established.

Author Contributions: Conceptualization, M.B. and T.K.; methodology, M.B.; software, P.J.Z.; validation, T.K., J.B.; formal analysis, T.K.; investigation, M.B.; resources, P.J.Z.; data curation, M.B.; writing—original draft preparation, M.B.; writing—review and editing, M.B., T.K. and P.J.Z.; visualization, M.B.; supervision, J.B.; project administration, M.B.; funding acquisition, T.K. All authors have read and agreed to the published version of the manuscript.

Funding: The project was co-financed in 2020–2023 by the European Regional Development Fund under the Smart Growth Operational Program 2014–2020, Priority Axis I: Support for R&D activities carried out by enterprises, Measure 1.1: R&D projects of enterprises, Sub-measure 1.1.1: Industrial research and development works carried out by enterprises. Project no. POIR.01.01.01-00-0335/19.

Institutional Review Board Statement: Not applicable.

Informed Consent Statement: Not applicable.

Data Availability Statement: The data presented in this study are available on request from the corresponding author due to confidentiality agreements with industrial partners.

Conflicts of Interest: The authors declare no conflicts of interest.

Abbreviations

The following abbreviations are used in this manuscript:

CFD	Computational Fluid Dynamics
CSD	Computational Solid Dynamics
Thermal-FSI	Thermal Fluid–Solid Interaction
rSOC	Reversible Solid Oxide Cell
SOFC	Solid Oxide Fuel Cell

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